28th AIRAPT and 60th EHPRG

23–28 July 2023

Edinburgh International Conference Centre,
Edinburgh, UK

iop.org

IOP Institute of Physics

Thank you to our sponsors and exhibitors for supporting The Joint 28th AIRAPT and 60th EHPRG International Conference 2023

Almax easyLab

Beijing Easy Material Technology Co. Ltd

Institute of Physics

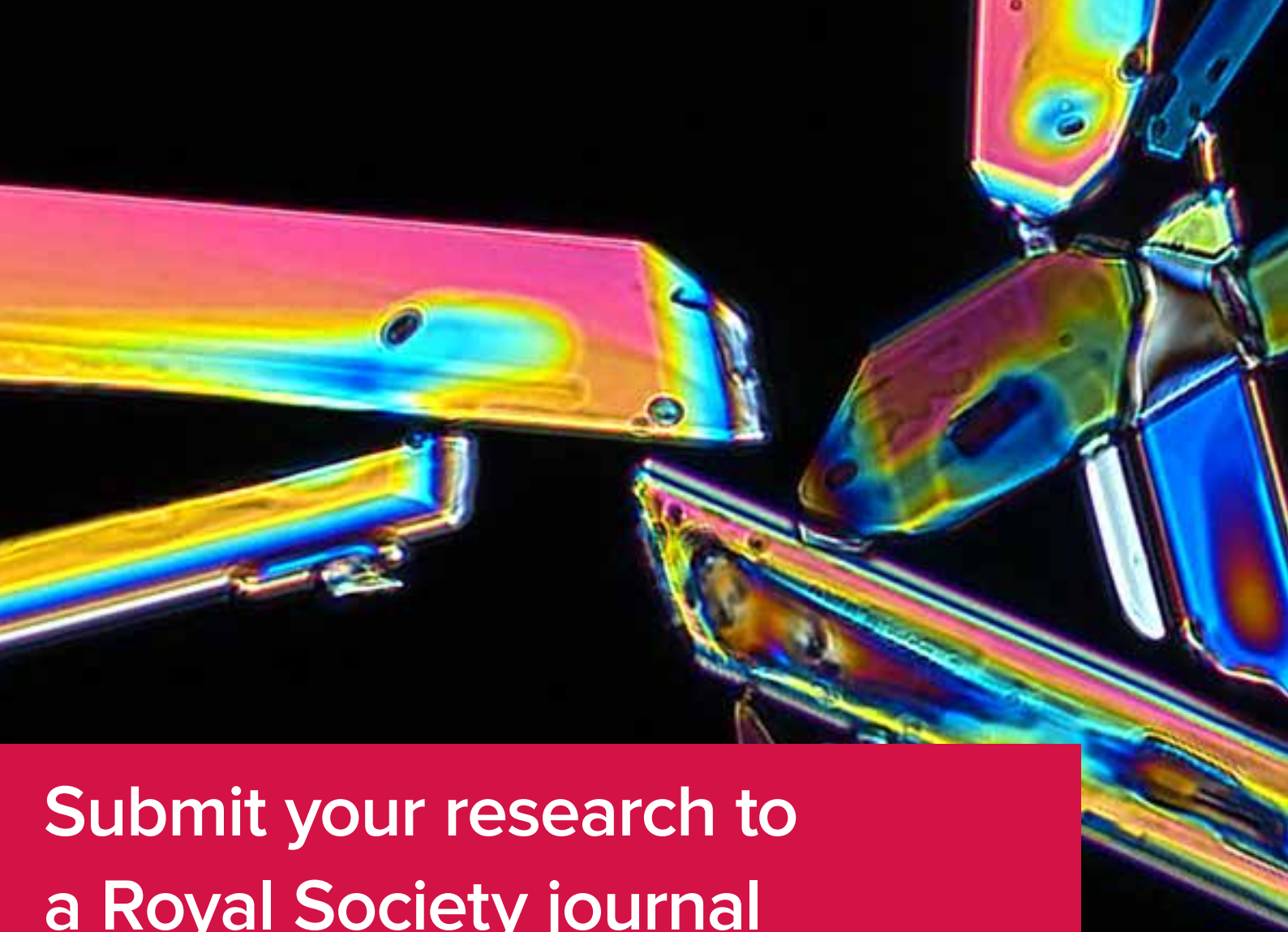
Royal Society Publishing

SARL BETSA

Technodiament

Teledyne Princeton Instruments

Abstract Book Contents:



Submit your research to a Royal Society journal

The Royal Society's journals *Proceedings A* and *Philosophical Transactions A* welcome submissions from researchers working in all areas of physics, maths and engineering. Publishing options include research, review and evidence synthesis papers, as well as the opportunity to guest edit your own theme issue. We are also preprint friendly and offer the option to publish Open Access.

Our authors benefit from:

- Efficient processing and fast decisions
- Rigorous and constructive peer review by experts in the field
- The guidance of international editorial boards
- High visibility and impact
- Open access and open peer review options
- Data archiving costs covered (Dryad/figshare)

To find out how to submit your work or submit a theme issue proposal, please visit **royalsociety.org/journals**

THE ROYAL SOCIETY PUBLISHING

Image: © Charlotte Johnson

宜捷材料
Easy Materials

北京宜捷材料科技有限公司
Beijing Easy Materials Technology Co.Ltd.

www.emtscience.com hp@emtscience.com

√ Customized design and processing √ Supply capacity with guaranteed quality √ Timely and efficient after-sales service

As an enterprise specializing in the development of special materials and customized mold processing, we are passionate about combining factors such as the functional goals that our products need to achieve, the material characteristics used to achieve functions, the diversification and convenience of product use, and the precision of processing and manufacturing processes. We are not only manufacturing products, but also hoping to collaborate with users to use them more reliably and conveniently.

The advantage we have is firstly that we have a wide user base that can blend and collide with each other to create many new product types and usage methods; Secondly, we have a strong material foundation, especially the research and development capabilities of special materials. So far, we have been able to independently manufacture NiCrAl non-magnetic steel alloys (with a hardness exceeding HRC58 and a tensile strength exceeding 1800Mpa), super titanium alloys (with a hardness exceeding HRC45 and a tensile strength exceeding 1500Mpa), titanium zirconium neutron transparent materials (which have been recognized by relevant users), and titanium zirconium hydrogen absorption and desorption alloy materials (which have been recognized by relevant users); Third, we have fully customized design capabilities, including drawing, simulation, processing and testing; The fourth is that we have a fully autonomous and well-equipped professional manufacturing factory. Our strong manufacturing capabilities not only enable us to independently manufacture precision electric high-pressure pump stations with a maximum pressure exceeding 400Mpa, sealed chambers with a pressure resistance exceeding 600MPa, and double-sided top presses with a maximum tonnage exceeding 2000 tons, but also greatly shorten the supply time and after-sales maintenance time of various products.

As a localized enterprise in China, we not only provide diversified high-pressure products (including diamond anvil presses, anvils, pressure tools, large sample size presses, etc.) to numerous high-pressure research groups and universities in our country, but also provide products to multiple overseas research units. We hope to embrace more users, provide timely and reliable product services for users, and also provide more development opportunities for enterprises.

The Joint 28th AIRAPT and 60th EHPRG International Conference 2023

Workshop Programmes: Sunday 23 July 2023

Workshop on the International Practical Pressure Scale (IPPS) 2023 Room: Lowther (Floor -1)		**Registration and Workshop on Transport Properties at High Pressure Room: Lammermuir (Floor -2)**	
9:30am to 10.00am	Arrival Refreshments	9:30am to 10.00am	Arrival Refreshments
10:00am to 11:00am	**Morning Workshop 1:** **Equations of State from 100 GPa to TPa pressures** 10:00am–10:10am Introduction by Jon Eggert 10:10am–10:20am Renata Wentzcovitch: How EOS tables should be used by our community 10:20am–10:30am Martin Gorman: Tantalum as an example 10:30am–10:40am Kamil Dziubek: Phase transitions and kinetics 10:40am–11:00am Discussion	10.00am to 12:10pm	**Morning Workshop 1** 10:00am–10:10am Stewart McWilliams: Welcome 10:10am–10:40am Longjian Xie: Viscosity measurements of silicate melts to lower-mantle conditions 10:40am–10:55am Bernhard Massani: Synchrotron X-ray microscopy of melting and melt dynamics in the laser-heated diamond cell 10:55am–11:10am Aigerim Karina: Probing dynamics in amorphous ice with X-ray photon correlation spectroscopy
11:00am to 11:20am	Morning Break	11:10am to 11:30am	Morning Break
11:20am to 1:00pm	**Morning Workshop 2:** **Equations of State from 100 GPa to TPa pressures** Static EOS experiments: 11:20am–11:30am Making accurate static EOS measurements 11:30am–11:40am Discussion Dynamic Compression EOS experiments: 11:40am–11:50am Jean-Paul Davis 11:50am–12:00pm Richard Briggs 12:00pm–12:10pm Discussion EOS table-building: 12:10pm–12:20pm Christine Wu 12:20pm–12:30pm Discussion 12:30pm–1:00pm: Conclusions and Planning		**Morning Workshop 2** 11:30am–12:00pm Sebastien Merkel: Deformation and microstructures of Earth minerals at mantle P and T using multigrain X-ray crystallography 12:00pm–12:30pm Thomas Meier: Versatility of Extreme NMR: from probing electronic and structural properties to superionicity in matter under extreme conditions 12:30pm–12:45pm Zena Younes: Thermal conductivity measurements using MHz X-ray free electron laser radiation 12:45pm–1:00pm Eric Edmund: Thermal conductivity of iron with direct thickness measurements at Mbar pressures

1:00pm to 2:00pm	Lunch (attendees to provide/buy own)	1:00pm to 2:00pm	Lunch sponsored by TRIREME (European Research Council)
2.00pm to 3:05pm	**Afternoon Workshop 1:** **Pressure Reference Points for Multi-anvil Systems** 2:00pm–2:05pm introduction by Yanbin Wang 2:05pm–2:25pm Agnes Dewaele: DAC isothermal compression data: PV tables and phase transformations 2:25pm–2:45pm Daisuke Yamazaki: High Pressure Generation in a Kawai-type Multianvil Apparatus Equipped with Sintered Diamond Anvils and Electrical Resistance of Fe2O3 at High Pressure 2:45pm–3:05pm Mikhail Eremets: Universal diamond edge Raman scale to 0.5 terapascal, the implication to metallization of hydrogen	2.00pm to 3:15pm	**Afternoon Workshop 1** 2:00pm–2:30pm Kenji Ohta: Pulsed light heating thermoreflectance technique for high pressure and high-temperature thermal conductivity measurements: Applications to (Mg,Fe)O, Pt and Fe 2:30pm–2:45pm Eric Lenhart: The thermal conductivity of liquid Fe-S-Si alloys at high pressure and the applicability of the Wiedemann-Franz Law 2:45pm–3:00pm Uwe Kleinschmidt: Electrical and thermal conductivity of fcc and hcp iron under conditions of the Earth's core from ab initio simulations
3:05pm to 3:15pm	Afternoon Break	3:00pm to 3:20pm	Afternoon Break
3:15pm to 5.00pm	**Afternoon Workshop 2:** **Pressure Reference Points for Multi-anvil Systems** 3:15pm–4:30pm Discussion on report of PRP characterization and calibration practice; Task Force recommendations; Task Force next phase focus. 4:30pm–5pm Next phase planning: election of next vice Chair and work emphasis for the next two years.	3:30pm to 6.00pm	**Afternoon Workshop 2** 3:20pm–3:50pm Sven Friedemann: Electrical transport measurements of metals and superconductors at high-pressures 3:50pm–4:05pm Israel Osmond: High-Pressure Metallisation of Barium Hydride Compounds 4:05pm–4:35pm Martin Preising: Transport Theory in Warm Dense Matter - An ab initio Perspective 4:35pm–5:05pm Andrew Krygier, Lawrence Livermore National Lab, USA: Heat conduction on micron-nanosecond scales during dynamic loading of condensed matter 5:05pm–5:10pm Christophe Thessieu: Current offerings for transport measurements at ALMAX Easylab
6.00pm to 8.00pm	**Registration and Welcome Reception** **Room: Lennox**		

The Joint 28th AIRAPT and 60th EHPRG International Conference 2023

Programme

Monday 24 July 2023

Time	Room	Programme
8:15am to 8:45am	Lennox	**Registration and Arrival Refreshments**
8:45am to 9am	Lennox	**Opening Ceremony**
9am to 9:50am	Lennox	**Plenary I Eva Zurek:** Chemically Complex Light-Element Superconductors from First-Principles Theory
9:50am to 10:15am	Lennox	**Morning Break**
10:15am to 12:15pm	Lennox	**Hydrides 1** **10:15am–10:45am Lilia Boeri:** Ab-initio design of high-Tc conventional Superconductors: how far is room-temperature Superconductivity? **10:45am–11:15am Hanyu Liu:** High superconductivity in light-element systems under high-pressure **11:15am–11:30am Taner Yildirim:** High-throughput search and discovery of near-room temperature superconductors under extreme pressures **11:30am–11:45am Siyu Chen:** Strong-correlation effects in high-pressure rare-earth superhydrides **11:45am–12:00pm Lewis Conway:** Accelerating the Prediction of High-Pressure Hydrides Using Data Derived Potentials **12:00pm–12:15pm Changqing Jin:** New Polyhydride Superconductors
	Lowther	**Phase Diagrams–Ionic Systems** **10:15am–10:45am Arthur Haozhe Liu:** High-pressure phase transitions studies using synchrotron X-ray techniques **10:45am–11:15am Marion Harmand:** Tracking phase transitions of Fe2O3 at planetary interiors conditions **11:15am–11:30am Anja Rosenthal:** The densities and phase transformations of subducted hydrous oceanic crust up to the Earth's transition zone: Insights from in-situ x-ray diffraction measurements **11:30am–11:45am Renata Wentzcovitch:** PBE-GGA predicts the B8↔B2 phase boundary of FeO at Earth's core conditions
	Menteith	**Multifunctional Materials** **10:15am–10:45am Catalin Popescu:** Cooling and energy conversion via pressure in barocaloric materials **10:45am–11:00am Francesco Capitani:** Metastable liquid-like CO2 confined in a mesoporous Metal-Organic Framework at high-pressure **11:00am–11:15am Josu Sánchez-Martín:** High-pressure Structural Stability of $Ni_3V_2O_8$ and $Co_3V_2O_8$: Raman and Infrared Spectroscopy (Ni, Co) and X-ray diffraction (Co) studies **11:15am–11:30am Xiaodong Yao:** Anomalous polarization enhancement in a vdW ferroelectric material under pressure

	Lammermuir	**Ice, Water and Clathrates** **10:15am–10:45am Katrin Amann-Winkel:** Water & amorphous ice: using X-rays to map the phase diagram **10:45am–11:15am Rachel J. Husband:** XFEL heating of low Z materials: a new pathway to superionic ice **11:15am–11:30am Fernando Izquierdo-Ruiz:** Molecular replacement in Clathrate Hydrates **11:30am–11:45am Ciprian Pruteanu:** Non-random fluid mixtures, present and future: the case of methane and water **11:45am–12:00pm Gunnar Weck:** Phase diagram of hot dense superionic ice probed by synchrotron X-ray diffraction **12:00pm–12:15pm Choong-shik Yoo:** Superionic Phases of H2O and H2O-He at High-pressure -Temperature Conditions: Structure, Bonding and Transition Mechanisms
	Moffat	**Magnetic Materials 1** **10:15am–10:45am Wenli Bi:** High-pressure effect on candidate Dirac materials EuMnPn2 (Pn = Sb, Bi) **10:45am–11:00am Shiyu Deng:** Pressure tuning and Evolution of Structural, Magnetic and Electronic Properties in TMPX3 van-der-Waals Compounds **11:00am–11:15am Mohamed Zayed:** Neutron scattering study of SrCu2(BO3)2 under high-pressure **11:15am–11:30am Angel M. Arevalo-lopez:** High-pressure ilmenite-type MnVO3: crystal and spin structures in the itinerant-localised-covalent regimes **11:30am–11:45am Zheng Deng:** Giant Exchange Bias Induced by Few Oersteds in a High-Pressure Stabilised Double Perovskite Y2NiIrO6
12:15pm to 2pm	**Lennox**	**Lunch**
1pm to 2pm	**Lowther**	**Meeting: "Women Under High-pressure ” group** Shanti Deemyad will lead this session, introducing the goals and direction of "Women in high-pressure ". Then successful scientists will share with the audience about their trajectories: Sakura Pascarelli, Chrystele Sanloup, Eva Zurek, Laura Henry. Followed by an open discussion
2pm to 4pm	**Lennox**	**Cores of Terrestrial Planets** **2:00pm–2:30pm Chris McGuire:** In-situ X-ray diffraction of laser-shock compressed binary compounds at Megabar pressures **2:30pm–2:45pm Anatoly Belonoshko:** Experimental evidence for the high-PT body-centered cubic Fe **2:45pm–3:00pm Efim Kolesnikov:** Development of strength and texture in hexagonal Fe-Si-C alloy at planetary cores conditions **3:00pm–3:15pm Tetsuya Komabayashi:** Chemical thermodynamics of Earth’s core materials under high-pressure **3:15pm–3:30pm Susanne Müller:** Effect of carbon on sound velocities of iron alloys and compounds at Earth’s inner core conditions **3:30pm–3:45pm Ian Ocampo:** In situ x-ray diffraction of iron oxides dynamically loaded to multi-megabar pressures **3:45pm–4:00pm Jac Van Driel:** Composition of the Martian Core

	Lowther	**Chemical Bonding 1** **2:00pm–2:30pm Stefano Racioppi:** Core-Electrons Chemical Bonding. Redefining the Chemistry of the Elements at High-pressure **2:30pm–3:00pm Hussien H. Osman:** Mechanism of electron-rich multicentre bonding in elemental crystals under pressure **3:00pm–3:15pm Francisco Javier:** High-pressure studies in compounds with multicentre bonds **3:15pm–3:30pm Madhavi Dalsaniya:** Theoretical investigation on the reactivity of fluorine and bromine at high-pressure : emergence of novel bromine fluorides **3:30pm–3:45pm Michael Pravica:** Inner shell chemistry at extreme conditions **3:45pm–4:00pm Alhaddad Toni:** Exceptional phonon point versus free phonon coupling in Zn-based semiconductor mixed crystals under pressure
	Menteith	**Nitrides, Borides and Carbides 1** **2:00pm–2:30pm Maxim Bykov:** High-pressure synthesis of binary and ternary polyntrides in laser-heated diamond anvil cells **2:30pm–3:00pm Florian Trybel:** Ultra-high complexity of synthesised meta-stable nitrides **3:00pm–3:15pm Julio Pellicer-Porres:** BN under high-pressure revisited **3:15pm–3:30pm Altair Soria Pereira:** Exploiting the reduction of Si melting temperature for the production of boron carbide-based composites under high-pressure **3:30pm–3:45pm Hitoshi Yusa:** High-pressure synthesis of light lanthanide dodecaborides (RB_{12}): Synthesis condition, valence fluctuation and bulk moduli **3:45pm–4:00pm Matteo Ceppatelli:** Synthesis of single-bonded cubic AsN from the high-pressure and high-temperature chemical reaction of arsenic and nitrogen
	Lammermuir	**Developments at XFELs & Lasers** **2:00pm–2:30pm Laura Robin Benedetti:** Progress in Time-Resolved X-ray Diffraction with Laser Compression at the National Ignition Facility (NIF) **2:30pm–3:00pm R. Stewart Mcwilliams:** Design of Static High-Pressure Experiments at Free Electron Lasers **3:00pm–3:15pm Samantha Clarke:** In situ X-ray diffraction of TATB on NIF **3:15pm–3:30pm Nicolas Jaisle:** Finite Element Method applied to MHz X-ray diffraction in Diamond Anvil Cell **3:30pm–3:45pm James McHardy:** Exploring hard X-ray free electron laser energy deposition through target imprinting **3:45pm–4:00pm Orianna Ball:** Dynamic Optical Pyrometry of Static High-Pressure Targets under X-ray Free Electron Laser Radiation
	Moffat	**Ceramics and Composites** **2:00pm–2:30pm Yogesh Vohra:** Synthesis and Properties of High Entropy Materials under Static and Dynamic Compression **2:30pm–3:00pm Bo Xu:** Heterogeneous Diamond-cBN Composites with Superb Toughness and Hardness **3:00pm–3:15pm Fang Peng:** Study on Stress, Strain and Densification of Superhard Materials and Ceramics during High-pressure Sintering **3:15pm–3:30pm Tao Liang:** Mechanical properties of high-pressure synthesised hexagonal silicon **3:30pm–3:45pm Volodymyr Svitlyk:** Extreme Zr-based synthetic phases for the safe disposal of nuclear waste
4pm to 4:30pm	**Lennox**	**Afternoon Break**

4:30pm to 6:30pm	**Lennox**	**Hydrides 2** **4:30pm–5:00pm Ion Errea:** Superhydrides on a quantum energy landscape **5:00pm–5:30pm Stanley Tozer:** A substituted La-based 556 K Tc superhydride superconductor **5:30pm–5:45pm Graeme J Ackland:** Hydrogen molecules in competition with superconductivity **5:45pm–6:00pm Hongbo Wang:** High-Tc superconductivity in clathrate calcium hydride CaH6 **6:00pm–6:15pm Mikhail Kuzovnikov:** Synthesis of novel rubidium superhydrides under high-pressure **6:15pm–6:30pm Tomas Marqueno:** Na-W-H and Na-Re-H ternary hydrides at high-pressures
	Lowther	**Chemical Bonding 2** **4:30pm–5:00pm Kuo Li:** Threshold distance of topochemical polymerization **5:00pm–5:15pm Samuel Dunning:** Diamond Nanothreads: Controlling Solid-State Reactivity via Reaction-Directing Heteroatoms **5:15pm–5:30pm Abdelmajid Elmahjoubi:** High-pressure Raman scattering and X-ray diffraction study of the highly-mismatched ternary semiconductor alloy Cd1-xBexTe ($x \leq 0.11$) **5:30pm–5:45pm Alvaro Lobato:** Enhancing thermoelectric power in skutterudites by tuning chemical interactions under pressure **5:45pm–6:00pm Piotr Rejnhardt:** Deuteration-enhanced Negative Thermal Expansion and Negative Area Compressibility in a 3-Dimensional Hydrogen Bonded Network **6:00pm–6:15pm Szymon Sobczak:** Structural and Electronic Insights into the Role of Anagostic Bonds in Metal Dithiocarbamate Complexes
	Menteith	**Minerals Under High-pressure** **4:30pm–5:00pm Samu Ishizawa:** Melting experiment of MgO under high-pressure by in situ time-resolved X-ray diffraction measurement with Bayesian estimation method **5:00pm–5:15pm Yanbin Wang:** Simultaneous measurements of ruby shift and unit cells of NaCl and Au in a diamond-anvil cell: new constraints on pressure scales to 20 GPa **5:15pm–5:30pm Christoph Otzen:** Lamellar amorphization in quartz and its relation to the formation of a rosiaite-structured high-pressure phase of silica **5:30pm–5:45pm Yunhua Fu:** Analysis of hydrogen concentration in anorthite from angrite by developed micro-NMR technique **5:45pm–6:00pm Taku Tsuchiya:** Effects of light elements on the water partitioning between liquid metal and molten silicate under high-pressure and temperature
	Lammermuir	**Facility Development 1** **4:30pm–5:00pm Olivier Mathon:** Static and dynamic high-pressure opportunities at ESRF XAS beamlines BM23 and ID24 **5:00pm–5:30pm Ioannis Tzifas:** Novel High-Pressure Irradiation Platform at GSI: Investigation of structural modifications under extreme conditions **5:30pm–5:45pm Jesse Smith:** Overview of beamline 16-ID-B of the High-Pressure Collaborative Access Team at the Advanced Photon Source **5:45pm–6:00pm Nenad Velisavljevic:** Overview of High-Pressure Collaborative Access Team (HPCAT) facility at the Advanced Photon Source at Argonne National Laboratory **6:00pm–6:15pm Helen Walker:** Developments in measuring collective excitations using inelastic Neutron Scattering under pressures up to 8kbar **6:15pm–6:30pm Yusheng Zhao:** Integrated Neutron Diffractometer at Extreme Conditions (INDEC) at China Spallation Neutron Source (CSNS)

	Moffat	**Nanoscale Systems** **4:30pm–5:00pm Zhidan Zeng:** Preservation of high-pressure materials in nanostructured diamond capsules **5:00pm–5:15pm Alexander Soldatov:** Response of a few-layer graphene to high shear stress **5:15pm–5:30pm Beatrice D'Alò:** High-pressure photoluminescence study of monolayer TMDs: an extensive investigation of the role of defects induced by sample/substrate interaction **5:30pm–5:45pm Riccardo Galafassi:** Investigation of environment and substrate roles on high-pressure tuning of graphene properties **5:45pm–6:00pm Camino Martín-Sánchez:** Monitoring gold nanoparticles at high-pressure through in situ small-angle x-ray scattering **6:00pm–6:15pm Christopher Schröck:** Swift heavy ion irradiation of bismuth nanowire networks pressurised in diamond anvil cells **6:15pm–6:30pm Marina Teresa Candela:** Cubic (Eu1-xYbx)2O3 nanophosphors under compression: a joint structural and spectroscopic study
6pm to 8pm	**Organiser's Room**	**AIRAPT Committee Meeting**
6:30pm to 8pm	**Lennox**	**Cocktail Reception**

The Joint 28th AIRAPT and 60th EHPRG International Conference 2023

Programme

Tuesday 25 July 2023

Time	Room	Programme
8:15am to 8:45am		**Arrival Refreshments**
8:45am to 9am	**Lennox**	**Bridgman Award Introduction**
9.00am to 9:50am	**Lennox**	**Bridgman Lecture** **Tetsuo Irifune:** Multi-anvil technology and applications to novel materials synthesis
9:50am to 10:15am	**Lennox**	**Morning Break**
10:15am to 12:15pm	**Lennox**	**Secular Evolution of the Earth** **10:15am–10:45am Kenji Ohta:** Inversion of the temperature dependence of thermal conductivity of hcp iron under high-pressure **10:45am–11:00am Jinhyuk Choi:** Layered redox processes of post-giant impact Earth, simulated and probed by European-XFEL **11:00am–11:15am Eric Edmund:** Thermal Conductivity of Bridgmanite at Lower Mantle Conditions **11:15am–11:30am Uwe Kleinschmidt:** Electrical and thermal conductivity of iron at Earth's core conditions from ab initio simulations **11:30am–11:45am Yongjae Lee:** Oxidation of iron by giant impact and its implication on the formation of reduced atmosphere in the early Earth **11:45am–12:00pm Isaac Taschimowitz:** Modelling the Density of Earth's Magma Ocean Using Machine Learning **12:00pm–12:15pm Duanwei He:** The mechanical state of the earth's crust and the force source of crustal plate movement
	Lowther	**Computational Methods** **10:15am–10:45am Chris Pickard:** Mapping and accelerating stochastic explorations of dense matter **10:45am–11:00am Stanimir Bonev:** First principles calculations of liquid entropy **11:00am–11:15am Hocine Chorfi:** Fine-tuning the strategy XtalOpt + Gibbs2 codes. Application to thermoelectric compounds (AgCl, PbTe and CoSb3): Phase diagrams pT **11:15am–11:30am Peter Cooke:** Simulating Shock Compression with Ephemeral Data Derived Potentials **11:30am–11:45am Vili Grigorova:** Use of FEA for temperature gradient determination inside a high-pressure sample assembly **11:45am–12:00pm Matthew Lane:** Molecular Dynamics to Explore the Role of Temperature, Water, and Porosity in Dynamic Shock Compression of SiO2 **12:00pm–12:15pm Maximilian Schörner:** Ab initio simulations for the ion-ion structure factor of warm dense matter in the hydrodynamic limit

	Menteith	**Dynamic Studies of Elements** **10:15am–10:45am Danae Polsin:** Structural Competitiveness in Ramp-Compressed Sodium **10:45am–11:00am Amy Coleman:** Probing off-Hugoniot states in laser-driven, high-pressure experiments **11:00am–11:15am Martin Gorman:** Time resolved observations of a phase transformation in dynamically compressed Pb **11:15am–11:30am Hye-Sook Park:** Studying high-Z material strength under high-pressure at the National Ignition Facility **11:30am–11:45am Saransh Singh:** Complex dynamics during a shock-induced phase transition in Zr **11:45am–12:00pm Cara Vennari:** Observation of defects in shocked diamond below the HEL
	Lammermuir	**Hydrogen (10:15am to 12:30pm)** **10:15am–10:45am Arnold Schwemmlein:** Toward Accessing the Solid Metallic State of Hydrogen via Ramp Compression of Solid parahydrogen **10:45am–11:15am Alexander Drozdov:** Metallization of hydrogen through a semi-metallic state **11:15am–11:45am Dominik Kraus:** Evidence for isolated hydrogen in laser-compressed hydrocarbons **11:45am–12:00pm Isaac Silvera:** The Metallic Hydrogens: Reflectance, Electrical Conductance, and Metastability **12:00pm–12:15pm Nakayama Atsuko:** Raman study of supercritical fluid phase of hydrogen at room temperature **12:15pm–12:30pm Eugene Gregoryanz:** Hydrogen and deuterium at very high compressions
	Moffat	**Molecular Compounds** **10:15am–10:45am Maria Rescigno:** High-pressure Plastic Phases of water and water-ammonia mixtures **10:45am–11:15am Hannah Shuttleworth:** Effects of high-pressure on the methane-nitrogen binary system **11:15am–11:30am Niccolo Avallone:** Molecular dynamics study of thermally-activated plastic transition in Ammonia Hemihydrate under intense pressure **11:30am–11:45am Frédéric Datchi:** Phase diagram and sound velocity of ammonia from Brillouin scattering in the laser heated diamond anvil cell **11:45am–12:00am Yang Song**: Synergetic Effect of High-pressure and Temperature Leading to Remarkably Enhanced CO2 Adsorption Capacity of ZIF-8 **12:00am–12:15pm Andrzej Katrusiak:** High-pressure preference for low-density polymorphs
12:15pm to 2.00pm	**Lennox**	**Lunch**
2.00pm to 4.00pm	**Lennox**	**Hydrides 3** **2:00pm–2:30pm Katsuya Shimizu:** Synthesis of Light-Element-Doped Lanthanum Superhydrides **2:30pm–2:45pm Maelie Causse:** Superionicity of H- in LaH10 superhydride **2:45pm–3:00pm Di Zhou:** Nuclear magnetic resonance in lanthanum polyhydrides up to 1.5 Mbar **3:00pm–3:15pm Bin Li:** Observation on Physical Properties of nitrogen-doped lutetium hydrides under pressures below 30 GPa **3:15pm–3:30pm Sun-Woo Kim:** Microscopic theory of colour in lutetium hydride **3:30pm–3:45pm Israel Osmond:** Observation of A15-type LaH~6 at Moderate Pressures **3:45pm–4:00pm Vasily S. Minkov:** Magnetic field screening and magnetic flux trapping in hydrogen-rich high-temperature superconductors

	Lowther	**Static Studies of Elements 1** **2:00pm–2:30pm Agnès Dewaele**: Mechanisms of phase transformation in metals under extreme conditions: examples of iron and titanium **2:30pm–2:45pm Emma Ehrenreich-Petersen**: Rapid Compression of Antimony in Dynamic Diamond Anvil Cells: Hunting the Phase Transitions **2:45pm–3:00pm Laura Henry**: Mesoscale mechanisms of the isostructural phase transition in Cerium **3:00pm–3:15pm Valery I Levitas**: Recent in-situ experimental and theoretical advances in severe plastic deformations, strain-induced phase transformations, and nanostructure evolution under high-pressure **3:15pm–3:30pm Christian Storm**: The Structure and Behaviour of Na-hP4 up to 300 GPa
	Menteith	**Nitrides, Borides and Carbides 2** **2:00pm–2:30pm Elena Bykova**: Applying methods of high-pressure crystallography in studies of high-pressure chemistry of metal borides **2:30pm–3:00pm Ken Niwa**: Crystal chemistry of binary nitrides and phosphides synthesised at high-pressure **3:00pm–3:30pm James Walsh**: Synthesis of metastable transition metal carbides using high-pressure **3:30pm–3:45pm Andrey Aslandukov**: The discovery of novel high-pressure yttrium nitrides in laser-heated diamond anvil cells using the Domain Auto Finder (DAFi) program **3:45pm–4:00pm Dominique Laniel**: High-Pressure Synthesis of Ultraincompressible and Recoverable Carbon Nitrides
	Lammermuir	**Next Gen Synchrotrons** **2:00pm–2:30pm Mohamed Mezouar**: ID27_II a unique beamline for science under extreme conditions **2:30pm–3:00pm Jiyong Zhao**: Perspectives of IXS and NRS for high-pressure studies in the APSU era **3:00pm–3:15pm Gilberto Fabbris**: Probing magnetism at extreme conditions at the APS-U POLAR beamline **3:15pm–3:30pm Ilya Kupenko**: New opportunities at the Nuclear Resonance Beamline of ESRF with submicron spatial resolution **3:30pm–3:45pm Changyong Park**: New HDCM and HDMM for Advanced Spectroscopy, Microscopy and Time-resolved XRD at HPCAT 16-ID-D and 16-ID-E Beamlines **3:45pm–4:00pm Maddury Somayazulu**: Tailored Software and Hardware development for emerging synchrotron high-pressure research at HPCAT
	Moffat	**Electronic Transitions 2** **2:00pm–2:30pm Alexander Tsirlin**: Pressure-induced magnetism collapse in 4d and 5d honeycomb compounds **2:30pm–2:45pm Bishnupada Ghosh**: Strain induced structural and electronic phase transitions in Transition metal dichalcogenides **2:45pm–3:00pm Roy Cohen**: The Pressure Driven Superconductor-Insulator-Transition in 2D Films **3:00pm–3:15pm Ece Uykur**: Dimensional crossover and re-entrant superconductivity in pressurised kagome metals AV_3Sb_5 **3:15pm–3:30pm Igor Abrikosov**: Revealing pressure induced electronic phase transitions at extreme conditions **3:30pm–3:45pm Yuming Xiao**: Synchrotron spectroscopies for the study of electronic and magnetic transitions under high-pressure at HPCAT
4pm to 6pm	**Lennox**	**Poster Session 1 and Refreshments**
6pm to 8pm	**Lennox**	**EHPRG General Assembly**

The Joint 28th AIRAPT and 60th EHPRG International Conference 2023

Programme

Wednesday 26 July 2023

Time	Room	Programme
8:30am to 9.00am	**Lennox**	**Arrival Refreshments**
9.00am to 9:50am	**Lennox**	**Plenary II Crystele Sanloup**: What does pressure-induced xenon chemistry tells us about planetary formation?
9:50am to 10:15am	**Lennox**	**Morning Break**
10:15am to 12:15pm	**Lennox**	**Outer Planets and Exoplanets 1** **10:15am–10:45am Michelle Marshall**: High-pressure phase transformations in ramp-compressed SiO2 **10:45am–11:00am Federica Coppari**: X-ray diffraction and laser-driven ramp-compression of iron at TPa **11:00am–11:15am Guillaume Morard**: Study of liquid silicates using laser-driven shock compression **11:15am–11:30am Yingwei Fei**: Measurements of melting and pressure calibration at extreme pressure **11:30am–11:45am Ashkan Salamat**: Evidence of symmetry lowering in dense H2O-ice above 300 GPa **11:45am–12:00pm Tsutomu Mashimo**: Measurement of Electrical Conductivity of Water and Heavy Water under Reverberating Shock Compression
	Lowther	**Computational Studies of Elements** **10:15am–10:45am Zhi Li**: Phase diagram of Iron at Earth's core conditions from deep learning **10:45am–11:15am Roman Martonak**: Study of polymerisation of high-pressure nitrogen by ab initio molecular dynamics **11:15am–11:45am John Tse**: Electronic and Dynamical Properties and Polymorphism in the Solid and Liquid Phases of Compressed Sodium **11:45am–12:00pm Sabri Elatresh**: Structural transitions and electride properties in the phase diagram of magnesium **12:00pm–12:15pm Wilfried B. Holzapfel**: Colourful systematic in the phase-diagrams of the elements
	Menteith	**Synthesis and Properties of Novel Materials 2** **10:15am–10:45am Frederico Alabarse**: Tuning thermal expansion and mechanical properties by high-pressure insertion of guest molecules **10:45am–11:15am Xiang Li**: High-pressure Synthesis and Physical Properties of New Functional Materials **11:15am–11:30am Francisco Javier**: Structural, Vibrational and Electronic Behavior of Two GaGeTe Polytypes under Compression **11:30am–11:45am Robin Turnbull**: Pressure-induced phase transition and band-gap decrease in semiconducting Na3Bi(IO3)6 **11:45am–12:00pm Jun Zhang**: A Ferrotoroidic Candidate with Well-Separated Spin Chains Synthesised at High-pressure

	Lammermuir	**Instrumentation and Techniques 1** **10:15am–10:45am Asami Sano-Furukawa**: Recent developments in neutron diffraction experiments at high-pressure and high temperature and application to Earth science **10:45am–11:00am Stefan Klotz**: HYDROMET: A new facility to study hydrogen embrittlement of materials at up to 2 kbar H2-pressure **11:00am–11:15am Kazuki Komatsu**: Nano-polycrystalline diamond anvil cells for neutron diffraction up to 100 GPa **11:15am–11:30am Antonio M. dos Santos**: In-Situ Pressure Control System for Neutron Scattering Cells: Applications for Low-Temperature Physics **11:30am–11:45am Longjian Xie**: Novel low-Z materials for combined X-ray and large-volume-press studies **11:45am–12:00pm Anna Makal**: Polymorphism of Luminescent Materials at High-Pressure and Why Crystal Orientation Matters
	Moffat	**Bio/Life Sciences and Soft Matter** **10:15am–10:45am Catherine Royer**: Pressure-based mapping of protein conformational landscapes **10:45am–11:00am Arvi Freiberg**: Towards the Understanding of Pressure-Induced Protein Phase Transitions **11:00am–11:15am Rohan Ajit Kulkarni**: Effects of extreme hydrostatic pressure on the wood-pulp fibre cell wall structure **11:15am–11:30am Sebastian Pawlus**: Is high-pressure an essential parameter for studying hydrogen-bonded materials? The case of monohydroxy alcohols **11:30am–11:45am Christian Roumestand**: Does similar folds mean similar folding pathways? A comparative high-pressure NMR study of the unfolding of two Ig-fold modules **11:45am–12:00pm Leonardo Chiappisi**: Pressure-induced phase transition in polymer brushes: thermodynamic predictions and structural studies **12:00pm–12:15pm Zhe Chen**: Assessment of changes in enzyme activity, bioactive compound, sugar, and sensory attribute during the storage of high-pressure treated pre-packaged squash cubes
12:15pm to 2.00pm	**Lennox**	**Lunch**
2.00pm to 4.00pm	**Lennox**	**Hydrides 4** (2pm to 4:15pm) **2:00pm–2:30pm Mikhail Eremets**: High temperature conventional superconductivity **2:30pm–2:45pm Sam Cross**: Superconductivity at 90 K in a lanthanum hydride film at 95 GPa **2:45 pm–3:00 pm Feng Du**: Tunnelling and Andreev spectroscopy studies on H3S **3:00pm–3:15pm Hiranya Pasan Vindana Wadhurawa Mudiyanselage**: Observation of superconducting gap in Carbonaceous Sulphur Hydride **3:15pm–3:30pm Dmitrii Semenok**: Non-Fermi-liquid behaviour of superhydrides **3:30pm–3:45pm Jonathan Buhot**: Superconductivity in YH4 Films at Very High-pressures **3:45pm–4:00pm Zhongyan Wu**: Superconductivity observed in yttrium lutetium ternary hydrides **4:00pm–4:15pm Guangtao Liu**: The synthesis and property study of ternary high-temperature superconducting polyhydride under high-pressure

	Lowther	**Synthesis and Properties of Novel Materials 1** **2:00pm–2:30pm Masashi Hasegawa**: Synthesis, Crystal Growth and Physical Properties of High-Entropy Transition-Metal Nitrides under High-Pressures and High-Temperatures **2:30pm–3:00pm Hongbo Lou**: Novel metallic glass states synthesised from extreme conditions **3:00pm–3:15pm Ben Heuser**: Recovery of Nanodiamonds Produced in Laser-Driven Shock-Experiments **3:15pm–3:30pm Qiaoshi Zeng**: Pressure-induced non-monotonic crossover of steady relaxation dynamics in a metallic glass **3:30pm–3:45pm Fabian Zimmerhofer**: Crystal Structure, Characterisation and Luminescence Properties of Mn(4+)-Doped K3Nb2O4F5 **3:45pm–4:00pm Elena Stellino**: High-Pressure Behaviour of δ-Phase of Formamidinium Lead Iodide by Optical Spectroscopies
	Menteith	**Equation of State 1** **2:00pm–2:30pm Gilbert 'Rip' Collins**: Converging to atomic pressures **2:30pm–3:00pm Jean-Paul Davis**: High-precision room-temperature isotherm of Pt to over 400 GPa from ramp-compression experiments at the Z machine **3:00pm–3:15pm Richard Briggs**: Ramp EOS measurements through phase transitions in tin up to 10 Mbar
	Lammermuir	**Instrumentation and Techniques 3** **2:00pm–2:30pm Jon Eggert**: Overview of TARDIS on NIF **2:30pm–3:00pm Emma McBride**: Direct Measurement of Temperature from Laser Compressed Argon at the LCLS **3:00pm–3:15pm Georgios Aprilis**: Measuring viscoelasticity inside the laser-heated Diamond Anvil Cell: Time-resolved Synchrotron Mössbauer Source spectroscopy **3:15pm–3:30pm Alexis Forestier**: Fast and confocal Brillouin spectroscopy for the study of molecular systems at planetary interiors conditions **3:30pm–3:45pm Silvia Pandolfi**: X-ray imaging of silicon under shock-compression at the LCLS: direct visualisation of high-pressure phase nucleation and multi-wave kinetics **3:45pm–4:00pm Guoyin Shen**: Multiple-axis diamond anvil cell: MDAC
	Moffat	**Magnetic Materials 2** **2:00pm–2:30pm Jing Song**: Enhanced Magnetic Ordering in Lanthanide Metals under Extreme Pressure **2:30pm–2:45pm Matthew Clay**: Neutron and X-ray Diffraction Study of Magnetic Ordering in Terbium at High-pressures and Low Temperatures **2:45pm–3:00pm Dominik Kurzydłowski**: Phase transitions in compressed palladium trifluoride: how Pd(II)Pd(IV)F6 becomes Pd(III)F3 **3:00pm–3:15pm Eduardo Poldi**: Cobaltates as prospective Kitaev quantum spin liquids: atomic, electronic and magnetic responses of Na3Co2SbO6 under pressure **3:15pm–3:30pm Ricardo Dos Reis**: Understanding quantum materials by X-ray techniques under high-pressure
4.00pm to 4:30pm	**Lennox**	**Afternoon Break**

4:30pm to 6:30pm	Lennox	**Outer Planets and Exoplanets 2** **4:30pm–5:00pm Mungo Frost**: Diamond Precipitation Dynamics from Hydrocarbons at Icy Planet Interior Conditions **5:00pm–5:15pm Ivan Oleynik**: Carbon at Extremes: Discovery Science with Machine Learning, Exascale Computers and Experiment **5:15pm–5:30pm Wan Xu**: Dense ammonia-containing composite systems in ice giants at high-pressures **5:30pm–5:45pm Anshuman Mondal**: Novel ammonia hydrates in the mid-mantle layers of icy (exo)planets **5:45pm–6:00pm Andreas Hermann**: First principles calculations of light element mixtures at planetary **6:00pm–6:15pm Michael Stevenson**: Chemistry of Low Z Mixtures at Icy Giant Conditions **6:15pm–6:30pm Martin Preising**: Material properties of matter in Saturn's interior from ab initio simulations
	Lowther	**Synthesis and Properties of Novel Materials 3** **4:30pm–5:00pm Martin Bremholm**: Discovery of a Seven-Coordinated CrSb2 High-pressure Polymorph **5:00pm–5:30pm Bingbing Liu**: Ultrahigh-pressure Generation at High-Temperature in a Walker-type Large-volume Press and its applications to the research of new carbon materials **5:30pm–5:45pm Julia-Maria Huebner**: Host-guest framework compounds based on silicon by high-pressure high-temperature synthesis **5:45pm–6:00pm Takuya Sasaki**: High-pressure synthesis and crystal chemistry of novel Cr-Ge compounds **6:00pm–6:15pm Timothy Strobel**: Boron-Stabilised Carbon Clathrates
	Menteith	**Electronic Transitions 1** **4:30pm–5:00pm Serge Desgreniers**: Photoluminescence of the Negatively Charged Split Silicon-Vacancy Defect in Diamond at Low-Temperature and High-pressure **5:00pm–5:15pm Keith Lawler**: Density driven changes in electronic properties of the binary M(IV) oxides (M=Sn, Ge, Ru) **5:15pm–5:30pm Daniel Errandonea**: High-pressure behaviour of Mg(IO3)2 **5:30pm–5:45pm Xiang Li**: Complex electronic and magnetic properties in Fe4O5 **5:45pm–6:00pm Jasmine Hinton**: Experimentally observed and computationally confirmed electronic topological transition in cadmium **6:00pm–6:15pm Anjana Joseph**: Pressure-induced phase transitions in 3D topological insulator TlBiTe2 **6:15pm–6:30pm Yang Ding**: Electronic Structure of Quantum Materials at High-pressure
	Lammermuir	**Static Studies of Elements 2** **4:30pm–5:00pm Shanti Deemyad**: Structural boundaries of lithium within its superconducting region **5:00pm–5:30pm Lisa Luhongwang Liu**: Pressure induced phase transition, crystallisation, and negative linear compressibility in crystalline and non-crystalline selenium **5:30pm–5:45pm Robin Fréville**: Phase diagram of tin under extreme conditions **5:45pm–6:00pm Daniel Sneed**: High-pressure structural systematics of Dy compressed in a neon pressure medium

	Moffat	**Instrumentation and Techniques 4** **4:30pm–4:45pm Simon Hunt**: Continuous peak fit: a new algorithm for fitting spotty, noisy or incomplete x-ray diffraction data **4:45pm–5:00pm Thomas Meier**: New Frontiers in nuclear magnetic resonance for high-pressure research and Geo-science **5:00pm–5:15pm Keizo Murata**: High-pressure medium, solidifying at pressure beyond 5 GPa at room temperature, and related topics **5:15pm–5:30pm Kirill Vlasov**: A diamond anvil cell setup for dielectric measurements of aqueous and non-aqueous solutions up to 5 GPa and 1073 K **5:30pm–5:45pm Eyal Yahel**: A novel differential thermal analysis measurements of phase transitions at high-pressure and temperatures **5:45pm–6:00pm Andreas Zerr**: Influence of elastic anisotropy on measured sound velocities of cubic solids
7.00pm to 11.00pm	**The National Museum of Scotland**	**Reception Drinks and Conference Dinner** The National Museum of Scotland, Chambers Street, Edinburgh EH1 1JF (15-minute walk from the EICC)

The Joint 28th AIRAPT and 60th EHPRG International Conference 2023

Programme

Friday 28 July 2023

Time	Room	Programme
8.00am to 8:30am	**Lennox**	**Arrival Refreshments**
8:30am to 9:10am	**Lennox**	**Jamieson Award Introduction and Lecture** **Akun Liang**: Pressure-induced band-gap increase in hydrated Ca(IO3)2
9:10am to 9:50am	**Lennox**	**EHPRG Award Introduction and Lecture** **Jean-Alexis Hernandez**: Exploration of planetary compounds at large terrestrial and icy planets' interior conditions
9:50am to 10:15am	**Lennox**	**Morning Break**
10:15am to 12:15pm	**Lennox**	Closing Ceremony

The Joint 28th AIRAPT and 60th EHPRG International Conference 2023

Poster Presentations

Poster Session Tuesday 25 July

Poster Board No.	First Name	Last Name	Paper Title
1	David	Abbasi Pérez	Simulation of Pressure Effects on Small Molecules Confined inside Carbon Nanotubes Using Density Functional Theory and Machine Learning Potentials
3	Marie-pierre	Adam	Optical properties of SiV and GeV colour centres in nanodiamonds under hydrostatic pressures up to 180 GPa
5	Sergejs	Afanasjevs	Extreme pressure-sensitivity of electrical resistivity in $Pt(bqd)_2$
7	Fernando	Aguado	Stability and High-Pressure behaviour of Paracetamol polymorphs through Raman spectroscopy
9	Frederico	Alabarse	Xpress beamline, Diffraction at Extreme Conditions – Elettra Sincrotrone Trieste
11	Monica	Amboage	Opportunities for high pressure research at beamline I18 of the Diamond Light Source
13	Shuto	Asano	High-pressure synthesis and characterisation of NiAs-type novel manganese mononitride
15	Francesco	Belli	Impact of ionic quantum fluctuations on the thermodynamic stability and superconductivity of LaBH8
17	Shrikant	Bhat	Novel Material Synthesis @ Large Volume Press Beamline P61B PETRA III
19	Khachiwan	Buakor	In situ X-ray diffraction study of (Fe,Mg)O under shock compression
21	Jonathan	Buhot	Raman spectroscopy under megabar pressures and high magnetic fields
23	Maelie	Causse	Prediction and synthesis of polyhydrides in the Y-Fe-H system
25	Amrita	Chakraborti	Superhard boron carbide: new insights into anomalous dynamic failure and how to reinforce it
27	Chung Ching	Chang	High-pressure synthesis of multi-components (Cr1-x-yMnxVy)P4 phosphides
29	Jin-Ming	Chen	Sequential spin state transition and intermetallic charge transfer in PbCoO3 under high-pressure

31	Leonardo	Chiappisi	The soft matter and chemistry support facilities at the Institut Laue-Langevin
33	Dimitrios	Christofilos	High-pressure Raman study of ibuprofen
35	Lewis	Clough	The high-pressure behaviour of Nd(XeF2)3(TaF6)3
37	Giuseppe	Cocomazzi	Investigating the melting temperature of silicates at extreme conditions using single pulse laser heating and time resolved XRD
39	Cassandra	Dailledouze	Application of Quantum Diamond Magnetometry to High-Tc Cuprate Superconductivity
41	Begoña	De Ancos	High pressure-assisted extraction of phenolic compounds from mango by-products
43	Koen	De Hantsetters	Finite element analysis to extent Boehler-Almax anvils to ultra-large apertures
45	Viktoriia	Drushliak	Temperature and high-pressure studies of layered perovskite Cs[C(NH2)3]PbI4
47	Utpal	Dutta	High-Pressure Study of Electrical Transport Properties of VBr3 and CrBr3: Possible Pressure Induced Metallisation
49	Matthias	Elender	Optical setup for fluorescence pressure measurements in piston-cylinder pressure cells with LED light source
51	Moran	Emuna	Effect of the incommensurate Bi-III phase on the Bi-Sb system under pressure
53	Alexis	Forestier	Superionicity of hot dense fcc ice evidenced by X-ray diffraction
55	Sven	Friedemann	Lifshitz transition at the onset of superconductivity in TiSe2
57	Sven	Friedemann	Clean-limit superconductivity in Hydrogen Sulphide H3S
59	Kazuhiro	Fuchizaki	Evaluation of a disposal type of 6–6 frame for high-pressure experiments
61	Satomi	Fujiwara	Raman study of supercritical fluid hydrogen coexisting with multilayer graphene at room temperature
63	Ken-ichi	Funakoshi	Structural changes in hydrous sodium silicate melts under high-pressure
65	Samuel	Gallego Parra	Characterisation of the ε'-Fe_2O_3 phase under extreme conditions
67	Tania	Garcia-Sanchez	High-pressure study of PbGa2S4
69	Hélène	Ginestet	MHz X-Ray Diffraction and X-Ray-Heating in the Diamond Anvil Cell: A Metrology Study on Fe

71	Nico	Giordano	Second Order Phase Transition and Stabilizing CH–H and CH–S Interactions in Naphthyl End-Capped Bithiophene at 3.5 GPa
73	Benny	Glam	Phase transition and sound velocity study of shock loaded CaF2
75	Alexander F	Goncharov	Thermal conductivity of deep Earth minerals and alloys measured at extreme pressure-temperature conditions
77	Geethanjali	Gopakumar	MetalJet X-ray sources for Experiments at Non-ambient Pressures and Temperatures
79	Christophe	Guillaume	Triple Coil Setup for Studies of Magnetic Properties at High-Pressure
81	Christophe	Guillaume	Innovative Design for Multimegabar Diamond Anvil Cell
83	Xin	He	Superconductivity Observed in Tantalum Polyhydride at High-Pressure
85	Antoine	Hilberer	Visible to mid-IR reflectivity of materials under extreme pressure
87	Jasmine	Hinton	Isothermal mode Gruneisen Tensor of Cadmium across electronic and structural phase boundaries
89	Mylaine	Holin	Analysis of ammonia-methane mixtures under high-pressure and high-temperature
91	Wilfried B	Holzapfel	Equation of State for Ice Ih with explicit contributions from proton-disorder and molecular defects
93	Shuhe	Hu	Pressure-Induced Emission Enhancement of π-conjugated Charge-Transfer Materials with Different Molecular Stacking
95	Agnieszka	Hućˊ	Structural transformations of chevkinite group minerals
97	Osamu	Ikeda	Pressure-induced magnetic transition of ε-FeOOH at 8 GPa
99	Almudena	Inchausti Valles	New insights in chemical and mechanical effects in ru(ii)-ru(iii) bonds
101	Kunlang	Ji	High field neutron study and complex magnetic structures of the NTO-type solid solution Ni2-xCoxScSbO6
103	Changqing	Jin	Superconductivity above 80 K in Polyhydrides of Hafnium
105	Changqing	Jin	Superconductivity above 210 K Discovered in Superhydrides of Calcium
107	Yeonhak	Jung	Reaction between the feldspars and water in the Earth's transition zone
109	Konstantin	Kamenev	Use of novel composite materials in construction of non-metallic high-pressure cells

111	Mikołaj	Kamiński	Ni2+ broadband infrared emission in varying temperature and pressure
113	Aigerim	Karina	Pressure dependence of dynamics in high-density amorphous ice
115	Jiří	Kaštil	Magnetic properties of layered van-der-Waals ferromagnets VI3 and CrI3 under high-pressures
117	Michał	Kaźmierczak	Intermolecular interactions in multicomponent crystals under pressure: a study case of 1,2-bis(4-pyridyl)ethane and fumaric acid cocrystal
119	Rustem	Khasanov	Three-wall piston-cylinder type pressure cell for muon-spin rotation/relaxation experiments
121	Egor	Koemets	Chemical interactions of iron and methane at extreme conditions
123	Tetsuya	Komabayashi	Melting experiments of the system Fe-Si-O under high-pressure with implications for the Earth's core
125	Petr	Král	Magnetism of geometrically frustrated Yb2Pt2Pb in elevated pressures
127	Joanna	Krzeszczakowska	Pressure-induced phase transitions and Equations of State for a luminescent arylacetylide-gold(I) compound.
129	Jorge	Laranjeira	Superconductivity in Novel Carbon Nanostructures
131	Eric	Lenhart	The thermal conductivity of liquid Fe-S-Si alloys at 2–5 GPa with implications for the dynamos of small outer Solar System planetary bodies
133	Tadeusz	Lesniewski	Evolution of the full energy structure of Mn4+ in fluoride phosphors under high-pressure
135	Valery I	Levitas	Plastic strain-induced phase transformations in Si: drastic reduction of transformation pressures, change in transformation sequence, and size effect
137	Valery I	Levitas	Simulations of multivariant Si I to Si II phase transformation in polycrystalline silicon with finite-strain scale-free phase-field approach
139	Qingchen	Li	Correlation effects on the structure and stability of Nickel Oxides under pressure
141	Hanns-Peter	Liermann	Present and Future Extreme Conditions Research at Low (PETRA III) & Ultra-Low (PETRA IV) Emittance Synchrotron Sources at DESY
143	Fuyang	Liu	Green luminescence in heavily carbon doped GaN synthesised by atomic substitution under high-pressure and high temperature

145	Jingyi	Liu	High-pressure Raman study of hcp metals Be, Os, and Re up to 200 GPa
147	Yuwei	Liu	High-pressure synthesis and study of structural and physical properties of Ba-based Ruddlesden-Popper 4d/5d transition metal oxides
149	Natalia	Majewska	Chemical and mechanical pressure influence on luminescence properties of near-infrared phosphors
151	Heehyeon	Sim	Hydration breakdown of serpentines along cold core geotherm
153	Seohee	Yun	Super-hydration and reduction of manganese oxide minerals at shallow terrestrial depths

Poster Session Thursday 27 July

Poster Board No.	First Name	Last Name	Paper Title
2	Ran	Aharoni	High Pressure EOS and Phase Transition in the Pb-Sb Alloy System
4	Matthew	Clay	A new metastable state in the rare-earth hexaboride EuB_6 induced by high pressure
6	Mikhail	Kuzovnikov	Lattice dynamics and heat capacity of multilayer graphane
8	Valery I	Levitas	Tensorial stress-plastic strain fields in α - ω Zr mixture, transformation kinetics, and friction in diamond anvil cell
10	Valery I	Levitas	New rules for coupled severe plastic deformation, strain-induced phase transformations, and nanostructure evolution under high-pressure
12	Edyta	Malinowska-Pańczyk	Hyperbaric storage of human milk at sub-zero temperature – impact on microbiota, leukocytes and basic nutrients
14	Tomas	Marqueno	Metallic hydroxides within the Earth's deep-water cycle
16	Philipp	May	Equation of state and diamond formation kinetics of C-H-O mixtures under ice giant interior conditions
18	Malcolm	McMahon	Are You Using the Wrong EoS in Dioptas?
20	Martin	Míšek	High-pressure study of the van-der-Waals ferromagnet CrBr3
22	Katharina	Mohrbach	Thermal conductivity of H2O ice VII from X-ray heating experiments at the European XFEL
24	Virginia	Monteseguro	Crystal-field mediated electronic transitions of EuX monochalcogenides (X = O, S, Se and Te) up to 35 GPs
26	Yoshihisa	Mori	Development of a high-pressure cell for SPS equipment
28	Hermann	Muhammad	Melting curve of black phosphorus and associated colossal volume jump
30	Alfonso	Muñoz	ScAlO3 perovskite under high pressure from first principles simulations.
32	Yuki	Nakamoto	Crystal structure and superconductivity of alkaline earth metal Strontium at low temperature and high-pressure
34	Satoshi	Nakano	High-pressure/high-temperature phase diagram of BaH_2 and the formation of barium polyhydride
36	Lucie	Nataf	XAS and XMCD under extreme conditions at the ODE beamline – SOLEIL Synchrotron

38	Ayako	Ohmura	The effect of pressure on superconductivity in AuxPd1-xTe2
40	Vitaly	Paris	Sound velocity, second shock velocity and off-Hugoniot measurements of lead compressed up to 83 GPa
42	Lea	Pennacchioni	Crystal structure and high-pressure phase behaviour of a CaCO3-SrCO3 solid solution
44	Ana Carmen	Perdigón Aller	High-pressure structural stability and luminescence studies of nanoclays for environmental applications
46	Juan	Pintor	Phase transitions and electronic properties of Fe2O3 under laser compression by ultrafast in-situ X-ray absorption spectroscopy
48	Christian	Plueckthun	Combining high-pressure and low temperature with single crystal resonant x-ray diffraction, P09, PETRA III
50	Aleksandra	Półrolniczak	Pressure-induced sorption in Cd(oba)(azpy) metal-organic framework in liquid and gaseous environment
52	Tomasz	Poreba	Pressure-tuned blue-to-orange light emission in polymorphic diphenylmaleic anhydride
54	Michael	Pravica	Studies of PFOA at extreme conditions
56	Clemens	Prescher	Investigating the iron phase diagram utilizing MHz diffraction at the European X-ray free electron laser
58	John	Proctor	Modelling of liquid internal energy and heat capacity over a wide pressure-temperature range from first principles
60	John	Proctor	Phase diagram of ethane to 450 K and 120 GPa
62	John	Proctor	Raman scattering study of liquid and solid propane to 60 GPa at 300 K
64	Benjamin	Pullicino	High-Pressure/High-Temperature Synthesis and Crystal Structure of two new Zinc Oxotellurate(VI) Compounds
66	Divyanshu	Ranjan	Characterising C-H demixing and Hydrogen metallization in Warm Dense Matter conditions
68	J. Manuel	Recio	On the high-pressure phase of 1T-HfSe2
70	Lukasz	Rogal	Transmission electron microstructure studies of Ti40Zr20Nb20Hf5Ta15 high entropy alloy after laser-heated diamond anvil cell experiments
72	Javier	Ruiz-fuertes	High-pressure phase of Iridium-based Sr2BIrO6 (B = Ca, Zn) Double Perovskites
74	Takeshi	Sakai	Equations of state of metals (Fe, Mo, Cu, W, Re, Pt, Au) and magnesium oxide (MgO) at multi-megabar pressure
76	Juan Ángel	Sans	Synchrotron-based structural characterization of Sr2FeIrO6 under high pressure

78	Misaki	Sasaki	Search for Superconductivity of Layered Iron Superhydrides Synthesised under High-Temperature and High-Pressure
80	Haritha	Sasidharan Vanaja	High-pressure structural study of CeAl2
82	Gordon	Scholz	Probing iron's spin state in FeS at conditions of the Martian core
84	Dmitrii	Semenok	Superconductivity in polyhydrides: 8 years after discovery of H3S
86	Gregory Alexander	Smith	Stoichiometric Determination of Clathrate-like Yttrium Hydride under Megabar Conditions
88	Yang	Song	Spacer Dependent and Pressure Tuned Structures and Optoelectronic Properties of 2D Hybrid Halide Perovskite
90	Altair	Soria Pereira	In situ and ex situ studies of silicate glasses and glass-ceramics under high-pressure
92	James	Spender	High-Pressure Investigation of the I-N System
94	Darko	Stojkovski	High-pressure and low-temperature studies of guanidinium iodobismuthate(III)
96	Marek	Szafrański	All-Inorganic Perovskites CsPbBr3 and CsPbCl3 under High-Pressure
98	Masashi	Tanaka	High-Pressure Effect on EuNi2As2
100	Minxue	Tang	In situ X-ray diffraction of the α-ε phase transition in iron at intermediate strain rates
102	Evgeny	Tararushkin	Classical atomistic simulations of the 10Å phase at high- temperatures and pressures
104	Tobias A.	Teichtmeister	Pr3Mo4B6O24(OH)3: High-Pressure/High-Temperature Synthesis of an Acentric Rare Earth Molybdenum Borate
106	Nicola	Thiering	In situ study of Fe2O3 at pressure and temperature conditions of the Earth's lower mantle
108	William	Thomas	High-pressure magnetic measurements of β-phase UH3
110	Pierre	Toulemonde	High pressure crystal structure study of non-superconducting Ln4Ni3O8 and (Ln1-xAx)NiO2 layered bulk nickelates (Ln = La, Pr, Nd ; A = Sr, Ca)
112	Kazunori	Umeo	Pressure Effects on the Specific Heat of the Thermoelectric Compound InTe
114	Erik	Uran	Hydrostatic behaviour of selected chemically inert pressure-transmitting media
116	Mercedes	Vasquez	Composition and pressure effects on thermal conductivity of terrestrial planetary cores: Canyon Diablo iron meteorite as a natural analogue

118	Sergio	Villa-cortes	The Isotope Effect and Critical Magnetic Fields of Superconducting YH$_{6}$: A Migdal-Eliashberg Theory Approach
120	Duojun	Wang	Electrical conductivity of clinochlore at high- pressure and temperature
122	Qinyan	Wang	Hornblende Crystal Populations of Appinites from the Jiagou Mesozoic Intrusion, Southeastern Margin of the North China Craton and their Genetic Implications
124	Marisa	Wood	Sound velocities in the Lunar Mantle
126	Fang	Xu	TiC-MgO composite: an X-ray transparent and machinable heating element for the multi-anvil high-pressure apparatus
128	Keishiro	Yamashita	Development of conical diamond anvil cell for single-crystal neutron diffraction under high-pressure
130	Daisuke	Yamazaki	Electrical resistance of Fe2O3 at high-pressure
132	Jiafeng	Yan	Synthesis and Structural Study of Lanthanum Aluminium Hydrides under High-Pressure
134	Yansun	Yao	Machine Learning Accelerated Simulation of Solid-Solid Phase Transitions under High-Pressure
136	Akira	Yoshiasa	Single crystal structure refinements and Debye temperatures of kashinite-bowieite (Ir2S3-Rh2S3) and erlichmanite-laurite (OsS2-RuS2) solid-solutions
138	Zena	Younes	Thermal conductivity of deep earth minerals using high pressure-temperature time-resolved powder X-ray diffraction at European XFEL.
140	Shuhua	Yuan	Negative linear compressibility in Se under pressure
142	Enrique	Zanardi	Phosphorus dimerization in GaP under high-pressure
144	Andreas	Zerr	Elastic moduli, anisotropy and refractive index of γ-Ge_3N_4 via laser ultrasonics, Brillouin light scattering, and first-principles calculations
146	Changling	Zhang	Record High Tc Element Superconductivity in Titanium at High-Pressure
148	Jianfa	Zhao	Superconductivity in Zirconium Polyhydrides with Tc above 70 K
150	Yongsheng	Zhao	Temperature and pressure-dependent incommensurate to commensurate on NbSe3
152	Xin	Zhong	Prediction of Above-Room-Temperature Superconductivity in Lanthanide/Actinide Extreme Superhydrides
154	Raimund	Ziegler	Synthesis and crystal structure of the zinc borate Zn3B4O9

Plenary Presentations

Multi-anvil technology and applications to novel materials synthesis

Prof. Tetsuo Irifune[1]
[1]*Geodynamics Research Center, Ehime University, Japan*

Bridgman Lecture: Tetsuo Irifune, July 25, 2023, 09:00–09:50

Multi-anvil apparatus, particularly the one developed by late Prof. Naoto Kawai of Osaka University, is called as Kawai-type multiainvil apparatus (KMA), where the sample is squeezed by 8 super-hard cubic anvils surrounded by 6 steel anvils. The 6–8 anvil assembly is compressed in a large-volume press with capacity of applying loads of up to several thousand tons. By using tungsten carbide as the second-stage cubic anvils of KMA, stable quasi-hydrostatic pressures to ~30 GPa and temperatures to 3000℃ are produced in sample volumes of a few mm3 to ~1 cm3, while pressures as high as 100 GPa can also be achieved by using harder anvils made of sintered diamond. KMA has been mainly used in geosciences, and greatly contributed to the mineralogy, chemistry, and physics of the Earth's deep interior.

We have been using KMA as a tool for novel materials synthesis, utilizing its capability of generating stable ultra-high pressure in relatively large sample volumes. The first such material we produced was bulk sample of nano-polycrystalline diamond (NPD), which is highly transparent and exhibits ultra-hardness, even harder than single crystal diamond. Using a large KMA operated in a 6000-ton press, we are able to make pure NPD rod samples with dimensions up to ~ 1cm in both diameter and length, which have successfully been applied to ultrahigh-pressure studies, as well as for some industrial applications.

Another example of novel materials produced by KMA technology is transparent nano-ceramics (TNC) of high-pressure phases converted from some glass starting materials at pressures greater than 10 GPa and at modest temperatures of 1000–1400℃, utilizing rapid nucleation and slow grain growth under such conditions. Some of the TNCs are highly transparent, depending on birefringence of the nanocrystals and their grain sizes, and harder than the corresponding single crystals by ~30% due presumably to the Hall-Petch effect.

Here I review developments of multi-anvil technology, particularly those in Japan, and its applications to novel materials synthesis, focusing mainly on the synthesis of NPD. Recent studies in applications of NPD to high-pressure sciences, achieved in collaboration with a number of research groups in the world, are also reviewed with some future perspectives.

What does pressure-induced xenon chemistry tell us about planetary formation?

Chrystele Sanloup[1]
[1]*Sorbonne University, Paris, France*

Plenary II: Crystele Sanloup, July 26, 2023, 09:00–09:50

While 2022 marked the 60ieth anniversary of the noble gases chemistry with the landmark synthesis of the first xenon (Xe) compound (1,2), its long-neglected impact on our knowledge of planetary processes is just coming to light. Xenon isotopes are indeed key to unravel planetary and atmosphere formation processes, and for this purpose, Xe is considered inert, volatile, and expected to degas to the atmosphere upon rock melting. But Xe is atypical. Compared to lighter noble gases, Xe is extremely fractionated both isotopically and elementally in the Earth's and Mars' atmospheres. These observations motivated experiments and theoretical calculations to test Xe chemical reactivity at the extreme pressures and temperatures of planetary interiors. Interestingly, Xe chemistry is strongly P-dependent, with Xe metals synthesized above 150 GPa, stoichiometric Xe-oxides between 50 and 100 GPa, i.e., in the P-T range of the Earth's lower mantle, and non-stoichiometric Xe-oxides observed even at the modest pressures of the Earth's crust (<1 GPa) (3).

This established pressure-induced chemistry of Xe at planetary interiors conditions, including in silicates as a trace element at moderate pressures, recently led us to evidence the retention of Xe and of its heaviest isotopes in minerals at depth (4). Unexpectedly, these results have cast light on the very early stages of terrestrial planets, revealing that upon each planetary embryos impacts, magma oceans are formed while atmosphere is massively lost, a scenario repeated about ten times.

Beyond Earth sciences, the understanding of Xe chemistry in planetary interiors has revealed a new synthesis pathway for high energy Xe compounds and opens applied research perspectives where similar conditions are found.

[1] Grandinetti, Nature 606, 659 (2022).
[2] Bartlett, Proc. Chem. Soc. 218 (1962).
[3] Sanloup, Front. Phys. 8, 157 (2020).
[4] Rzeplinski et al., Nature 606, 713-717 (2022).

Pressure-induced band-gap increase in hydrated Ca(IO3)2

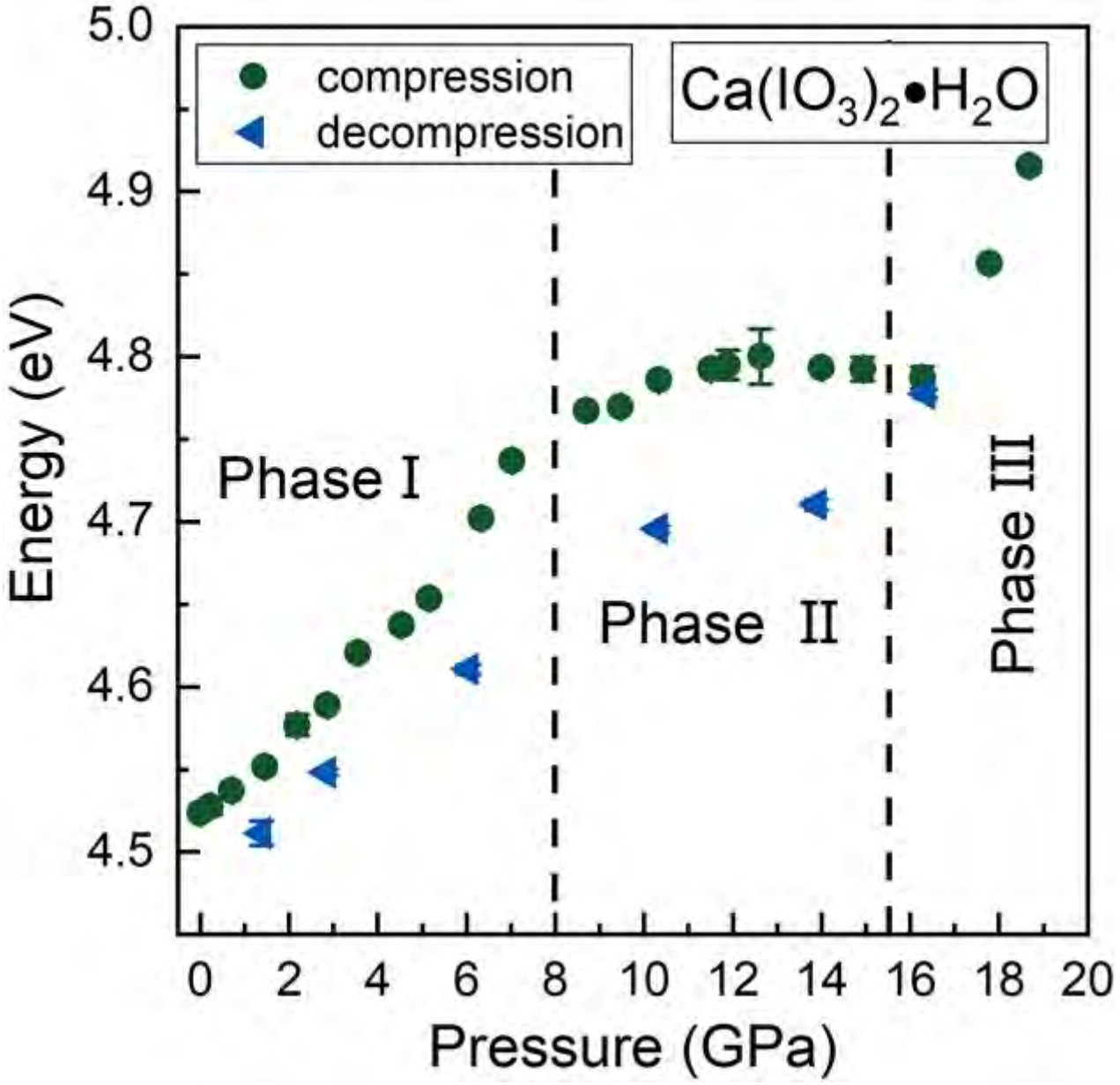
Akun Liang[1,2], Lan-Ting Shi[3], Robin Turnbull[1], Francisco Javier Manjón[4], Jordi Ibáñez[5], Catalin Popescu[6], M Jasmin[7], Jaspreet Singh[8], Kanchana Venkatakrishnan[8], Ganapathy Vaitheeswaran[9], Daniel Errandonea[1]

[1]University of Valencia, Burjassot, Spain, [2]CSEC, The university of Edinburgh, United Kingdom, [3]Institute of High Energy Physics, Chinese Academy of Sciences (CAS), Beijing, China, [4]Universitat Politècnica de València, Spain, [5]Geosciences Barcelona (GEO3BCN), Spain, [6]CELLS-ALBA Synchrotron Light Facility, Spain, [7]TKM College of Arts and Science, India, [8]Indian Institute of Technology Hyderabad, India, [9]University of Hyderabad, India

Jamieson Award Introduction and Lecture, July 28, 2023, 08:30 - 09:10

The search for the next generation of nonlinear optical (NLO) materials has led to the synthesis and characterization of many new metal iodates [1,2]. However, finding an ideal NLO crystal with a high laser damage threshold, excellent thermal stability, a wide transparency window, and a large second-harmonic generation (SHG) response remains a challenge. This work is inspired by our previous high-pressure studies on metal iodates and the finding of the general inverse correlation between the bandgap of metal iodates (which only contain non-transition or closed-shell metal) and the distance of average I-O covalent bonds [3]. In this study [4], we report on the first instance of a metal iodate, hydrated Ca(IO3)2, with an opened bandgap achieved by applying external pressure. The bandgap increased from 4.52 eV to 4.92 eV without saturation at increasing pressure (Figure 1). This is explained by: ⅰ) molecular orbital (MO) diagrams established from theoretical calculations of the density of state (DOS) and crystal orbital overlap population (COOP), and ⅱ) the pressure dependence of the bond distance of the primary, short, strong I-O covalent bonds and secondary, long, weak I-O halogen bonds, as obtained from powder X-ray diffraction measurements. In addition, two reversible isostructural phase transitions were observed in the pressure range of 6.6–8.0 and 13.0–15.5 GPa, characterized by nonlinear changes in the bandgap energy, crystal lattice parameters, and the occurrence of extra peaks and peak splitting in the Raman spectra.

[1] Peng, G. et al. Angew. Chemie - Int. Ed. 60, 17415–17418 (2021)
[2] Chen, J. et al. Angew. Chemie - Int. Ed. 58, 11666–11669 (2019)
[3] Liang, A. et al. Phys. Rev. Mater. 6, 044603 (2022)
[4] Liang, A. et al. Phys. Rev. B 106, 235203 (2022)


compression
decompression
Ca(IO3)2•H2O
Phase I
Phase II
Phase III
Energy (eV)
Pressure (GPa)
5.0
4.9
4.8
4.7
4.6
4.5
0
2
4
6
8
10
12
14
16
18
20

Inertial Confinement Fusion and High-Pressure Science on the National Ignition Facility*

Peter Celliers[1]
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Plenary III: Peter Celliers, July 27, 2023, 09:00–09:50

On 5 December 2022 an experiment on the US National Ignition Facility (NIF) delivered a 2.05 MJ laser pulse to a target containing a spherical diamond shell and a layer of frozen DT fuel. The resulting implosion released more than 3.1 MJ of energy in the form of neutrons generated by D-T fusion reactions. This achievement is the culmination of six decades of effort that began with ideas formulated shortly after the invention of the laser. The conditions in the fusion fuel during the experiment reach up to 500 Gbar in pressure and many keV in temperature, which exceed the pressures and temperatures in the interior of our sun. In this talk I will give a short overview of the history of the inertial confinement fusion (ICF) effort and some details of the recent experiments that led to this important result. While the ICF effort has played a central role in NIF's activities, many of the large suite of x-ray and optical diagnostics developed for ICF combined with the exquisite pulse-shaping of the laser provide an unmatched capability for high pressure science. This combination has already produced many important data sets and is opening up an exciting new era of experimental research. I will review these capabilities and highlight several recent results of interest to the high-pressure science community.

*This work was performed under the auspices of the U.S. Department of Energy by LLNS, LLC, under Contract No. DE-AC52-07NA27344.

Chemically Complex Light-Element Superconductors from First-Principles Theory

Dr. Eva Zurek[1]
[1]*Department Of Chemistry, University at Buffalo, United States*

Plenary I: Eva Zurek, July 24, 2023, 09:00–09:50

Advances in ab-initio crystal structure prediction algorithms, methods for calculating electron-phonon interactions, and machine learning have opened the door towards the rational discovery of conventional superconductors with superior behavior. Herein, we report theoretical studies of various light-element based superconductors that are discovered using the XtalOpt evolutionary algorithm for crystal structure prediction, or via high-throughput calculations on prototype structures known to be conducive towards superconductivity. Ternary hydride-based superconductors are discussed, focusing on their potential stabilization at low pressures, effects of configurational entropy on their stability, and anharmonic effects on their superconducting properties. Moreover, we show how a chemical pressure analysis can be useful in designing ternary or quaternary clathrate superhydride superconductors. Finally, we consider boron-carbon based superconducting materials inspired by the superhydrides.

Exploration of planetary compounds at large terrestrial and icy planets' interior conditions

Jean-Alexis Hernandez[1]
[1]*European Synchrotron Radiation Facility, France*

EHPRG Award Introduction and Lecture, July 28, 2023, 09:10–09:50

As of mid-2023, more than 5430 exoplanets have been discovered and more than 50 % are in size between the Earth and Neptune. Depending on the composition of their host star and their orbital characteristics, a whole zoology of exoplanets is expected, ranging from hot and dense super-Mercury-like planets to icy giants with thick H-He atmospheres. In order to constrain the interior models of such planets, including the Earth, the structure and the properties of potential planetary compounds have to be investigated at pressures of 100s of gigapascals and temperatures of several 1000s Kelvin. At such conditions, various phenomena occur in materials such as dissociations, superionicity, melting and metallization, affecting the dynamics of the planets, and making both experimental and computational investigations more challenging.
In this presentation, I will present an overview of the experimental and theoretical studies I carried out with my collaborators on the phase diagram and properties of hot dense ices and silicates. Moreover, I will emphasize how the complementarity of atomistic simulations and high-pressure experiments benefits to our understanding of matter at these extreme condition.

Invited Speaker Presentations

Core-Electrons Chemical Bonding. Redefining the Chemistry of the Elements at High-pressure

Stefano Racioppi[1], Eva Zurek[1]
[1]*State University of New York at Buffalo, Buffalo, United States*

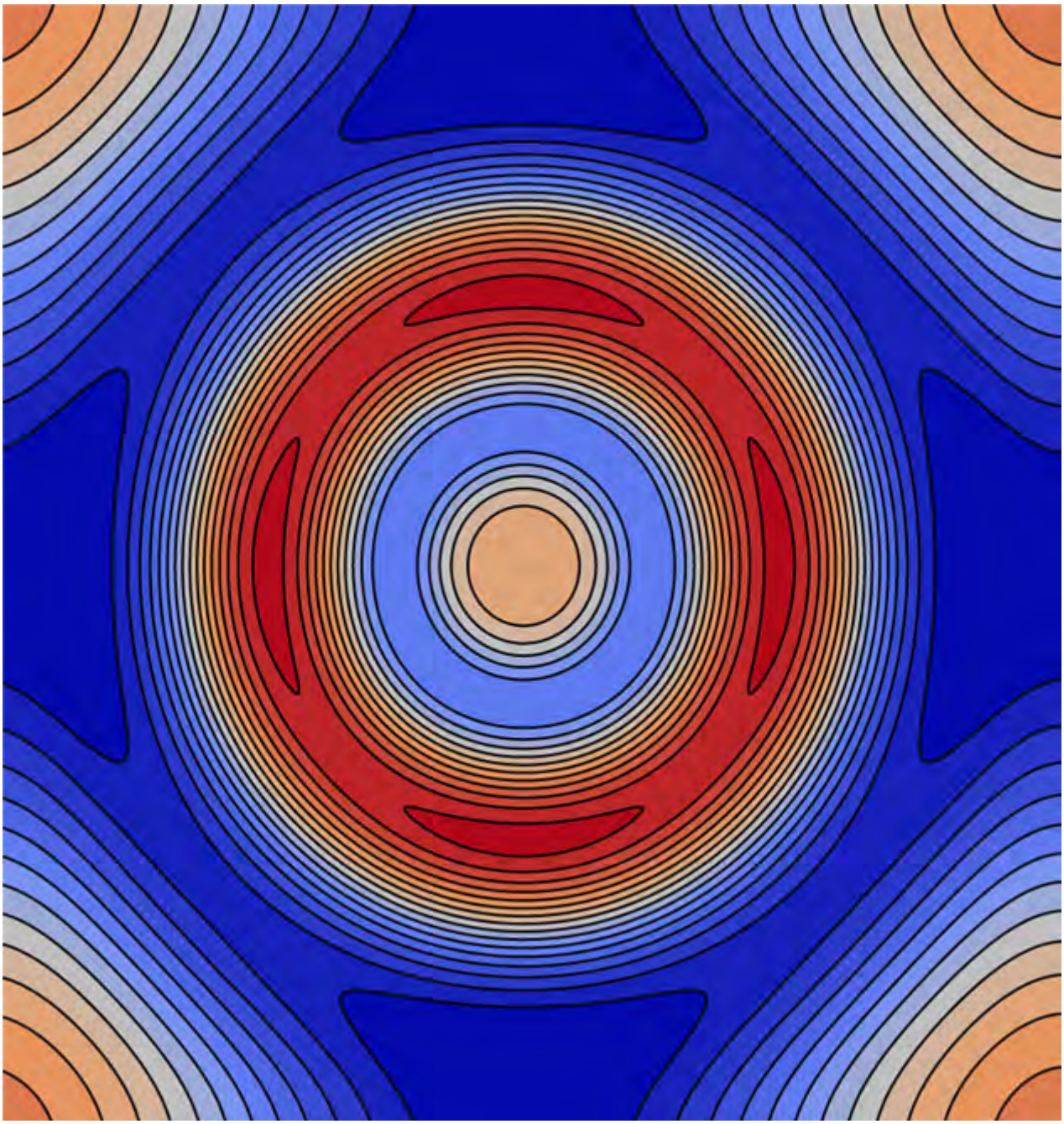
Chemical Bonding 1, July 24, 2023, 14:00–16:00

Dividing the electronic structure of atoms into core and valence regions is one of the very first ideas thought in chemistry classes. Traditionally, the core-valence separation is based on atomic energy levels,[1] and this delimitation has an important chemical implication: Valence electrons participate in chemical bonding, core electrons do not.[2] Despite its simplicity and practical usefulness, especially in quantum chemical calculations, this separation is, nonetheless, an approximation, which can work very well in some cases, but less in others.

The core-valence boundary become blurrier when matter is squeezed. At high-pressure, the electronic structure of atoms often change from the configuration at ambient pressure.[3] With enough compression, the core levels may become more accessible, with important consequences on the chemistry of the elements.[4][5] Generally, such drastic transition is expected only applying very high-pressure s. However, we want to show that, sometimes, core electrons can be activated with just a mild compression.

Through density functional theory (DFT) calculations, we will show that alkali elements have a richer chemistry than what thought. In particular, that the core-electrons of the heavier elements, K, Rb and Cs, can be activated already at few GPa of pressure.

[1] V. A. Rassolov, J. A. Pople, P. C. Redfern, L. A. Curtiss, Chem. Phys. Lett. 2001, 350, 573–576.
[2] G. N. Lewis, J. Am. Chem. Soc. 1916, 38, 762–785.
[3] R. J. Hemley, N. W. Ashcroft, Phys. Today 1998, 51, 26–32.
[4] C. S. Yoo, Matter Radiat. Extrem. 2020, 5, 018202.
[5] M. Miao, Y. Sun, E. Zurek, H. Lin, Nat. Rev. Chem. 2020, 4, 508–527.



What is a phase diagram?

Kamil Dziubek[1]
[1]*Lens – European Laboratory for Non-linear Spectroscopy, Sesto Fiorentino, Italy*

Phase Diagrams – Molecular Systems, July 27, 2023, 14:00–16:00

A phase diagram, defined as a graphical representation of the physical states of materials under varied temperature and pressure conditions, is one of the basic concepts in high-pressure research. Its general definition refers to the equilibrium state and stability limits of particular phases, which set the stage for its terms of use. In the literature, however, a phase diagram often appears as an umbrella category for any pressure–temperature chart that presents not only equilibrium phases, but also metastable states, especially in view of the recent results obtained using emerging experimental techniques [1].

The current state of affairs requires a deep reflection on the definition of the phase diagram. By providing insight into issues and potential solutions, this contribution will set the stage for in-depth discussions aimed to reach a consensus on the most significant working definitions, which will hopefully result in issuing official recommendations supported by AIRAPT.

[1] Dziubek, K.F. (2022). Crystals 12, 1186.

Structural boundaries of lithium within its superconducting region

Prof. Shanti Deemyad[1]
[1]*Physics and Astronomy, University of Utah, Salt Lake City, United States*

Static Studies of Elements 2, July 26, 2023, 16:30–18:30

Below 100GPa, lithium has the highest superconducting transition temperature among the elements and is the only alkalis that exhibits superconductivity at ambient pressure. The high-pressure superconductivity of lithium is attributed to deformations of its Fermi surface and the formation of Fermi surface hot spots. Theoretical calculations assume structural phase boundaries extrapolated from those measured at temperatures well above superconducting region of lithium. However, there is disagreement in literature, even at high temperature, on the location of these boundaries. Here we measured the structural boundaries of lithium up to 60GPa and between 10–70K and within the superconducting region of lithium. Specifically, we address the inconsistency in prior studies regarding the presence of hR1 phase at low temperature [1]. Moreover, using novel and high precision experimental techniques, we measured the pressure dependence of distortions of Fermi surface of lithium based on quantum oscillations and Shubnikov-de-Haas (SdH) effect to pressures exceeding 4.7GPa[2]. Together, we explain the origin of pressure induced superconductivity in lithium and its complex superconducting phase diagram based on direct measurements of its structural phase boundaries at low temperature and changes in its electronic structure.

In addition, we could resolve the distortions of the Fermi surface at ambient pressure with sufficient accuracy to identify three distinct SdH peaks. Together with theoretical calculations and comparative studies on sodium, we demonstrate that these peaks originate from the presence of two different low temperature structures. The low temperature structure of lithium has been debated for many years. This work sheds new light onto this problem and provides experimental evidence for the existence of a mixed low temperature phase of lithium.

[1] Saffarian-Deemyad, Iren, William Holle, Audrey Glende, Mason Burden, Adam Dockery, Julia St. Andre, Alice Leppert, Curtis Kenney-Benson, Jesse Smith and Shanti Deemyad “Structural boundaries of lithium within its superconducting region” Manuscript under preparation

[2] Bhowmick, Tushar, Sabri F. Elatresh, Audrey D. Grockowiak, William Coniglio, Mohammad Tomal Hossain, Elisabeth J. Nicol, Stanley W. Tozer, Stanimir A. Bonev, and Shanti Deemyad. "Structure and pressure dependence of the Fermi surface of lithium." Physical Review B 106, no. 4 (2022): L041112.

High superconductivity in light-element systems under high-pressure

Hanyu Liu[1]
[1]*International Centre for Computational Method and Software, College of Physics, Jilin University, Changchun, China*

Hydrides 1, July 24, 2023, 10:15–12:15

The search for high superconductivity in light-elements systems under high-pressure has attracted great attention in high-pressure community. In this talk, I mainly focus on the investigation of high superconductivity among light-elements compounds, such as superhydrides and boron-carbon compounds at moderate pressure, by employing a state-of-the-art technique, a heuristic algorithm based on particle swarm optimisation CALYPSO. These results may be helpful to design and discovery of high-temperature superconductors at moderate pressures in the near future.

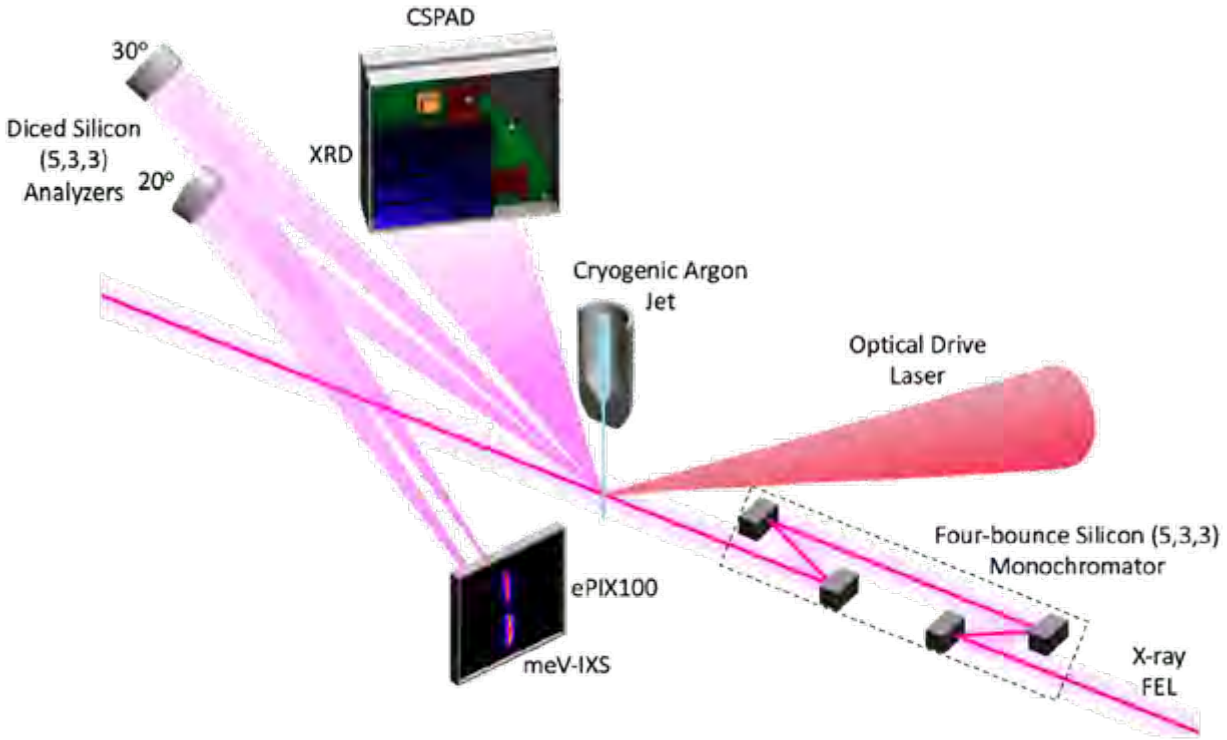
Direct Measurement of Temperature from Laser Compressed Argon at the LCLS

Dr. Emma McBride[1,2], Dr. Adrien Descamps[1,2], LCLS LQ85 Collaboration, Prof. Tom White[3], Prof. Giulio Monaco[4], Prof. Gianluca Gregori[5], Prof. Siegfried Glenzer[2]
[1]Queen's University Belfast, United Kingdom, [2]SLAC National Accelerator Laboratory, United States, [3]University of Nevada at Reno, United States, [4]Universita di Trento, Italy, [5]University of Oxford, United Kingdom

Instrumentation and Techniques 3, July 26, 2023, 14:00–16:00

Direct and accurate measurements of temperature and transport properties are essential for understanding the behaviour of matter at simultaneous extreme pressures and temperatures. While X-ray diffraction measurements from shock compressed matter have allowed in situ measurements of structure and density, the direct measurement of bulk temperature remains a challenge. In shock compression experiments, it is often estimated from hydrodynamic simulations or inferred using streaked optical pyrometry, which requires a priori knowledge of the material properties at extreme conditions. For temperatures less than 4000 K, the intensity recorded on the detector decreases and the accuracy of the technique degrades. This limitation is particularly hindering for the investigation of high-pressure, moderate temperature states of matter such as the one generated using double shock or quasi-isentropic compression. Furthermore, due to the small penetration depth of optical photons in solid density materials, this technique only gives access to the surface temperature, leaving the bulk temperature unknown.

Here, I will present high-resolution millielectronvolt inelastic X-ray scattering measurements conducted at a hard X-ray Free Electron Laser as an avenue to measure the direct temperature of a laser-compressed system. Experiments conducted at the MEC endstation of the LCLS hard X-ray Free Electron Laser couple a high-repetition rate chirped short pulse laser with a high repetition rate cryogenic jet of argon to directly measure acoustic modes in laser compressed liquid argon, allowing the direct measurement of temperature of the bulk system. In addition, I will discuss future opportunities for developing this technique.

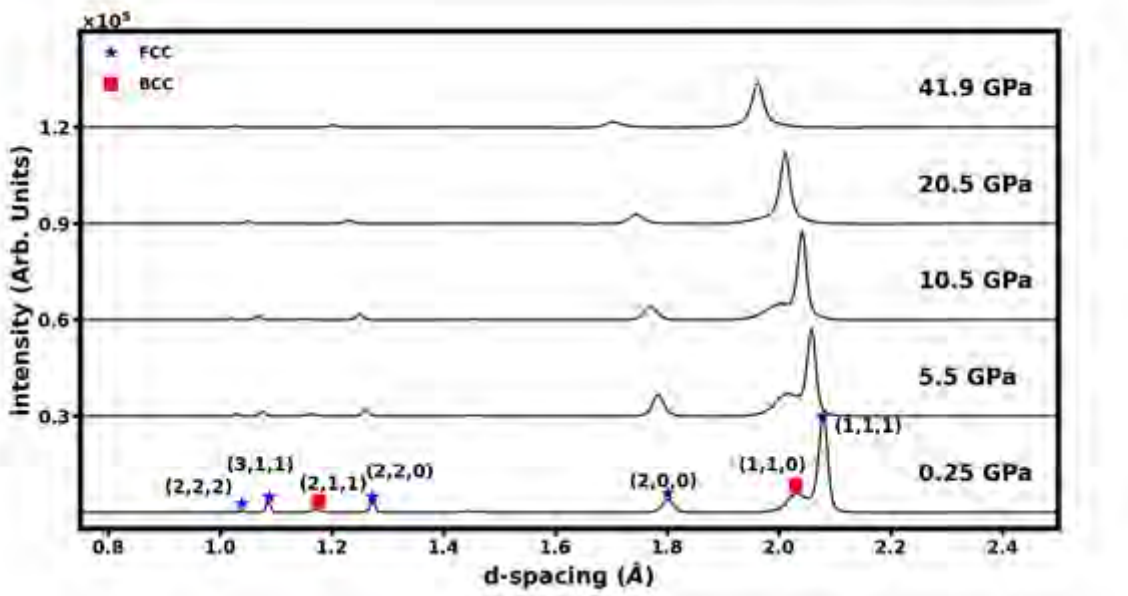


Synthesis and Properties of High Entropy Materials under Static and Dynamic Compression

Professor Yogesh Vohra[1]
[1]*University of Alabama at Birmingham, Birmingham, United States*

Ceramics and Composites, July 24, 2023, 14:00–16:00

High-entropy materials represent a new direction in materials science where five or more constituent elements are incorporated in a variety of alloys, oxides, nitrides, and borides. The high-entropy materials are thermodynamically stable at high temperatures and provide tunability in physical and mechanical properties that is only possible in compositionally complex systems. This talk will review recent synthesis and study of high-entropy materials under extremes of temperatures and pressures. We have synthes d a series of high-entropy transition metal borides, e.g., (HfMoNbTaZr)B10 at high-pressures and high-temperatures staring from ball-milled metal oxide precursors and boron powder. A single hexagonal AlB2-type phase of (HfMoNbTaZr)B10 has been synthes d and studied to 10 GPa and 2273 K in a Paris-Edinburgh press. The synthes d materials are recovered and studied in a diamond anvil cell by both axial X-ray diffraction for equation of state measurements and radial X-ray diffraction for shear strength measurements. The hexagonal AlB2-type phase of (HfMoNbTaZr)B10 is stable to 220 GPa pressure (30% volume compression). The measured nano-indentation hardness of high-entropy borides is 20 GPa and thermal oxidation studies show better performance in oxidizing environment to 1573 K compared to single element boride like TiB2. In a separate effort on high entropy alloys, Laser Powder Bed Fusion (LPBF) method have been able to 3-D print high-entropy alloys AlCoCrFeNi2.1 and Ni40Co20Fe10Cr10Al18W2 in far from equilibrium body-Centreed cubic (BCC)/face-Centreed cubic (FCC) nanostructures. Phase transitions and equation of state of high-entropy alloys have been documented and studied to 318 GPa. The thermal equation of state data on high entropy alloy and high entropy borides will be presented. The static high-pressure data on high-entropy alloys is complemented by laser shock compression studies and the BCC-FCC phase transition pressures under shock compression are compared with corresponding diamond anvil cell studies.

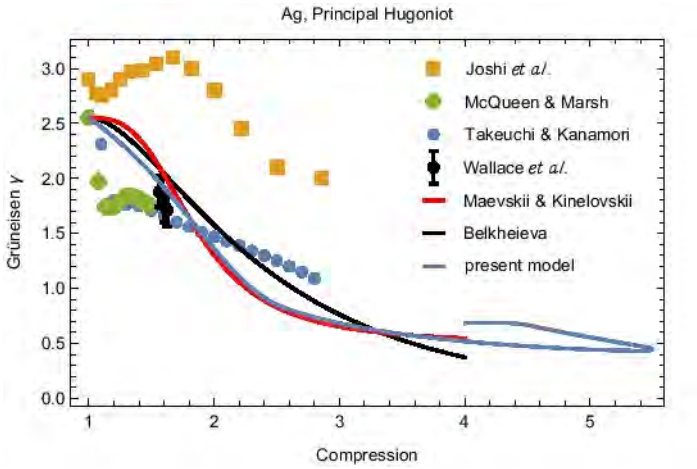


Analytic Model of Principal Hugoniot in a Wide Pressure Range

Dr. Leonid Burakovsky[1], Dr. Dean Preston[1], Dr. Scott Ramsey[1], Dr. Roy Baty[1]
[1]*Los Alamos National Laboratory, Los Alamos, United States*

Equation of State 2, July 27, 2023, 14:00–16:00

Over several decades of research, there has been continuous interest in the understanding of shock-wave phenomena and the proper modeling of the shock Hugoniots, both principal and second-shock ones, and the thermodynamic quantities associated with them, such as the isentropic (adiabatic) bulk modulus (BS), Grüneisen parameter (γ), Mach number (M), pressure (P), energy (E), etc., all being on the Hugoniot and, thus, being functions of a Hugoniot variable, e.g., particle velocity (Up) or degree of compression (η). In our talk we present an analytic model of the principal Hugoniot in a wide pressure range. We discuss the way the model is constructed as well as its theoretical basis. The model allows one to obtain analytic expressions for P, E, BS, γ and M as functions of Up at all $0 \le Up \le \infty$ or, equivalently, as functions of η at all $1 \le \eta \le \eta_{max}$, where η_{max} is the point of maximum compression referred to as a turnaround point since at this point the $\eta = \eta(Up)$ behavior changes from increasing with Up to decreasing with Up. We also compare predictions of the model to the results of the available experimental and independent theoretical studies for several materials of common interest, such as aluminum, iron, copper, silver, platinum, lithium fluoride, and selected lanthanides.



Enhanced Magnetic Ordering in Lanthanide Metals under Extreme Pressure

Dr. Jing Song[1]
[1]*Institute of Physics, Chinese Academy of Sciences, Beijing, China*

Magnetic Materials 2, July 26, 2023, 14:00–16:00

At atmospheric pressure all lanthanide metals order magnetically at temperatures below ambient. Magnetic ordering at To results from the so-called Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. Under sufficiently high-pressure, however, one anticipates that the 4f state of a given lanthanide should become unstable, leading to exotic physics arising from competition between the RKKY interaction and Kondo screening. Four-point electrical resistivity measurements on the lanthanide metals reveal that To soars to anomalously high values at extreme pressures. The giant superconducting pair-breaking effect found in the dilute magnetic alloys Y-Ln give evidence that the record high To values are an heretofore unrecognised feature of a Kondo lattice.

Novel metallic glass states synthesised from extreme conditions

Hongbo Lou[1], Qiaoshi Zeng[1]
[1]*Centre for High-pressure Science and Technology Advanced Research, Shanghai, China*

Synthesis and Properties of Novel Materials 1, July 26, 2023, 14:00–16:00

Liquid and glass are two closely associated states of matter. The existence of two or more structurally different but chemically identical liquids or glasses, referred to as liquid or glass polymorphism, has been attracting extensive and enduring research interest over decades, which, however, remains an intriguing topic of intense debates. In this talk, I will show the observation of three different metallic glass states via quenching of the high-pressure liquids and the following decompression by in situ high-temperature high-pressure synchrotron X-ray diffraction. First-order-like transitions are identified between them with discontinuous changes in their structures and properties in two prototype multicomponent glass-forming metallic alloys.

Pressure Tuned 2D Superconductivity in Black Phosphorus

Jinlong Zhu[1], Dr. Meiling Jin[1], Dr. Ying Liu[1], Mr. Chenkai Li[1]
[1]*Southern University of Science and Technology, Shenzhen, China*

Novel Superconductors 1, July 27, 2023, 10:15–12:15

The interactions between conducting layer and electron storage layer of superconducting, and its modulations from weak van der Waals interaction to strong covalence bonding, is important of understanding the micro-parameters of superconductors and resulted Tc. Layered black phosphorus (BP) studied here hosts rich scenario of phase transitions and related quantum phenomena as a function of pressure. The revisiting of P-T phase diagram unveiled that all three phases exhibit superconducting states with pressure higher than 5.0 GPa. The dimensional characters of superconductivities were demonstrated by angle-dependent upper critical field, suggesting that superconductivities in A17 phase and cubic phase are of three-dimensional (3D) characters, while in A7 phase the superconductivity shows two-dimensional (2D) character. This 2D behaviour is related to distortion entangled weakening of interlayer coupling in A7 phase. Further, DFT calculations indicate structure of nanoflake forming 2D Fermi surface contributes to the 2D superconductivity in A7 BP.

Preservation of high-pressure materials in nanostructured diamond capsules

Zhidan Zeng[1]
[1]*Centre for High-pressure Science and Technology Advanced Research (HPSTAR), Shanghai, China*

Nanoscale Systems, July 24, 2023, 16:30–18:30

High-pressure induces dramatic changes and novel phenomena in materials that are usually not preservable after pressure release. Herein we proposed an approach to preserving high-pressure volatiles using nanostructured diamond capsules (NDCs). As a demonstration, we pressurised argon into enclosed nano-pores of glassy carbon precursors in a diamond anvil cell (DAC), then converted the glassy carbon into nanocrystalline diamond by laser heating under higher pressure, and eventually synthesised NDCs capable of permanently preserving high-pressure argon even after releasing the pressure in the DAC. With NDCs, various vacuum-based diagnostic probes, including electron microscopy, can be employed to characterise high-pressure argon directly. Synchrotron X-ray diffraction and transmission electron microscopy study show nm-sized argon crystals at ~22.0 GPa embedded in the nanocrystalline diamond matrix. Moreover, the preserved pressure of the argon sample inside NDCs can be readily tuned by controlling the NDCs synthesis pressure. To test the general applicability of the NDC process, we show high-pressure neon can also be encapsulated in NDCs as well. In principle, the NDC strategy can be applied to liquid and solid samples as well. Therefore, it could provide a unique approach to retaining high-pressure materials and their novel properties for ambient applications.

Recent developments in neutron diffraction experiments at high-pressure and high temperature and application to Earth science

Asami Sano-Furukawa[1,2], Sho Kakizawa[3], Yuichiro Mori[4], Hiroyuki Kagi[4], Jun Abe[5], Ken-ichi Funakoshi[5], Takanori Hattori[1]

[1]J-PARC Centre, JAEA, Tokai, Japan, [2]IMSS, KEK, Tokai, Japan, [3]JASRI, Sayo, Japan, [4]The University of Tokyo, Bunkyo-ku, Japan, [5]CROSS, Tokai, Japan

Instrumentation and Techniques 1, July 26, 2023, 10:15–12:15

Hydrogen is an essential constituent of the Earth. It takes various bonding forms depending on the surrounding environment, such as crystal structure, pressure, and temperature and influences the mineral's various physical properties and rock's differentiation. For example, hydrogen affects the melting temperature, viscosity, and electrical conductivity of minerals. So where and how much hydrogen is present in the Earth's interior has been an important issue. Neutron experiments with high sensitivity to hydrogen can be a powerful tool to answer this question. However, there have been relatively few examples of high-pressure and high-temperature experiments using neutrons as probes, mainly due to sample volume matters.

This situation has changed significantly with the advent of high-intensity pulsed neutron facilities. In the high-pressure neutron diffractometer PLANET at MLF in J-PARC, a large volume 6-axis multi-anvil press, and precise optics have enabled stable neutron diffraction experiments at high-pressure and high temperature [1-3]. High-temperature experiments, previously limited to several GPa, can now be performed routinely at pressures above 10 GPa. This sample environment has promoted unique research, as exemplified by determining the amount of hydrogen in the iron alloys that form the Earth's core [4]. In this presentation, recent results of neutron diffraction experiments at PLANET will be presented, as well as the on-going developments.

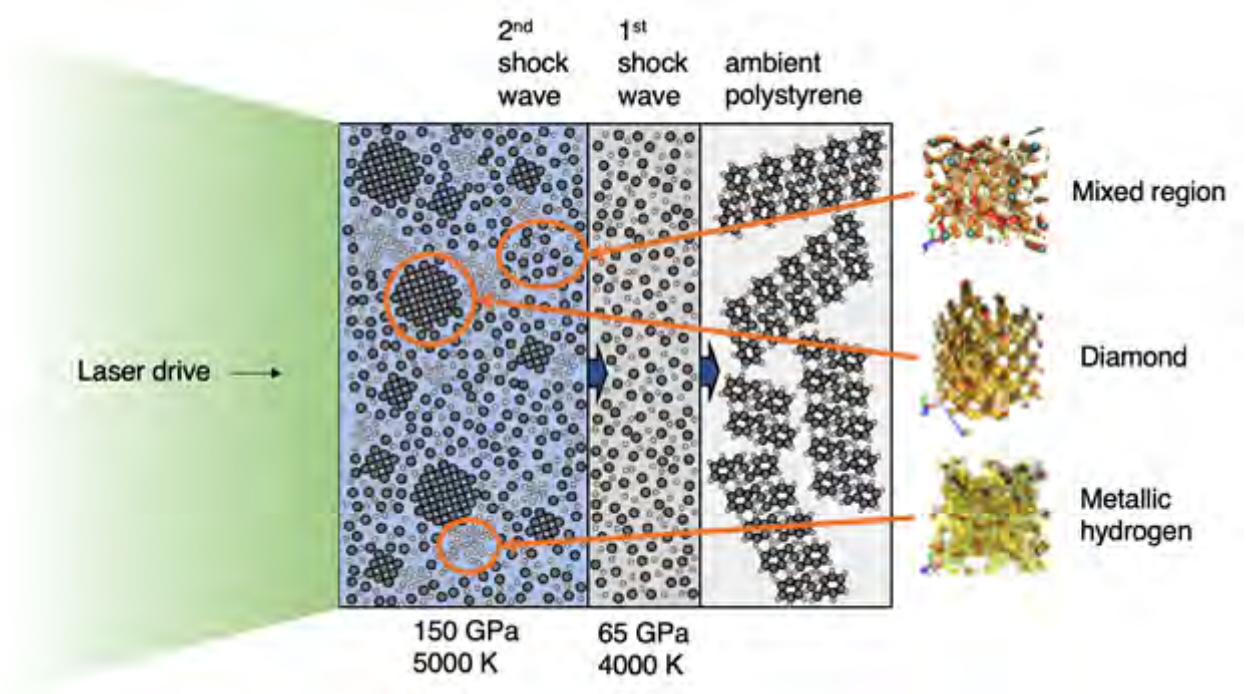
[1] Hattori et al,. Nucl. Instrum. Methods Phys. Res. A. 780, 55-67, 2015.
[2] Sano-Furukawa et al., Rev. Sci. Instrum. 85, 113905, 2014.
[3] Sano-Furukawa et al., High Press. Res. 41, 65-74, 2021.
[4] Mori et al., J. Mineral. Petrol. Sci. 116, 309-313, 2021.

Evidence for isolated hydrogen in laser-compressed hydrocarbons

Dominik Kraus[1,2]
[1]University of Rostock, Rostock, Germany, [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Hydrogen, July 25, 2023, 10:15–12:30

We demonstrate a significantly simplified experimental approach for investigating liquid metallic hydrogen, which is crucial to understand the internal structure and evolution of giant planets. Plastic samples were shock-compressed and then probed by short pulses of X-ray s generated by free electron lasers. By comparison with ab initio simulations, we provide evidence for the creation of isolated hydrogen in shock-compressed plastics at 150 GPa and 5,000 K and thus in a regime where hydrogen is predicted to be metallic. Being the most common form of condensed matter in our solar system, and ostensibly the simplest of all elements, hydrogen is the model case for many theoretical studies, and we provide a new possibility to benchmark models for conditions with extreme pressures and temperatures. Moreover, this approach will also allow probing the chemical behaviour of metallic hydrogen in a mixture with other elements, which, besides its importance for planetary physics, may open up promising pathways for the synthesis of new materials.



High-pressure effect on candidate Dirac materials EuMnPn2 (Pn = Sb, Bi)

Wenli Bi[1], Greeshma C. Jose[1], Raimundas Sereika[1], Rongying Jin[2], Weiwei Xie[3], William Shelton[4], Dongzhou Zhang[5], Yuming Xiao[6], Barbara Lavina[6], Jiyong Zhao[6], Esen E. Alp[6], Yogesh K. Vohra[1]
[1]University of Alabama at Birmingham, Birmingham, United States, [2]University of South Carolina, Columbia, United States, [3]Michigan State University, East Lansing, United States, [4]Louisiana State University, Baton Rouge, United States, [5]University of Hawaii at Manoa, Honolulu, United States, [6]Argonne National Laboratory, Lemont, United States

Magnetic Materials 1, July 24, 2023, 10:15–12:15

$EuMnPn_2$ (Pn = Sb, Bi) has attracted much attention as magnetic Dirac semimetal candidates [1–6]. Due to the strong coupling of Eu magnetism and charge transport properties, $EuMnPn_2$ provides a rich platform to control topological states by manipulating magnetism. In this work, we have investigated the pressure control of crystal structure, Eu local moment magnetism, and the electronic state using synchrotron X-ray diffraction, time-domain Mössbauer spectroscopy in ^{151}Eu, and X-ray absorption spectroscopy. In both $EuMnSb_2$ and $EuMnBi_2$, X-ray absorption experiments at Eu L_3 edge as well as isomer shift measurements show a continuous and significant transition of valence state from Eu2+ toward Eu3+ with increasing pressure. Surprisingly, despite the large valence transition, an enhancement of magnetic ordering temperature in Eu ions has been observed in both systems. And magnetic order in $EuMnSb_2$ and $EuMnBi_2$ persists up to 33 and 28 GPa, respectively. The similar and distinct responses to external pressure in these two materials will be discussed in detail.

[1] A. F. May, M. A. McGuire, and B. C. Sales, Effect of Eu Magnetism on the Electronic Properties of the Candidate Dirac Material EuMnBi2, Phys. Rev. B 90, 075109 (2014).
[2] H. Masuda, H. Sakai, M. Tokunaga, M. Ochi, H. Takahashi, K. Akiba, A. Miyake, K. Kuroki, Y. Tokura, and S. Ishiwata, Impact of Antiferromagnetic Order on Landau-Level Splitting of Quasi-Two-Dimensional Dirac Fermions in EuMnBi2, Phys. Rev. B 98, 1 (2018).
[3] Y. Shiomi, H. Watanabe, H. Masuda, H. Takahashi, Y. Yanase, and S. Ishiwata, Observation of a Magnetopiezoelectric Effect in the Antiferromagnetic Metal EuMnBi2, Phys. Rev. Lett. 122, 127207 (2019).
[4] J. R. Soh, P. Manuel, N. M. B. Schröter, C. J. Yi, F. Orlandi, Y. G. Shi, D. Prabhakaran, and A. T. Boothroyd, Magnetic and Electronic Structure of Dirac Semimetal Candidate EuMnSb2, Phys. Rev. B 100, 1 (2019).
[5] D. Gong, S. Huang, F. Ye, X. Gui, J. Zhang, W. Xie, and R. Jin, Canted Eu Magnetic Structure in EuMnSb2, Phys. Rev. B 101, 224422 (2020).
[6] Z. L. Sun, A. F. Wang, H. M. Mu, H. H. Wang, Z. F. Wang, T. Wu, Z. Y. Wang, X. Y. Zhou, and X. H. Chen, Field-Induced Metal-to-Insulator Transition and Colossal Anisotropic Magnetoresistance in a Nearly Dirac Material EuMnSb2, Npj Quantum Mater. 6, 94 (2021).

Melting experiment of MgO under high-pressure by in situ time-resolved X-ray diffraction measurement with Bayesian estimation method

Mr. Osamu Ishizawa[1], Dr. Kenji Ohta[1], Mr. Ryoto Ebina[1], Dr Saori Kawaguchi[2], Dr Manabu Kodama[3], Professor Shuichiro Hirai[3]
[1]Tokyo Institute of Technology, EPS, Japan, [2]JASRI, Japan, [3]Tokyo Institute of Technology, Mech. Eng., Japan

Minerals Under High-pressure, July 24, 2023, 16:30–18:30

MgO is the end member of (Mg,Fe)O, the second most abundant component in the lower mantle, and its melting behavior provides necessary information for understanding the properties of the lower mantle and magma ocean solidification scenarios in the early Earth. However, due to the high melting point of MgO at high-pressure s, direct melting experiments have only been carried out below 50 GPa [1]. The determination of the melting curve of MgO up to 136 GPa, the lowermost mantle pressure, is limited to estimation from melting experiments of (Mg,Fe)O [e.g. 3] or theoretical calculations [e.g. 2]. Theoretical melting curves are consistent up to 50 GPa, but they show variations depending on the calculation method above 100 GPa. Therefore, high-pressure melting experiments of MgO are needed to obtain more reliable melting curves covering the entire lower mantle.

In this study, we performed melting experiments of MgO in the range of about 40 to 130 GPa using a laser-heated diamond anvil cell (LHDAC). The sample was heated for 1 s, and in situ high-speed X-ray diffraction (XRD) measurements acquiring 100 frames per second were performed in all experiments. The time-varying MgO (200) diffraction peak was analyzed using the Bayesian estimation method to determine whether or not it was melting. As a result, the melting curve of MgO estimated by extrapolation [1] was revised downwards at high-pressure. The heating and melting determination method developed in this study can be applied to simulate solidification in magma oceans of the early Earth and to reproduce chemical reactions in celestial collisions.

[1] Kimura, T. et al. Melting temperatures of MgO under high-pressure by micro-texture analysis. Nat. Commun. 8, 15735 (2017).
[2] Alfe, D. Melting curve of MgO from first-principles simulations. Phys. Rev. Lett. 94, 235701 (2005).
[3] S. Fu, J. Yang, Y. Zhang, J. Liu, E. Greenberg, V. B. Prakapenka, T. Okuchi, and J. F. Lin, Earth Planet. Sci. Lett. 503, 1 (2018).

Calibrating the initial slope of a ruby gauge based on primary piston gauges

GUOYIN SHEN[1], Jesse Smith[1], Curtis Kenney-Benson[1]
[1]*Argonne National Laboratory, Lemont, United States*

In a recent report by the task group on the International Practical Pressure Scale (IPPS)[1], there is a call for more accurate calibration of the initial slope of a ruby gauge for better pressure determination at low pressures (<10 GPa). The published initial slopes were either based on the linear coefficient averaged over a pressure range of 0–20 GPa, which tends to over-estimate the initial slope because of nonlinearity, or back-extrapolated using a large pressure range, which may involve unknown uncertainties. We have calibrated the initial slope against the two well-established reference points based on primary piston gauges: the melting pressure of mercury (1254MPa at 298K)[2] and the transition pressure of Bi I-II (2520MPa at 298K)[3]. The calibration of the initial slope links the luminescence-based ruby gauge to the more fundamental primary piston gauges, and improves the accuracy of the ruby gauge, particularly for pressure determination at low pressures (<10 GPa).

1. Shen, G., et al., High-pressure Research, 2020. 40(3): p. 299-314.
2. Molinar, G.F., et al., Metrologia, 1991. 28(4): p. 353-354.
3. Getting, I.C., Metrologia, 1998. 35(2): p. 119-132.

Pressure-induced magnetism collapse in 4d and 5d honeycomb compounds

Prof. Alexander Tsirlin[1], Dr. Bin Shen[2], Dr. Angel Arevalo-Lopez[3], Dr. Ece Uykur[4], Prof. Philipp Gegenwart[2]

[1]Felix Bloch Institute, Leipzig University, Leipzig, Germany, [2]EP VI, EKM, University of Augsburg, Augsburg, Germany, [3]University of Lille, Lille, France, [4]Helmholtz-Zentrum Dresden-Rossendorf, Germany

Electronic Transitions 2, July 25, 2023, 14:00–16:00

Transition-metal compounds with honeycomb networks of 4d and 5d magnetic ions are under active scrutiny as potential hosts for novel magnetic states, such as Kitaev spin liquid that can have important implications for topological quantum computing [1]. Experimental realisation of this exotic state requires fine tuning of magnetic interactions via external stimuli such as hydrostatic or chemical pressure. Our tuning attempts uncovered an unusual instability, the formation of metal-metal bonds that leads to an abrupt magnetism collapse [2]. This transition is quite different from the more familiar magnetism collapse in Mott insulators. It may occur at pressures as low as 1 GPa and does not involve any significant changes in the bandwidth or correlation strength.

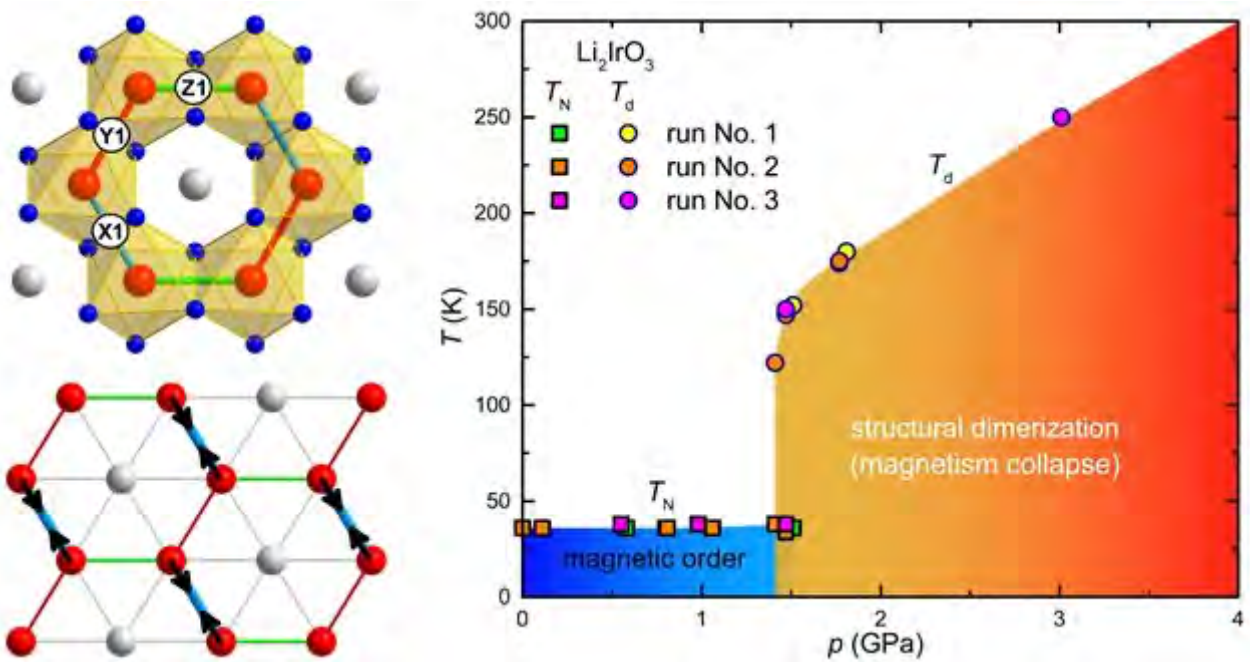
In this talk, I will summarise our recent results on the magnetism collapse due to metal-metal bonds in 4d and 5d honeycomb compounds. We use a combination of high-pressure XRD, magnetisation measurements under pressure, and ab initio calculations to study the suppression of magnetism in Li_2IrO_3 and other honeycomb iridates, as well as ruthenium trihalides, RuX_3 with X = Cl, Br, and I.

We show that critical pressure of magnetism collapse in iridates is controlled by the unit-cell volume and, consequently, by the size of the alkaline-metal ion [3,4]. Additionally, effects of local disorder can further suppress the magnetic phase and even bring the transition to ambient pressure. We discuss both temperature and pressure dependence of the magnetism collapse transition [5] and uncover its microscopic origin.

A similar magnetism collapse transition was observed in the van der Waals honeycomb magnet α-$RuCl_3$. Interestingly, $RuBr_3$ and RuI_3 were previously known in the chain-like nonmagnetic beta-form only. Their magnetic honeycomb polymorphs are obtained under high-pressure, yet we show that pressurizing the magnetic polymorph, α-$RuBr_3$, leads to a magnetism collapse transition already at 2 GPa. On the other hand, no such transition could be observed in the iodide.

Our results reveal a new mechanism of magnetism collapse due to metal-metal bonds in 4d/5d compounds and highlight its major differences from the conventional suppression of magnetism in pressurised Mott insulators.

[1] H. Takagi et al. Nature Rev. Physics 1, 264 (2019)
[2] V. Hermann, A.A. Tsirlin et al. Phys. Rev. B 97, 020104(R) (2018)
[3] M. Majumder, A.A. Tsirlin et al. Phys. Rev. Lett. 120, 237202 (2018)
[4] B. Shen, A.A. Tsirlin et al. Phys. Rev. B 104, 134426 (2021)
[5] B. Shen, A.A. Tsirlin et al. Phys. Rev. B 105, 054412 (2022)


Z1
Y1
X1
Li2IrO3
TN Td
run No. 1
run No. 2
run No. 3
Td
structural dimerization
(magnetism collapse)
TN
magnetic order
T (K)
p (GPa)
0
50
100
150
200
250
300
1
2
3
4

High-pressure phase transitions studies using synchrotron X-ray techniques

Prof. Arthur Haozhe Liu[1], Dr. Lisa Luhongwang Liu[2,3]
[1]HPSTAR, Beijing, China, [2]SHARPS, Shanghai, China, [3]UIUC, Urbana, United States

Phase Diagrams – Ionic Systems, July 24, 2023, 10:15–12:15

The current state-of-the-art synchrotron X-ray techniques combined with diamond anvil cell (DAC) and large volume press (LVP) techniques make phase transition studies one of most active, burgeoning fields in the high-pressure community. The structural evolution of material under pressure is the long-term active research subject, which in fact strongly depends on the development of corresponding high-pressure and synchrotron technologies. The selected research cases for various types of material, such as phase determination in several metal hydrides, puzzling behaviors in various types of nano materials, and order parameter effect in high entropy materials under high-pressure conditions, will be presented. The contributions from the first principles calculations and synergetic effort in synchrotron sources will be discussed based on these scientific cases.

Diamond Precipitation Dynamics from Hydrocarbons at Icy Planet Interior Conditions

Dr. Mungo Frost[1]
[1]*Slac National Accelerator Laboratory, Menlo Park, United States*

Outer Planets and Exoplanets 2, July 26, 2023, 16:30–18:30

The formation of diamond from hydrocarbons at high-pressure and temperature is important to understanding the interiors of icy planets, meteorite impact events and inertial confinement fusion. However, there is large discrepancy between static and dynamic compression experiments in the conditions at which this reaction is observed. In laser-heated diamond anvil cells (DACs) diamond is observed in samples quenched from 2500 K above 10 GPa, while laser driven shock studies find no diamond formation below 150 GPa and 4000 K. Recent X-ray free electron laser heated pump-probe experiments on DAC compressed polystyrene between 19 and 27 GPa allowed in situ observation of the reaction with 220 ns time resolution. Diamond formation was observed, but only after 30 □s, suggesting the origin of this discrepancy is reaction kinetics. Compared to dynamic compression results, the reduced pressure and temperature conditions of diamond formation has implications for icy planetary interiors, where diamond subduction plumes provide a source of internal energy and could drive convection in the conductive ice layer which is proposed to give rise to their complex magnetic fields.

High-pressure Generation in a Kawai-type Multianvil Apparatus Equipped with Sintered Diamond Anvils and Electrical Resistance of Fe2O3 at High-pressure

Daisuke Yamazaki[1]
[1]*Okayama University, Japan*

The Kawai-type multianvil apparatus (KMA) has been widely employed to clarify the structure and state of the deep Earth [1]. The most important advantage of the KMA over the diamond anvil cell is the capability to compress a large volume sample (>1 mm3) in an octahedral pressure medium under a quasihydrostatic environment owing to squeezing by eight cubic anvils [2]. Moreover, by adopting an internal heating system, we can heat the sample homogeneously and stably, which makes it possible to measure physical and chemical properties of minerals under high-pressure and temperature conditions. However, in the conventional KMA, the attainable pressure has been limited to ~30 GPa [3]. To extend the pressure range in KMA, we have been developing the experimental technique in KMA by using sintered diamond (SD) anvil [4].

We conducted pressure generation in a large volume press (SPEED mk.II) at SPring-8 synchrotron facility. For the cell assembly, we used Cr-doped MgO as pressure medium, BN+TiB2 as heater because of high transparency for X-ray and soft fired pyrophyllite as gasket. Sintered starting material of the mixture of Mg0.9Fe0.1SiO3+5wt % Al2O3 bridgmanite and gold was prepared as sample and pressure standard. We finally succeeded to generate pressure to 120 GPa, based on Au gold scale [5], by using “C2-grade” SD anvils at press load of 13 MN at an ambient temperature after pre-heating of 800K.

In recent years, the pressure limit in KMA has been expanded not only by using SD anvil but also by using “binderless” WC anvil “TJS01”. Pressure more than 50 GPa is attainable in WC-KMA [6], indicating that the determination of pressure fix point more than 50 GPa is urgent issue. Ito et al. [1] reported preliminary result on the electrical resistance of Fe2O3 with increasing pressure at room temperature and suggested its drastically decrease at ~58 GPa. We measured electrical resistance at high-pressure up to ~55 GPa and temperature to ~900 K to clarify the relationship between electrical resistance and phase present. As a result, we did not observe the phase transformation during significant decrease of electrical resistance. This may indicate that the change in electrical resistance is caused by the change of state of electron.

[1] E. Ito: in Treatise on Geophysics (2nd Edition) (Elsevire, 2015), pp. 233-261.
[2] N. Kawai and S. Endo, Rev. Sci. Instrum. 4, 425 (1970).
[3] T. Kunimoto et al., High Press. Res. 36, 97 (2016).
[4] D. Yamazaki and E. Ito, High Press. Res. 40, 3 (2020).
[5] T. Tsuchiya, J. Geophy. Res. 108, 2003JB002446 (2003).
[6] Ishii et al., Engineering, 5, 434 (2019).

Mechanism of electron-rich multiCentre bonding in elemental crystals under pressure

Hussien H. Osman[1], Alberto Otero-de-la-Roza[2], Placida Rodríguez-Hernández[3], Alfonso Muñoz[3], Francisco Javier Manjón[4]

[1]Departamento de Física Aplicada-ICMUV, MALTA Consolider Team, Universitat De València, Valencia, Spain, [2]Departamento de Química Física y Analítica, MALTA Consolider Team, Universidad de Oviedo, Spain, [3]Departamento de Física, Instituto de Materiales y Nanotecnología, MALTA Consolider Team, Universidad de La Laguna , Spain, [4]Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Universitat Politècnica de València , Spain

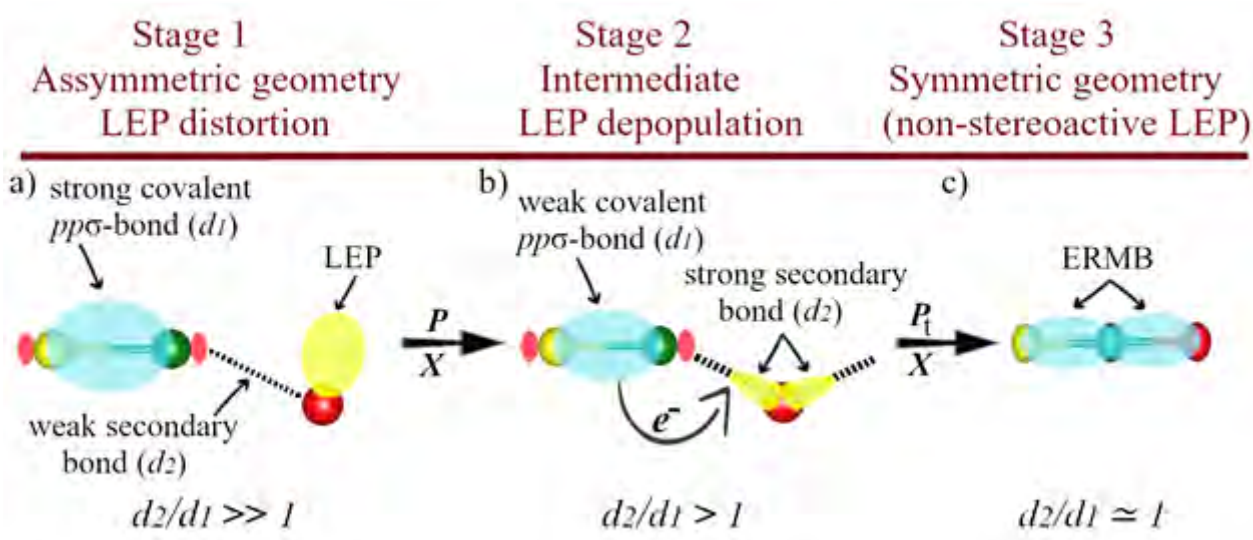
Chemical Bonding 1, July 24, 2023, 14:00–16:00

The unconventional bonding in the crystalline phases of phase change materials (PCMs) has been discussed in the literature using different chemical bonding models.1-8 One of those models proposes that PCMs feature electron-rich multiCentre (ERM) bonds related to materials with a pre-ERM bonding scenario characterised by a combination of a primary covalent ppσ-bond and a secondary bond in which the lone electron pairs (LEPs) are involved.2,4-8 Since the pre-ERM bonding scenario occurs in group-V (As, Sb, Bi) and -VI (Se, Te) elements,9 we show, by means of quantum-mechanical calculations, that these elements develop ERM bonds at high-pressure as they approach sixfold coordination. Interestingly, polonium, in both its α- and β- phases, is the only element that shows ERM bonds at room pressure. We also show that the ERM bond formation mechanism, which can show up to three stages (see Fig. 1), depends on the type of LEP present in secondary bonds. This work provides a comprehensive understanding of the ERM bond formation that is key to improving the performance of advanced materials, such as PCMs, topological insulators, and highly efficient thermoelectrics of the IV-VI and V2-VI3 families.

Fig. 1. Graphical representation of the mechanism of ERM bond formation in a 3c-4e model system under the effect of hydrostatic pressure (P) or change of chemical composition (X).

Keywords: MultiCentre bond, hypervalent bond, metavalent bond, lone electron pairs, high-pressure

[1] P. B. Littlewood, Crit. Rev. Solid State Mater. Sci. 1983, 11, 3, 229.
[2] A.V. Kolobov, P. Fons, J. Tominaga, and S.R. Ovshinsky, Phys. Rev. B 2013, 87, 165206.
[3] M. Wuttig, V. L. Deringer, X. Gonze, C. Bichara, J.-Y. Raty, Adv. Mater. 2018, 30, 51, 1803777.
[4] T. H. Lee, S. R. Elliott, Adv. Mater. 2020, 32, 28, 2000340.
[5] T. H. Lee, S. R. Elliott, Phys. Status Solidi RRL 2021, 15, 2000516.
[6] J. Hempelmann, et. al., Adv. Mater. 2021, 33, 37, 2100163.
[7] J. Hempelmann, et. al., Angew. Chem., Int. Ed. 2022, 61, 17, e202115778.
[8] T. H. Lee, S. R. Elliott, Nat. Commun. 2022, 13, 1 1458.
[9] M. Kastner, Phys. Rev. Lett. 1972, 28 355.


Stage 1
Assymmetric geometry
LEP distortion
Stage 2
Intermediate
LEP depopulation
Stage 3
Symmetric geometry
(non-stereoactive LEP)
a) strong covalent
ppσ-bond (d1)
LEP
weak secondary
bond (d2)
d2/d1 >> 1
P
X
b)
weak covalent
ppσ-bond (d1)
strong secondary
bond (d2)
e-
d2/d1 > 1
P1
X
c)
ERMB
d2/d1 ≃ 1

Tuning thermal expansion and mechanical properties by high-pressure insertion of guest molecules

Frederico Alabarse[1], Benoit Baptiste[2], Boby Joseph[1], Julien Haines[3]
[1]Xpress Beamline – Elettra Synchrotron Facility, Trieste, Italy, [2]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, (IMPMC), CNRS – Sorbonne Université – IRD – MNHN, Paris, France, [3]ICGM, CNRS, Université de Montpellier, ENSCM, Montpellier, France

Synthesis and Properties of Novel Materials 2, July 26, 2023, 10:15–12:15

Microporous aluminophosphate $AlPO_4$-17, with a hexagonal erionite structure, is the oxide which exhibits the highest coefficient of negative thermal expansion (NTE). The NTE mechanism in this material is rationalised by a structural contraction around the empty pores that occurs with increasing temperature. $AlPO_4$-17 is also extremely compressible and shows pressure induced amorphisation (PIA), in which novel compression behaviour was observed with an anomalous pressure-induced softening (PIS) effect (negative value for B'). The insertion of small molecules into the pores of $AlPO_4$-17 offers a means to modify its thermal expansion and mechanical properties. In the present study, high quality single-crystal (SC) and powder X-ray diffraction (XRD) measurements were used to monitor the NTE and the respective structural response to pressure in $AlPO_4$-17 in penetrating pressure transmitting media (PTM). The experiments were performed at the Xpress beamline of Elettra Synchrotron Facility.

Dehydrated $AlPO_4$-17 was loaded with O_2, N_2 and Ar cryogenically and compressed by using a diamond anvil cell to promote the guest molecules insertion in the pores of the structure. Ruby, Sm^{2+}:SrB_4O_7 and Au were loaded along with the sample to monitor in situ the P-T dependence. The insertion of O_2 molecules at high-pressure (HP) into $AlPO_4$-17 was found to tune its very strong NTE. The structure of the oxygen-filled material was determined in situ at HP by SC-XRD. Powder XRD allowed us to determine the thermal expansion coefficient upon cooling at a pressure of 0.38 GPa, by using a closed-cycle He-cryostat. Whereas the volumetric thermal expansion only exhibits a small change with respect to $AlPO_4$-17 (empty pores) at ambient pressure, the thermal expansion for the oxygen-filled material along the main crystallographic directions are surprisingly different. While the thermal expansion along the 'a' direction decreases almost to zero upon molecular insertion, the negative expansion along 'c' becomes 7 times larger ($-2.2 \cdot 10^{-5}$ K^{-1}), if compared to the empty $AlPO_4$-17.

At HP and room T in penetrating N_2, O_2 and Ar PTM guest species insertion completely modified $AlPO_4$-17 structural response to pressure. Collapse in the 'a' direction no longer occurred and this plane exhibited close to zero area compressibility. PIA and PIS were also suppressed as this elastic instability was removed. Crystal structure refinements indicate that up to 24 guest molecules are inserted per unit cell and that this insertion is responsible for reductions in compressibility observed at HP. A phase transition to a new hexagonal structure with cell doubling the 'a' direction was observed above 4.4 GPa in fluid O_2.

Such highly anisotropic thermal expansion properties observed are of great interest for mechanical and optical applications. Molecular guest insertion is thus a very powerful tool for tuning the thermal expansion properties of porous materials with close to zero thermal expansion. HP, variable temperature XRD is the technique of choice to determine the effect of guest content on the thermal expansion properties of these porous materials. The insertion of non-volatile guest species or the polymerisation of a guest molecule under pressure can be used as a strategy to recover composites for potential applications.

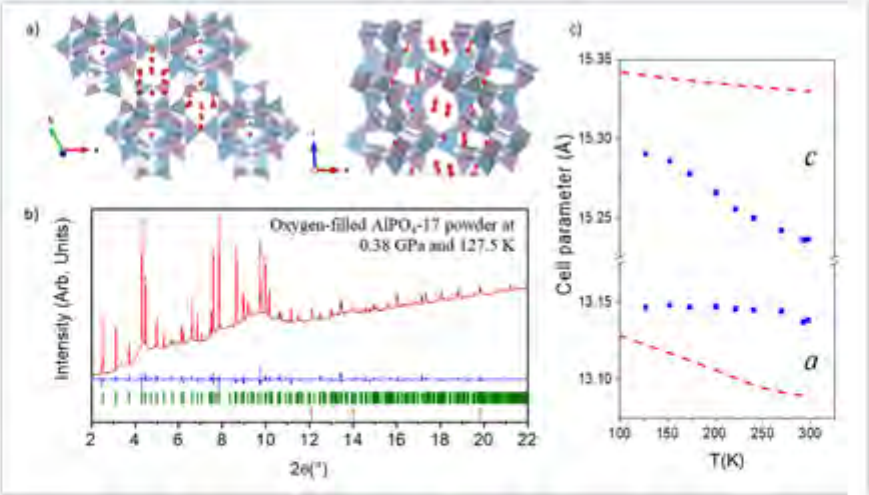


Figure 1: (a) Views of the crystal structure of O_2–filled $AlPO_4$-17 at 0.5 GPa obtained from single-crystal diffraction. (b) Experimental (black), calculated (red) and difference (blue) XRD profiles (λ=0.4958 Å) for oxygen-filled $AlPO_4$-17 powder at 0.38 GPa and 127.5 K. Upper (green) and lower (orange) vertical bars indicate the calculated positions of the Bragg reflections of $AlPO_4$-17 and Au (*P-T* calibrant), respectively. (c) Unit cell parameters (blue square symbols) of oxygen-filled $AlPO_4$-17 powder at 0.38 GPa as a function of temperature. Data (red dashed line) for empty $AlPO_4$-17 at ambient pressure are from Attfield and Sleight, Chem. Mater. 10, 2013-2019 (1998).

Perspectives of IXS and NRS for high-pressure studies in the APSU era

Jiyong Zhao[1]
[1]*Argonne National Laboratory, Argonne, United States*

Next Gen Synchrotrons, July 25, 2023, 14:00–16:00

High-pressure study has been an important part of programs at Advanced Photon Source, including the momentum-resolved high resolution inelastic X-ray scattering (HRIXS) at Sector 30, resonant inelastic X-ray scattering (RIXS) at Sector 27, and nuclear resonant scattering (NRS) at Sector 3 and Sector 30. Information acquired from techniques such as sound velocities, phonon electron couplings, hyperfine interactions, magnetic phase transitions and melting under high-pressure with either high temperature or low temperature have great impact on scientific research.

With the upcoming APS storage ring upgrade, we expect these programs to expend in performance and scope, especially for applications on high-pressure research using smaller beam size introduced by the upgrade. Detailed upgrades will be described for these beamlines, and future perspectives on the user program will be given in this talk.

Mechanisms of phase transformation in metals under extreme conditions: examples of iron and titanium

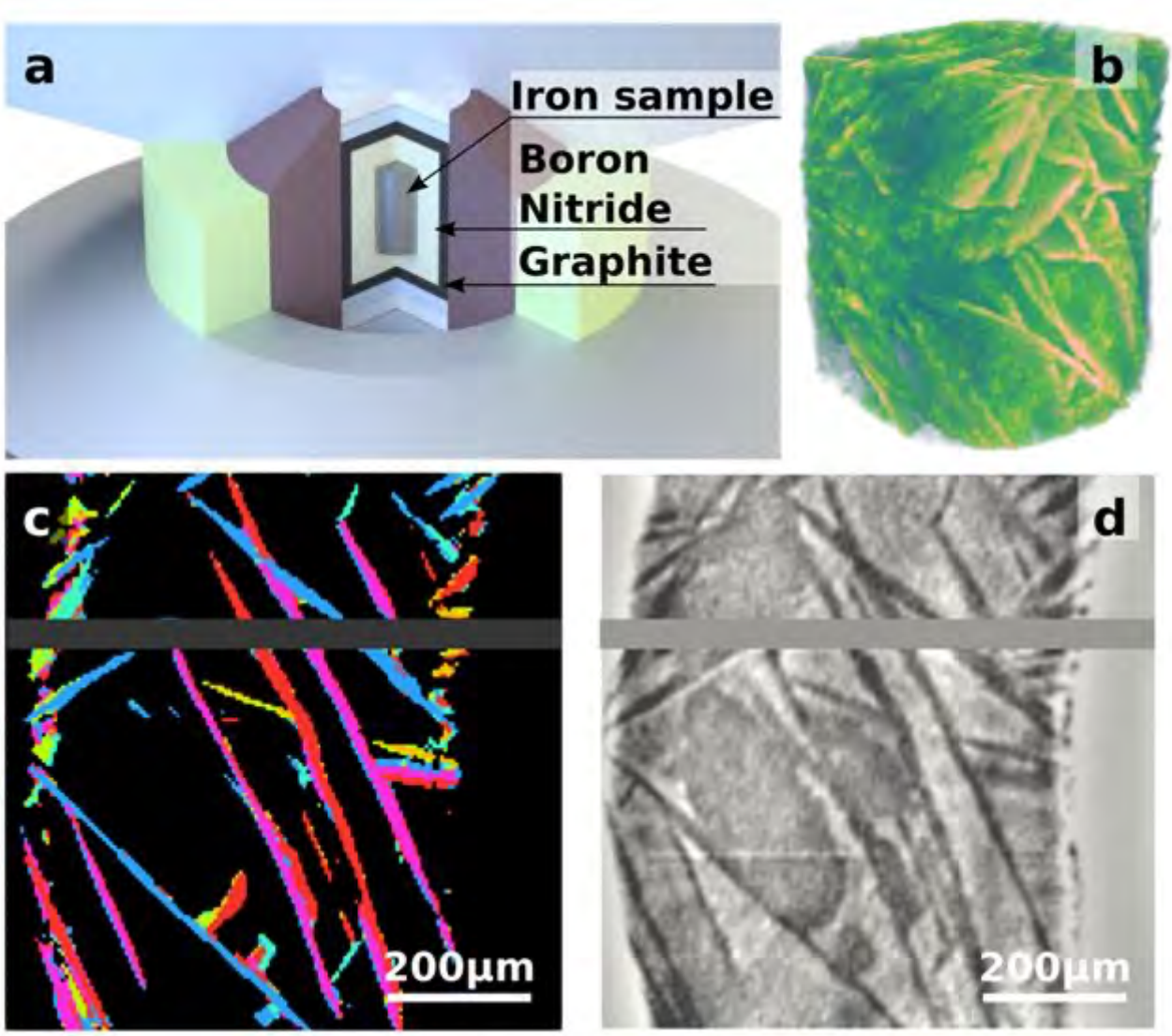
Agnès Dewaele[1,2], Robin Fréville[1,2], Laura Henry[1,2], Eglantine Boulard[3], Volodymyr Svitlyk[4], Alexei Bosak[4], Gaston Garbarino[4], Nicolas Guignot[5], Andrew King[5], Christophe Denoual[1,2], Nicolas Bruzy[1,2]

[1]CEA, DAM, DIF, 91297 Arpajon Cedex, France, [2]LMCE, CEA and Universite Paris Saclay, 91680 Bruyères-le-Châtel, France, [3]IMPMC, CNRS and Sorbonne Université, 75005 Paris, France, [4]ESRF, 38043 Grenoble, France, [5]Synchrotron Soleil, 91192 St Aubin, France

Static Studies of Elements 1, July 25, 2023, 14:00–16:00

Solid-solid phase transformations under extreme conditions exhibit multiscale mechanisms which give rise to various microstructures; they need to be understood if one wants to tailor these microstructures. It is known that the transformation path is affected by external parameters (stress, strain rate, system size and defects…). However, X-ray diffraction and imaging evidences characteristic features for α-γ-ε transformations in iron, regardless of these parameters. These transformations take place in the 0-15 GPa, 300-900 K pressure-temperature domains that can be obtained in diamond anvil cells as well as Paris-Edinburgh presses. Using these two devices, we observe martensitic orientation relations and wide planar interfaces between parent and daughter phase for α-ε, and a microstructure memory effect; martensitic orientation relations and stacking faults for γ-ε; reconstructive features such as annealing twinning for α-γ [1,2]. We present displacive or reconstructive mechanisms for these transitions. We used these differences to produce quality single crystal epsilon-iron and measure its single crystal elastic constants.
We have also studied the mechanisms of pressure-induced α-ω phase transformations in titanium; martensitic orientation relations and interfaces are found which constraint its modelling.

[1] R. Fréville et al., Phys. Rev. B 107, 104105, 2023
[2] E. Boulard et al., Acta Mat. 192, 30, 2020



Figures: a) schematic of an iron sample assembly in the Paris-Edinburg press. b) 3D rendering of the density (yellow: ϵ-Fe, green: α-Fe) upon the α-Fe ⟶ ϵ-Fe transition. c) ϵ-Fe platelets orientation variants, materialised by different colors, d) Reconstructed absorption contrast 2D slice. Dark (light) zones correspond to ϵ-Fe (α-Fe).

Ultra-high complexity of synthesised meta-stable nitrides

Florian Trybel[1], Dominique Laniel[1], Igor A. Abrikosov[1]
[1]Theoretical Physics Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, Sweden, [2]Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, United Kingdom

Nitrides, Borides and Carbides 1, July 24, 2023, 14:00–16:00

High-pressure can lead to a surprisingly strong modification of crystal chemistry and the formation of new and highly complex phases. We employ density-functional-theory-based calculations to complement in-situ structure refinement from high-pressure single-crystal X-ray diffraction from polycrystalline samples in diamond anvil cells in order to analyse structural stability, obtain a deeper understanding of high-pressure chemistry and find functional properties of novel synthesised phases.

This synergy revealed unexpectedly complex and metastable nitrides [1,2,3] with up to 250 atoms in the unit cell -- significantly too large to be relaxed from random or even sensible random atomic positions -- and phases only stabilised through dynamic or thermal effects [3]. The identified structures do not only reveal that high-pressure compounds can show complexity beyond any imagination, but are also particularly interesting, as they show new chemistry, e.g., long sought-after aromatic hexazine [N6]4- anions in K_9N_{56} [1], surprising dynamical effects in the P-N system [3] or multi-functionality -- a combination of high hardness, wide band gap, piezoelectricity -- in recoverable polymeric C-N compounds [2] with an outstanding potential for technical applications. I will present our recent findings in nitride systems to hopefully initiate discussions on how similarly complex (meta-stable) but promising phases can be efficiently identified, characterised, and in the future utilised.

[1] Laniel, Trybel, et al. "Aromatic hexazine [N6] 4− anion featured in the complex structure of the high-pressure potassium nitrogen compound K9N56." Nature Chemistry (2023): 1–6.
[2] Laniel, Trybel, et al. "Synthesis of Ultra-Incompressible Carbon Nitrides Featuring Three-Dimensional Frameworks of CN4 Tetrahedra Recoverable at Ambient Conditions." arXiv preprint arXiv:2209.01968 (2022).
[3] Laniel, Trybel, et al. "Revealing Phosphorus Nitrides up to the Megabar Regime: Synthesis of ′-P3N5, δ-P3N5 and PN2." Chemistry–A European Journal 28.62 (2022): e202201998.

Synthesis, Crystal Growth and Physical Properties of High-Entropy Transition-Metal Nitrides under High-Pressures and High-Temperatures

Prof. Dr. Masashi Hasegawa[1], Takuya Sasaki[1], Chung-Ching Chang[1], Ryo Kanzaki[1], Ken Niwa[1]
[1]*Department of Materials Physics, Nagoya University, Nagoya, Japan*

Synthesis and Properties of Novel Materials 1, July 26, 2023, 14:00–16:00

High-entropy materials such as high-entropy alloys and high-entropy ceramics have attracted much attention in recent years. These materials have crystal structures with unique atomic arrangements in which disorder and periodicity coexist. They also exhibit attractive physical and chemical properties such as high toughness, catalytic ability, and energy storage. Metallic nitrides composed of transition metals have excellent properties such as superconductivity, high hardness, and wear resistance, and are expected to be applied to electronic devices and industrial materials. In this study, we attempted to synthesise transition metal nitrides with high entropy under high-temperature and high-pressure above the ~GPa region using a multi-anvil high-pressure generator. Quinary transition metal nitrides having the NaCl-type structure have been successfully synthesised in a bulk form by chemical reactions between alloy and ammonium chloride, which are useful for high-pressure syntheses of novel monocomponent metal nitrides [1,2]. We have also succeeded in growing their single crystals [3]. The obtained crystals show a cubic shape with a habit consistent with the NaCl-type structure. The formation process was clarified by in-situ high-temperature and high-pressure synchrotron XRD measurements. Physical properties such as compressive and thermal expansion behaviours will also be presented and discussed in this talk.

[1] T. Sasaki, T. Ikoma, K. Sago, Z. Liu, K. Niwa, T. Ohsuna, M. Hasegawa, Inorg. Chem., 58 (2019) 16379.
[2] N.A. Gaida, T. Sasaki, Z. Liu, K. Niwa, M. Hirozawa, T. Ohsuna, M. Hasegawa, Appl. Phys. Lett., 116 (2020) 123102.
[3] R. Kanzaki, T. Sasaki, N.A. Gaida, K. Niwa, M. Hasegawa, Special Issue of Rev. High Press. Sci. Technol., 32 (2022) 100.

Photoluminescence of the Negatively Charged Split Silicon-Vacancy Defect in Diamond at Low Temperature and High-pressure

Professor Serge Desgreniers[1], Mr. Michael Tokiyoshi Hamel[1]
[1]*Laboratoire de physique des solides denses, Department of Physics, University of Ottawa, Ottawa, Canada*

Electronic Transitions 1, July 26, 2023, 16:30–18:30

Although very rare in natural diamond, silicon is often present in laboratory-made diamond. The non-intentional deposition of Si is due to plasma etching of silica components present in a system for sample growth by chemical vapour deposition. Combined with two neighbouring vacancies, silicon forms a quantum defect – the split silicon-vacancy system (V-Si-V or SiV, for short) – with a characteristic photo-induced luminescence at around 740 nm, for its negatively charged state (SiV-). The SiV- defect in diamond, acting as a colour centre, presents in relatively narrow photoluminescence line, a desirable characteristic for applications like nanoscale sensing or use as single photon emitters for quantum storage and computing. The SiV- electronic levels are necessarily influenced by the increase of density resulting from the application of high-pressure to diamond. In this contribution, we present results of photoluminescence spectroscopy of the SiV- colour centre as a function of pressure up to 20 GPa at room (295 K) and low temperature (11 K) in different pressure transmitting media and compare them to that of the nitrogen-vacancy (NV0 and NV-) defects. SiV defects are obtained from growth of polycrystalline and single-crystal diamond by chemical vapour deposition in presence of undoped Si, followed by sample annealing. The pressure dependence of the photoluminescence corresponding to the zero-phonon line of SiV- in polycrystalline diamond compressed in nitrogen used as the pressure transmitting medium, recorded at 295 ± 1K (orange) and 11 ± 1K (green) is illustrated. Although the pressure induced spectral shift of the zero-phonon line of the SiV- defect is not as pronounced as that observed, for instance, for the NV system (1.23 meV/GPa and 3.78 meV/GPa, at 11 K, for the SiV- and NV- defects, respectively), the relatively strong photoluminescence signal with a minimal contribution from phonon-assisted transitions makes the SiV- defect a suitable system for an in-situ pressure gauge imbedded in the diamond anvil and in close proximity with a sample under compression.

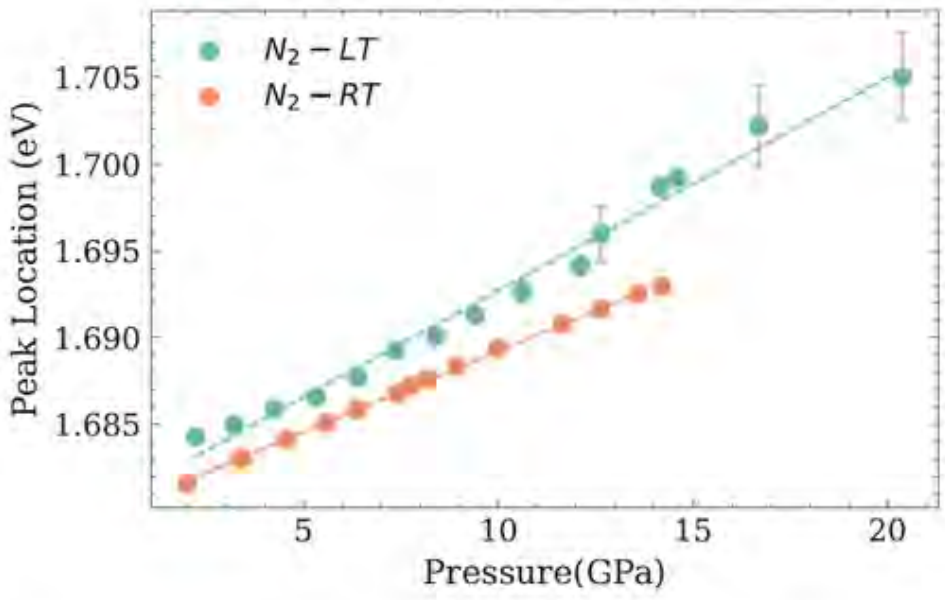


Figure 1. Pressure dependence of the zero-phonon photoluminescence of SiV^- in polycrystalline diamond, recorded at 295 ± 1K (orange) and 11 ± 1K (green). Samples were compressed in N_2, used as the pressure transmitting medium. Dotted lines correspond to linear fits with pressure coefficients of 0.97 and 1.23 meV/GPa, for the room and low temperature data points, respectively.

Cooling and energy conversion via pressure in barocaloric materials

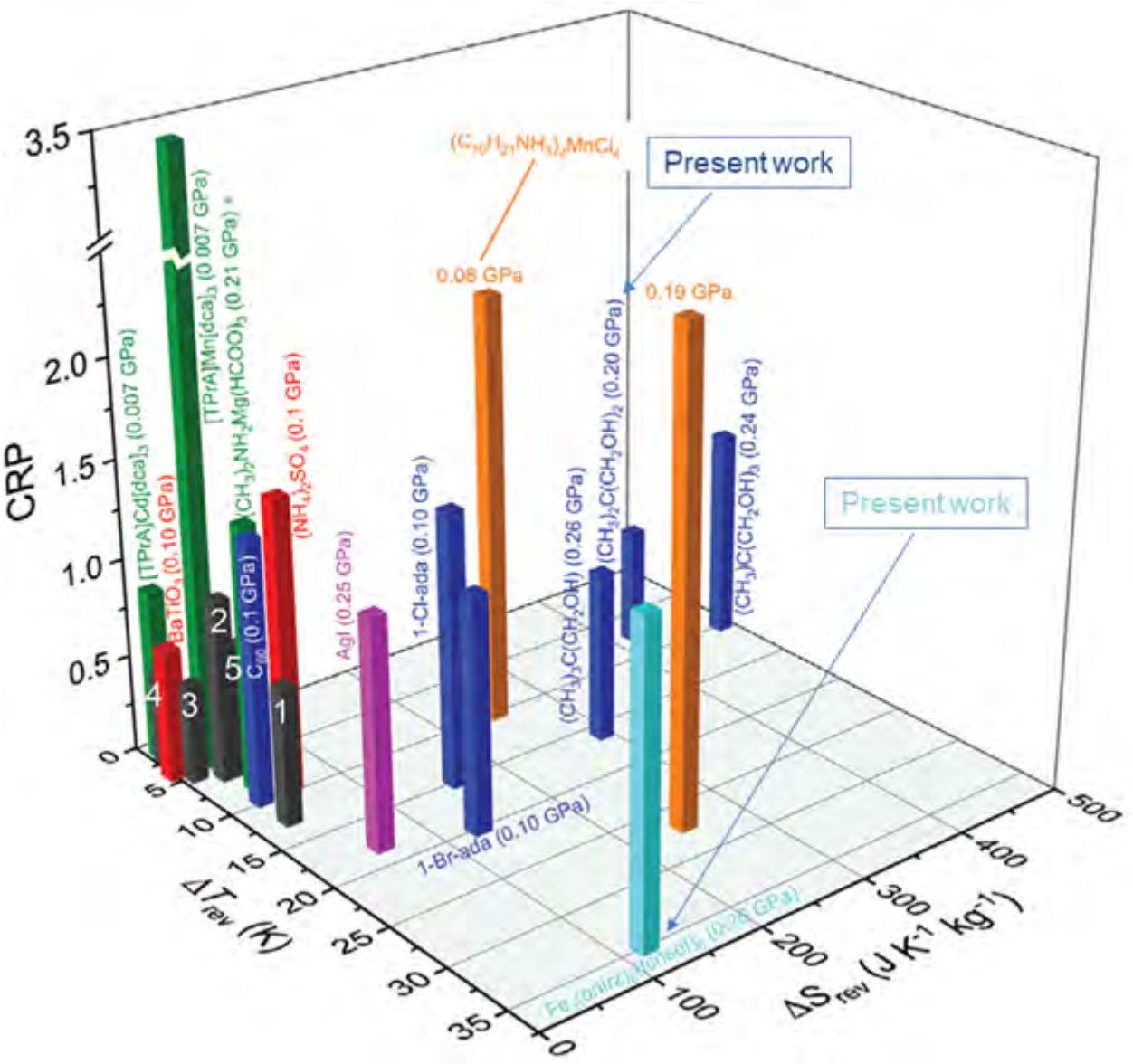
Catalin Popescu[1]
[1]*ALBA Synchrotron, Cerdanyola Del Valles, Spain*

Multifunctional Materials, July 24, 2023, 10:15–12:15

Conventional refrigeration technologies are based on compression of greenhouse gases that are environmentally threatening (hydrofluorocarbons and hydrochlorofluorocarbons) [1]. The urgent need to reduce their footprint follows the European climate strategy aiming to reduce by 2030 greenhouses gas emissions to at least 55% by fostering energy efficiency and renewable energy[2]. The need to replace this technology led to solid state cooling devices which overcome many environmental issues. The study of materials with caloric effects at first-order phase transitions is one of the best alternatives for solid state cooling devices and emerges as leading research field in Materials Science[3].

Here, we present recent advances in barocaloric performance of different materials. In particular, we report on plastic crystals that exhibit colossal barocaloric effects with entropy changes an order of magnitude larger than any other caloric materials so far[4]. More recently, we showed evidence of giant barocaloric in spin-crossover molecular material[5]. The performance of this material largely outperforms those previously reported for spin-crossover compounds with a temperature change of an order of magnitude larger. Furthermore, the present work has implications on both scientific and instrumental levels. We will present a new infrastructure for measuring X-ray diffraction at low pressures and moderate temperatures matching the application pressure range of barocaloric materials.

[1] Cazorla,C et al. Nature 567, 470 (2019)
[2] European Commission, 2030 climate & energy framework (https://climate.ec.europa.eu/eu-action/climate-strategies-targets/2030-climate-energy-framework_en)
[3] L. Manosa, A. Planes; Adv. Mater. 29, 1603607 (2017).
[4] Lloveras, P. et al. Nat. Comm. 10, 235203 (2019)
[5] Romanini, M. et al. Adv. Mat. 33, 2008076 (2021)
[6] Li, J. et al. Adv.Funct. Mat. 31, 2105154 (2021)


CRP
3.5
2.0
1.5
1.0
0.5
0
ΔT_{rev} (K)
5
10
15
20
25
30
35
ΔS_{rev} (J K^{-1} kg^{-1})
0
100
200
300
400
500
$(C_{10}H_{21}NH_3)_2MnCl_4$
0.08 GPa
0.19 GPa
Present work
Present work
[TPrA]Cd(dca)$_3$ (0.007 GPa)
$BaTiO_3$ (0.10 GPa)
[TPrA]Mn(dca)$_3$ (0.007 GPa)
$(CH_3)_2NH_2Mg(HCOO)_3$ (0.21 GPa)
$(NH_4)_2SO_4$ (0.1 GPa)
C_{60} (0.1 GPa)
AgI (0.25 GPa)
1-Cl-ada (0.10 GPa)
1-Br-ada (0.10 GPa)
$(CH_3)_3C(CH_2OH)$ (0.26 GPa)
$(CH_3)_2C(CH_2OH)_2$ (0.20 GPa)
$(CH_3)C(CH_2OH)_3$ (0.24 GPa)
Fe$_{0.89}$Mn$_{0.11}$(pz)[Ni(CN)$_4$] (0.25 GPa)
1
2
3
4
5

Crystal chemistry of binary nitrides and phosphides synthesised at high-pressure

Ken Niwa[1], Shuto Asano[1], Takuro Yamamoto[1], Keita Nishidozono[1], Taku Matsuo[1], Takuya Sasaki[1], Masashi Hasegawa[1]
[1]Nagoya University, Nagoya, Japan

Nitrides, Borides and Carbides 2, July 25, 2023, 14:00–16:00

Recent advances in high-pressure techniques have made it possible to synthesise new nitrogen-based compounds. In particular, the high-pressure crystal chemistry of nitrides has been advanced by combining laser-heated diamond anvil cells (LHDAC) and synchrotron X-ray diffraction measurements. Novel nitrogen-based compounds synthesised under ultrahigh-pressure exhibit interesting chemical and physical properties that derive from their unique chemical bonds and electronic states. Recent studies have shown that almost all transition metals form highly coordinated nitrogen-based compounds above about 30 GPa, some of which can be recovered at ambient pressure. On the other hand, transition metal pernitrides synthesised under high-pressure crystallise in a crystal structure similar to that of phosphides, indicating that there is a similarity between the crystal structures of nitrides and phosphides. Therefore, further high-pressure studies of nitrides and phosphides will lead to a further understanding of novel functional compounds. To further understand the high-pressure crystal chemistry of binary nitrides and phosphides, we have conducted the synthesis experiments of new early transition metal-nitride and -phosphide using LHDAC to approximately 80 GPa. For nitride synthesis experiments (V-N, Cr-N, Nb-N, Mo-N), small pieces of elements or mononitride nitrides were loaded into the sample chamber of the DAC with molecular nitrogen. After elevated pressure, the samples were heated by infrared laser irradiation. For the synthesis of phosphides (Nb-P, Mo-P, Ta-P, W-P), existing transition metal phosphides were synthesised in a vacuum quartz tube and loaded into the sample chamber of the DAC. Synthesis was performed by introducing an infrared laser into the sample under high-pressure, and the synthesised compounds were characterised by synchrotron X-ray diffraction and Raman scattering measurements under high and ambient pressure. Characterisation of the synthesised samples revealed the presence of a new high-pressure nitrogen-rich phase in all these systems. It was also found that the new high-pressure phase of phosphides is composed of highly coordinated transition metals and that the crystal structure has never been found in pernitrides, which were also synthesised under high-pressure. In this presentation, we will discuss the crystal chemistry of the early transition metal nitrides and phosphides synthesised under high-pressure.

Structural Competitiveness in Ramp-Compressed Sodium

Danae Polsin[1,2], Amy Lazicki[3], Xuchen Gong[1,2], Stephen Burns[1], Federica Coppari[3], Linda Hansen[5], Brian Henderson[1], Margaret Huff[1,2], Malcolm McMahon[4], Marius Millot[3], Reetam Paul[3], Raymond Smith[3], Jon Eggert[3], Gilbert Collins[1,2], J. Ryan Rygg[1,2]
[1]University of Rochester, Rochester, United States, [2]Laboratory for Laser Energetics, Rochester, United States, [3]Lawrence Livermore National Laboratory, Livermore, United States, [4]The University of Edinburgh, Edinburgh, United Kingdom, [5]Sandia National Laboratory, Albuquerque, United States

Dynamic Studies of Elements, July 25, 2023, 10:15–12:15

At high-energy-density conditions, a new realm of quantum behaviour emerges including electron localisation, structural complexity, core-electron chemistry, and more. Sodium (Na) behaves particularly bizarre at these conditions because of its very high compressibility. Normally a shiny ideal metal, Na transforms to a topological insulator at 200 GPa. This topologically insulating phase (hP4) is due to the valence electrons occupying interstitial positions of its crystalline lattice rather than the orbitals Centred on ionic cores. Using lasers as high-pressure drivers, we report the structural and electronic properties of Na at the most extreme compressions yet studied. X-ray diffraction measurements to 480 GPa and 2000 K reveal unexpected new phases. Simultaneous reflectivity measurements suggest a dramatic drop in the conductivity of both the solid and fluid phases. These data together with ab initio evolutionary structure searches reveal a rich structural competitiveness than extends to greater than 300 GPa and thousands of degrees Kelvin. Recent experiments on ramp-compressed sodium at the National Ignition Facility will be discussed.

This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856, the U.S. Department of Energy, Office of Science, Fusion Energy Sciences funding the award entitled High Energy Density Quantum Matter under Award Number DE-SC0020340, the University of Rochester, and the New York State Energy Research and Development Authority. Partial funding for this research is provided by the Centre for Matter at Atomic Pressures (CMAP), a National Science Foundation (NSF) Physics Frontiers Centre, under Award PHY-2020249.

Ultrahigh-pressure Generation at High Temperature in a Walker-type Large-volume Press and its applications to the research of new carbon materials

Prof, Ms Bingbing Liu[1]
[1]*Jilin University, State Key Lab of Superhard Materials, Changchun, China*

Synthesis and Properties of Novel Materials 3, July 26, 2023, 16:30–18:30

High-pressure has been used as an important technique to create new materials. Carbon is the focus in material research and particularly the discovery of a new carbon material usually triggered a new research field. Searching for novel carbon materials under high-pressure has always been an important topic in the fields of both high-pressure and materials science, and the related study strongly depends on high-pressure technology. In this presentation, I will introduce latest progress on the development of large volume press (LVP) technologies and their applications to the study of new carbon materials. The main contents include: 1) We developed advanced LVP technology by designing the cell assembly based on domestically produced WC anvils which can reach ultrahigh-pressure above 40 GPa at high temperature in a Walker-type Large-volume Press. By using this technique, we synthesised an amorphous carbon bulk material with nearly pure sp3 bonds, which shows the highest thermal conductivity, hardness. The microstructure of amorphous carbon has been further tuned by modulating the contained diamond-like short/medium range orders, in which C70 was used as precursor because of its higher percentage of hexagonal carbon rings on the cage. The obtained bulk amorphous carbon is transparent. Our study opens a new way for the structure tuning of sp3 hybridised amorphous carbon. 2) We developed a new strategy of combining high-pressure with co-crystal to create new carbon structures and obtained a series of long range ordered crystal with amorphous nanoclusters as building blocks (OACC) from compressing fullerene cocrystals. OACC structure is a new structure in solids besides the well-known crystal, amorphous and quasicrystal, which extends the categories of solid materials from atomic structure point of view. We further synthesised bulk OACC material with millimeter size by using the LVP technology and discovered that this is a new superhard material with optical band gap comparable to that of amorphous silicon but much higher hardness.

Novel High-Pressure Irradiation Platform at GSI: Investigation of structural modifications under extreme conditions

Ioannis Tzifas[1], Dr. Maria- Eugenia Toimil-Molares[1,4], Dr. Kay-Obbe Voss[1], Christopher Schroeck[1,3], Professor Maik Lang[2], Professor Christina Trautmann[1,4]
[1]GSI Heavy Ion Accelerator, Darmstadt, Germany, [2]University of Tennessee, Knoxville, United States, [3]Goethe Universität, Frankfurt, Germany, [4]Technical University of Darmstadt, Darmstadt, Germany

Facility Development 1, July 24, 2023, 16:30–18:30

We present a newly-built high-pressure irradiation platform at the GSI heavy ion accelerator facility, where materials are simultaneously exposed to high static pressures and high-energy heavy ion irradiation. Energetic ions can produce unique defect configurations and chemical changes in materials, yielding structural modifications, including point and cluster defects, amorphisation, and crystalline-to-crystalline phase transformations. The platform was recently complemented Raman spectroscopy. Pioneering experiments at the SIS-18 accelerator at GSI revealed that the combination of pressure (range 2-50 GPa) and ion irradiation (179Au, 238U of GeV kinetic energy) can lead to the synthesis of new phases far from the thermodynamic equilibrium and to the possibility to recover a high-pressure phase upon pressure release [1,2]. The compression is achieved by using Diamond Anvil Cells (DACs), while the irradiation takes place through the metallic gasket. To prevent beam-induced coloration of the diamonds, the beam size is minimised by a remote-controlled adjustable collimation system. Structural changes of the sample in the DAC are monitored by online Raman spectroscopy through the diamond anvils. The aim of this development is to provide a user platform in Cave A with SIS-18 beams and at a later stage in the APPA Cave of the new FAIR facility.

[1] Lang, M., Zhang, F., Zhang, J., Wang, J., Schuster, B., Trautmann, C., Neumann, R., Becker, U., Ewing, R.C. Nanoscale manipulation of the properties of solids at high-pressure with relativistic heavy ions. Nat. Mater 2009, 8(10): p. 793-797 https://doi.org/10.1038/nmat2528

[2] Glasmacher UA, Lang M, Keppler H, Langenhorst F, Neumann R, Schardt D, Trautmann C, Wagner GA (2006) Phase transitions in solids stimulated by simultaneous exposure to high-pressure and relativistic heavy ions. Phys Rev Lett 96:195701-1–195071-4, https://doi.org/10.1103/PhysRevLett.96.195701

Measurement of high-pressure crystal structure and the pressure-temperature melt conditions in shock-compressed silicon carbide

Raymond Smith[1], Zixuan Ye[2], Saransh Singh[1], Marius Millot[1], Kien Nguyen Cong[4], Dayne Fratanduono[1], David Erskine[1], Sally Tracy[3], Ivan Oleynik[4], Jon Eggert[1], June Wicks[2]
[1]Lawrence Livermore National Laboratory, Livermore, United States, [2]Johns Hopkins University, Baltimore, United States, [3]Carnegie Institution for Science, Washington DC, United States, [4]University of South Florida, Florida, United States

Phase Diagrams – Metals, July 27, 2023, 10:15–12:15

Silicon Carbide (SiC) has many attractive properties including low density, high strength, high melting point, low wear coefficient and high chemical stability that leads to its extensive use in a wide range of industrial applications including as abrasives, shielding material on space craft, personal armour and as a potential ablator material for fusion capsules. Silicon carbide is also important in geology and planetary science. SiC grains – found in meteorites and impact sites – have an unusual isotopic signature which indicate that they are pre-solar in origin and provide constraints on stellar nucleosynthesis and on the stellar sources for the origin of the solar system. Several studies have also explored possible interior structure of carbon-rich planets in which SiC is a likely main constituent, but experimental data for the high-pressure, high-temperature properties of SiC is currently unavailable to test these models.

Here we report on laser-driven nanosecond X-ray diffraction and shock-decay experiments on the Omega-EP laser facility located at the Laboratory for Laser Energetics (NY, USA). We present new data on the high-pressure crystal structure, microstructural texture evolution, and pressure-temperature conditions for melt in uniaxially compressed single-crystal SiC samples. We employ a forward X-ray diffraction model which reproduces the azimuthal texture around the Debye-Scherrer cones and places a constraint on the 4H->B1 phase transformation at ~100 GPa. We also present Hugoniot data to 1 TPa. Our data is compared against recent quantum molecular dynamic simulations.

Toward Accessing the Solid Metallic State of Hydrogen via Ramp Compression of Solid parahydrogen

Arnold Schwemmlein[1], Ryan Rygg, Raymond Jeanloz, Peter Celliers, Jon Eggert, Paul Loubeyre, Zaire Sprowal, Gilbert Collins
[1]*Laboratory For Laser Energetics, United States*

Hydrogen, July 25, 2023, 10:15–12:30

The equation of state of hydrogen at high-pressureshas received significant interest from both material and planetary science. One particular region of interest is at temperatures and pressures around 1500K and 200-300GPa, where recent studies at the National Ignition Facility and the Z Pulsed Power Facility observed an insulator–metal transition during ramp compression of liquid deuterium. Similar ramp compression experiments were conducted at the Laboratory for Laser Energetics with solid para-hydrogen. These targets have ~2kB/molecule lower initial entropy in order to enable lower temperature quasi-isentropic compression. Pressure histories of the compressed hydrogen up to 400GPa were determined from velocimetry data. Experimental results of this recent pilot study compressing hydrogen into the conducting regime will be discussed.

This material was funded by the Centre for Matter at Atomic Pressures (CMAP), a National Science Foundation (NSF) Physics Frontiers Centre, under Award PHY-2020249.

Synthesis of metastable transition metal carbides using high-pressure

Dr James Walsh[1], Paul Marshall, Scott Thiel, Zeynep Alptekin, Dr Yue Meng, Dr Dean Smith, Dr Matthew Whitaker
[1]*University of Massachusetts Amherst, Amherst, United States*

Nitrides, Borides and Carbides 2, July 25, 2023, 14:00–16:00

The synthetic phase space opened up by high-pressure is vast, and no doubt harbours countless undiscovered metastable materials with the potential to propel next-generation technologies. However, this phase space remains only partially explored, being limited by: (1) the difficulties involved in precisely targeting specific chemical compositions under the constraints of extreme pressure methods, which makes doped and multi-element phases difficult to access; and by (2) the high computational costs required to search for low-symmetry and/or multi-element phases using theory-based approaches, which inherently biases searches toward well-ordered phases with small unit cells. Here, we will present results from our studies into the use of high-pressures to access novel transition metal carbides (TMCs), including new experimental and theoretical approaches that move us beyond the current frontiers in high-pressure materials discovery.
We will present results from our work on the high-pressure synthesis of novel first-row TMCs using both laser-heated diamond anvil cell and large volume press methods [1,2], outlining a novel approach to precursor preparation that allows us to reliably and repeatably target specific chemical compositions in the diamond anvil cell. We will also present computational results from our recent data-driven study on zirconium carbide, which under normal synthesis conditions exhibits a remarkably high degree of sub-stoichiometry at the carbon site [3]. The use of cluster expansion methods allows us to survey a broad range of phase space at a much lower cost than would be permitted with first principles approaches alone, revealing details on the effect that pressure has on the range of sub-stoichiometry that can be synthetically accessed. These data-driven tools augment structure searching methods by allowing us to examine the stability of substoichiometric candidate phases in our systems of interest.

[1] Marshall, P. V.; Alptekin, Z.; Thiel, S. D.; Smith, D.; Meng, Y.; Walsh, J. P. S., Chem. Mater., 2021, 33, 9601–9607.
[2] Marshall, P. V.; Thiel, S. D.; Cote, E. E.; Meng, Y.; Whitaker, M. L.; Walsh, J. P. S., In Preparation.
[3] Thiel, S. D.; Walsh, J. P. S., Adv. Theory Simul., 2022, 5, 2200439.

In-situ X-ray diffraction of laser-shock compressed binary compounds at Megabar pressures

Chris McGuire[1], Saransh Singh[1], Andy Krygier[1], Travis Volz[1], Sally Tracy[2], Francesca Miozzi[2], Cara Vennari[1], Trevor Hutchinson[1], Richard Briggs[1], Jon Eggert[1]
[1]Lawrence Livermore National Laboratory, Livermore, United States, [2]Carnegie Institution of Washington, Washington, United States

Cores of Terrestrial Planets, July 24, 2023, 14:00–16:00

In this talk, I will discuss X-ray diffraction experiments at the Dynamic Compression Sector's laser-shock compression end-station at the Advanced Photon Source. A 100 J Nd:glass long-pulse laser drives a shock wave by laser ablation through a planar target package, generating stress states in the sample comparable to the pressures at the Centre of the Earth. The ability to probe these states directly with picosecond hard X-ray s (E = 24 or 36 keV) has opened a frontier in planetary science, allowing new experimental data to be collected on the structure of geomaterials. In an experiment on metallic Fe3C and Fe-C alloy, we determined the structure and density of Fe-C liquids compressed to peak stresses between 1.8 to 3.3 Mbar (1 Mbar = 106 atmospheres), extending the pressure range of in-situ X-ray diffuse scattering measurements of liquid iron alloys by a factor of ~5. In an experiment on the wide band-gap semiconductor GaN, we observed coexistence of a new high-pressure phase and liquid at stresses of approximately 2.5 Mbar. We also observed crystallisation of the ambient structure of GaN from the compressed liquid within several nanoseconds after release of the shock wave. Implications for the phase diagrams of Fe-C and Ga-N under dynamic compression will be discussed.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Discovery of a Seven-Coordinated CrSb2 High-pressure Polymorph

Emma Ehrenreich-Petersen[1], Mads F. Hansen[1], Justin Jeanneau[1], Davide Ceresoli[2], Francesca Menescardi[3], Martin Ottesen[1], Vitali Prakapenka[4], Sergey N. Tkachev, **Martin Bremholm**[1]
[1]Dept. of Chemistry and iNANO, Aarhus University, Aarhus C, Denmark, [2]Consiglio Nazionale delle Ricerche – Istituto di Scienze e Tecnologie Molecolari, Milano, Italy, [3]Dipartimento di Chimica, Università degli Studi di Milano, Milano, Italy, [4]Centre for Advanced Radiation Sources, University of Chicago, Chicago, United States

Synthesis and Properties of Novel Materials 3, July 26, 2023, 16:30–18:30

We have investigated the high-pressure behaviour of MSb2 compounds with M = Cr, Fe, Ru, and Os using synchrotron powder X-ray diffraction. We find that all compounds maintain their marcasite structure up to pressures exceeding 50 GPa, except for CrSb2, which undergoes a structural phase transition at 10 GPa to a metastable MoP2-type structure, with Cr atoms coordinated to seven Sb atoms. Our density functional theory calculations confirm the MoP2-type structure is more favourable than marcasite at elevated pressure. Our results also provide valuable insights into the high-pressure behaviour of MSb2 compounds and demonstrate a new pathway to a metastable polymorph which can possibly also be realised from other marcasite structures. Furthermore, we performed laser-heating experiments on CrSb2, which resulted in the CuAl2-type structure at pressures both below and above the phase transition, i.e. the CuAl2-type is most favorable structure at high-pressure. Our findings shed light on the structural behaviour of CrSb2 under high-pressure and suggest possible pathways for synthesizing novel polymorphs of MSb2 compounds. Finally, we will discuss the crystal chemistry and properties of the studied compounds, as well as results from computational structure searches for novel metal diantimonides.

Progress in Time-Resolved X-ray Diffraction with Laser Compression at the National Ignition Facility (NIF)

Dr Laura Robin Benedetti[1], Dr. M. G. Gorman[1], Dr. S. R. Nagel[1], Dr. N. Palmer[1], P. Nyholm[1], R. B. Petre[1], Dr. C. Stan[1], Dr. J. Eggert[1], Dr. D. K. Bradley[1], N. Bhandarkar[1], A. Carpenter[1]
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Developments at XFELs & Lasers, July 24, 2023, 14:00–16:00

We report on progress in the development of an experimental platform to measure X-ray diffraction at several times during a single laser-driven dynamic compression experiment.

The platform consists of a laser-driven helium-alpha X-ray source, a dual-function target that both holds the physics package and acts as a shield to protect the X-ray detector, and hCMOS sensors with integration times as small as 1-2 ns. A developmental instrument that includes two hCMOS sensors, each collecting four images over twelve ns, has been tested on fifteen NIF experiments.

We present preliminary diffraction data across a laser driven phase transition. We discuss data quality, ongoing challenges, and improvements to both detector and target.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, LLNL-ABS-845172.

Hydrocarbons under high-pressure: Full-colour luminescence by altering molecular packing

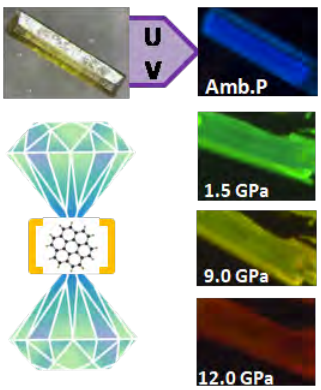
Takeshi Nakagawa[1], Yang Ding[1]
[1]*Centre For High-pressure Science & Technology Advanced Research, China*

Other Molecular Systems, July 27, 2023, 10:15–12:15

Recently, the use of high-pressure has proven to be an effective approach to uncover the relationship between the crystal structure and material properties. Pressurisation can effectively alter the molecular packing of organic materials and by combining various spectroscopic technique, we can investigate pressure-induced changes in the optical properties, intermolecular interaction, molecular conformation, phase transformation, and more. Here, we introduce recent investigation results on a optical properties of a large Polycyclic Aromatic Hydrocarbons (PAHs), where we employed high-pressure to obtain deeper insight of the structure-optical property relationships. In particular, we are interested in a physical phenomenon known as piezochromism, a pressure-dependent changes in the emission colour of luminescent materials. Piezochromic luminescence is a direct consequence of the perturbation to the electronic band-gap energy of the electronic transition in luminescent materials. Such behaviour is often found in van der Waals materials, where the molecular packing is sensitive to the changes in external stimuli. Pressure can induce different piezochromic behaviours in materials with different molecular structures via distinct piezochromisms, such as, the generation, enhancement, or quenching of fluorescence. We combined various spectroscopic techniques with Diamond Anvil Cell to investigate structure-to-property relationships.

PAHs are known as both carbon-rich and hydrogen-rich organic molecules and their outstanding tuneability of crystal structure and molecular packing have been attracting continuous research interest for their possibilities for technological application, such as organic optoelectronic and photovoltaic devices, semiconductors, and nanoelectronics.

In this work, we prepared coronene (C24H12) that exhibits blue fluorescence at ambient conditions, which, via high-pressure compression, realised full-colour emission under UV-light. During compression, we discovered that the tuneable piezochromic luminescence of coronene is strictly related to the molecular packing, that is, crystal structure transitions observed are associated with each emission colour changes from blue to green, and to red. We combined in-situ photoluminescence, UV-visible absorption, Raman, infrared spectroscopy, and synchrotron powder XRD measurements to demonstrate their outstanding tuneability and high stability of coronene crystal structure allows significant modifications of chromaticity of their emission. This work not only sheds light on the structure-optical property relationships of hydrocarbon, but also paves the way to develop a single molecular system with different molecular packing that exhibit RGB emission even at ambient conditions. Single-component materials with such optical properties, which can be prepared without complex and costly organic synthesis procedures, are an important discovery for application in various optoelectronic materials.



XFEL heating of low Z materials: a new pathway to superionic ice

Rachel J. Husband[1], Hanns-Peter Liermann[1], Malcolm McMahon[2]
[1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany, [2]The University of Edinburgh, Edinburgh, United Kingdom

Ice, Water and Clathrates, July 24, 2023, 10:15–12:15

Water (H2O) transforms to two forms of superionic ice (SI) at high-pressuresand temperatures, which are characterised by the fast diffusion of mobile, fluid-like protons within a solid oxygen sublattice. Determining the stability fields, structural behaviour, and transport properties of these phases is of interest for a wide range of disciplines ranging from fundamental physics to planetary science – for example, to understand how SI in the interiors of Neptune and Uranus contributes to their magnetic fields. Structural behaviour at static high-pressure is typically investigated using IR laser-heated diamond anvil cells coupled with X-ray diffraction (XRD) at synchrotron sources; however, these studies are complicated by a number of challenges including difficulties in sample confinement and chemical reactivity during prolonged heating and the low scattering power of H2O, all of which motivate the development of alternative methods to create and probe these states.

Here, we present the results of an X-ray heating study performed at the High Energy Density (HED) instrument which used the MHz pulse trains produced by the European X-ray Free Electron Laser (European XFEL) to create and probe high temperature states of statically compressed H2O samples. This experiment utilised a pump-probe X-ray heating scheme in which samples were irradiated with a series of XFEL pulses at 2.2 MHz, where each pulse provided a snapshot of the sample as it cooled from the hot state created by the previous pulse. Pulse-resolved, MHz XRD capabilities allowed us to clearly identify an isostructural transition during heating in the 25-70 GPa pressure range, consistent with the formation of bcc-SI, and evidence of fcc-SI was observed at the highest pressure. The large volume of XRD data generated requires new approaches to data analysis, which will be discussed. The results from this study demonstrate that stepwise XFEL heating is a viable method for the study of reactive, low Z materials at high P-T conditions.

Acknowledgements: This work is presented on behalf of European XFEL Proposal 2590

Phase diagram of Iron at Earth's core conditions from deep learning

Zhi Li[1], Sandro Scandolo[1]
[1]The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy

Computational Studies of Elements, July 26, 2023, 10:15–12:15

Iron is considered to be the main component of the Earth's core. Substantial efforts have been made to determine its phase diagram and elastic properties at extreme conditions, which is at the heart of understanding the thermodynamic evolution of the core and interpreting the seismic data. However, it remains debated about how the atoms in solid iron are arranged at Earth's core conditions, where possible candidates include hexagonal close-packed (hcp), body-centred cubic (bcc), and face-centred cubic (fcc) structures. As crystal structure and physical properties are closely related, the uncertainty is also present in interpreting the seismic data, and the origin of the low shear wave velocity in the inner core remains mysterious.

Atomistic simulations have provided important insights into the mineralogy of the core, but they are challenged by the large sizes and time scales required to achieve statistical convergence. Here we have constructed a deep-learning interatomic potential for iron to overcome these limitations. To check the performance of such potentials, we have examined the elastic and plastic behaviour of hcp iron and the effects of structural defects at inner core conditions [1], which compares very well with previous results. We then compute the Gibbs free energy of the bcc, fcc, hcp and liquid phases by performing large-scale molecular dynamics simulations. The calculated free energy allows for determining the phase stability of solid iron in Earth's core [2]. Based on the phase diagram, we provide a more plausible explanation for the cause of the low shear velocity of seismic waves in the inner core.

[1] Li, Z., & Scandolo, S. (2022). Elasticity and viscosity of hcp iron at Earth's inner core conditions from machine learning-based large-scale atomistic simulations. Geophysical Research Letters, 49, e2022GL101161
[2] Li, Z., & Scandolo, S. (2023), submitted.

Superhydrides on a quantum energy landscape

Ion Errea[1]
[1]*University of The Basque Country, Spain*

Hydrides 2, July 24, 2023, 16:30–18:30

Reaching superconductivity at ambient conditions is one of the biggest scientific dreams since more than a century ago. The discoveries in the last few years at high-pressuresplace hydrogen-based compounds as the best candidates for making it true. The prospects are higher than ever. As the recent history shows, first-principles calculations are expected to guide the experimental quest in the right track and contribute to the characterisation of the properties of these superhydrides. In this talk I will discuss how ionic quantum fluctuations and the consequent anharmonicity largely affect the crystal structure and the vibrational properties of superconducting hydrides, generally stabilizing high-critical temperature compounds at much lower pressures than expected otherwise, but not always. I will describe when and why quantum anharmonic effects enhance or suppress superconductivity, providing several examples of current interest.

Tracking phase transitions of Fe2O3 at planetary interiors conditions

Marion Harmand
[1]*CNRS, Sorbonne University, Paris, France*

Phase Diagrams – Ionic Systems, July 24, 2023, 10:15–12:15

Iron and oxygen are two of the most abundant elements in terrestrial planets and iron oxides play a major role in the mantle and core mineralogy of Earth and Super Earth exoplanets. Even when iron is present in only small amounts in the Earth's mantle, the ratio of Fe2+ to Fe3+ within a rock determines, in part, the mineral phase stabilities and the silicate mineral assemblage of the rock. The multiple iron oxidation states strongly affect the speciation of the fluid phases, chemical differentiation, melting, and physical properties of planetary interiors and ultimately contribute to determine the state of hydrosphere and atmosphere. Therefore, it is now well established that the nature and properties of iron oxides at pressure and temperature conditions modify the planetary interior structures and global redox state of the Earth and Super-Earths. In order to extend phase diagram to higher pressure and temperature, dynamic compression by laser is often a first choice. While several laser-compression experiments have been exploring the FeO phase diagram, very little is reported on Fe2O3 using such technic. In that context, we present laser compression experiments on Fe2O3, coupled with ultrafast time-resolved X-ray diagnostics to track physical properties during the shock and release. X-ray diffraction at LULI, SACLA and LCLS facilities as well as complementary X-ray absorption spectroscopy at ESRF were performed on Fe2O3. On Fe2O3, we have accurately measured its equation of state up to 700 GPa at LULI and determined its melting pressure under shock. Our diffraction measurements also showed that the high-pressure phases observed in static compression are not identical to those revealed by dynamic compression.

High-pressure synthesis of binary and ternary polyntrides in laser-heated diamond anvil cells

Maxim Bykov[1], Dr. Elena Bykova[2], Mr. Lukas Brüning[1], Mr. Pascal Jurzick[1], Dr. Alexander Goncharov[4], Prof. Leonid Dubrovinsky[3]

[1]University Of Cologne, Cologne, Germany, [2]Goethe University Frankfurt, Frankfurt, Germany, [3]University of Bayreuth, Bayreuth, Germany, [4]Carnegie Institution for Science, Washington, United States

Nitrides, Borides and Carbides 1, July 24, 2023, 14:00–16:00

The high-pressure chemistry of nitrogen and nitrogen-rich compounds has been the focus of many studies in recent years, due to both fundamental and practical interests. Poly-nitrogen compounds are considered potential high-energy density materials, owing to the remarkable differences in the average bond energy between the single N-N bond, the double N=N bond, and the triple N≡N bond.

In this work, we systematically studied various binary nitride systems (Na-N, K-N, Be-N, Fe-N, Re-N, W-N, Os-N, Pd-N, Ta-N) featuring either mostly ionic or combined ionic-covalent element-nitrogen bonding. Based on crystal chemical considerations, we developed a set of empirical rules that led to the rationalisation of the synthesis, crystal structures, and chemical bonding.

Increasing the complexity of the systems from binary to ternary compounds imposes great challenges for synthesis, due to the inherent inhomogeneity of the samples in diamond anvil cells. Therefore, phase-pure synthesis usually requires a proper choice of precursors and minimisation of the number of reagents in the system. In this talk, we will also discuss our attempts to approach ternary polynitrides through the following synthetic routes:

– Azide-mediated oxidation of transition metals
– Synthesis from the elements
– Synthesis via single-source precursor route
– Nitridation of alloys

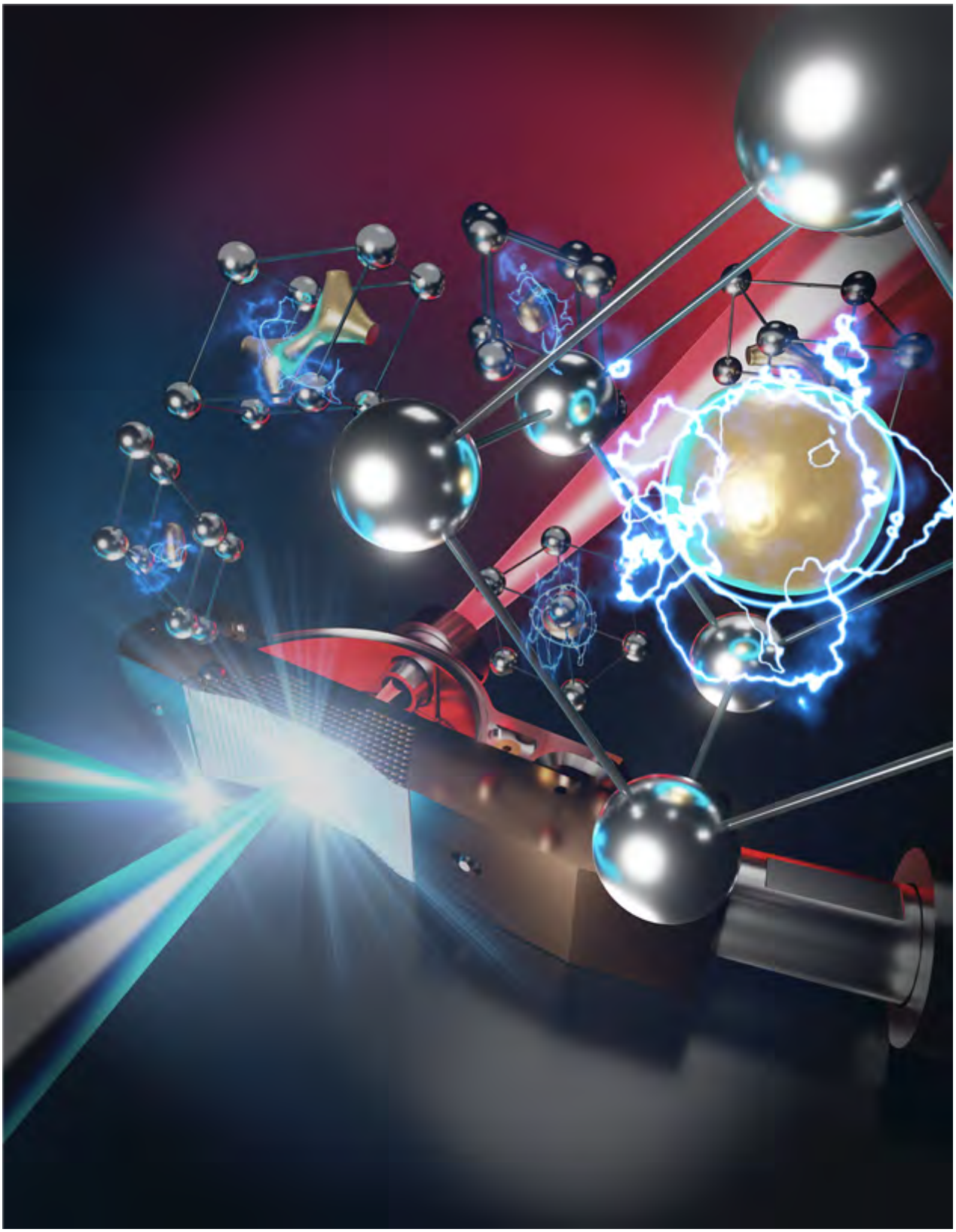
Overview of TARDIS on NIF

Dr. Jon Eggert[1], Prof. Ryan Rygg[2], Dr. Ray Smith[1], Dr. Amy Lazicki[1], Dr. Chris Wehrenberg[1], Dr. Andy Krygier[1], Dr. Martin Gorman[1], Dr. Richard Kraus[1], Dr. Samantha Clarke[1], Dr. Amy Coleman[1], Dr. Dayne Fratanduono[1], Dr. Federica Coppari[1], Dr. Marius Millot[1], Dr. Dave Braun[1], Dr. Damian Swift[1], Prof. Justin Wark[3], Prof. Gilbert Collins[2], Dr. Jim McNaney[1]
[1]Lawrence Livermore National Laboratory, Livermore, United States, [2]University of Rochester, Rochester, United States, [3]University of Oxford, Oxford, United Kingdom

Instrumentation and Techniques 3, July 26, 2023, 14:00–16:00

Over 150 TARget Diffraction In Situ (TARDIS) shots have been fielded at the National Ignition Facility (NIF) over the past 10 years. These shots – including about 30% 'Discovery Science' shots proposed by academic collaborators – range from about 20 to 2000 GPa and represent both the highest-pressure and the longest laser-driven diffraction measurements ever made. In this talk, I will give a brief history of the design considerations, campaigns and results, and plans for future diffraction experiments on NIF.

This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under contract number DE-AC52-07NA27344.



Effects of high-pressure on the methane-nitrogen binary system

Hannah Shuttleworth[1], Mikhail Kuzovnikov[1], Eugene Gregoryanz[1], Miriam Peña Álvarez[1], Ross Howie[1,2]

[1]Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh, United Kingdom, [2]Centre for High-pressure Science and Technology Advanced Research (HPSTAR), Shanghai, China

Molecular Compounds, July 25, 2023, 10:15–12:15

The understanding of binary compound phases is crucial in forming models for planetary satellite compositions. In our solar system, absorption spectra of Titan in particular have been found to contain both methane and nitrogen [1]. Simple molecular binary systems are known to form van der Waals compounds and/or react with the application of pressure, yet experimental work investigating the dense methane-nitrogen system remains scarce [2].

Through a series of high-pressure X-ray diffraction and Raman spectroscopy measurements, we observe the formation of two novel CH4-N2 van der Waals compounds above 5 GPa, each dependent on the relative content of the gas mixture. With further compression of the system above 100 GPa, we observe the disappearance of the Raman signatures associated with molecular nitrogen suggesting the emergence of a novel covalent bonded C-N-H compound. With theoretical predictions demonstrating that such compounds may be recoverable to ambient conditions [3], this result demonstrates great potential in yielding sought-after high-energy density materials.

[1] L. C. Kouvaris, F.M. Flasar, Icarus 91 (1991)
[2] C. Aldous, Thesis (2011)
[3] F. Peng et al., Phys. Rev. Materials 4 (2020)

Study of polymerisation of high-pressure nitrogen by ab initio molecular dynamics

Dominika Melicherova[1], **Prof. Roman Martonak**[1]
[1]*Faculty Of Mathematics, Physics And Informatics, Comenius University in Bratislava, Bratislava, Slovakia*

Computational Studies of Elements, July 26, 2023, 10:15–12:15

We study properties of nitrogen at high-pressure and temperature (100-120 GPa, 2000-3000 K) where molecular and polymeric phases compete both in solid and liquid phase. We employ ab initio MD simulations with the SCAN functional. We study the pressure-induced polymerisation in liquid nitrogen for system sizes up to 288 atoms, in order to reduce finite-size effects. The transition is studied both upon compression and decompression and for the largest system it takes place between 110-115 GPa, which further improves the agreement with experimental data. We also simulate the molecular crystalline ε-phase close to the melting line and analyse its structure. We show that the molecular crystal in this regime is highly disordered, in particular due to pronounced orientational disorder of the molecules. Its short-range order and vibrational density of states are very close to those of the molecular liquid indicating that the system likely represents a high-entropy plastic crystal.

High-pressure phase transformations in ramp compressed SiO2

Michelle Marshall[1], Donghoon Kim[2], Danae Polsin[1], Ian Ocampo[3], J. Ryan Rygg[1], Gilbert Collins[1], Thomas Duffy[3], Raymond Smith[4], Jon Eggert[4]
[1]University of Rochester, Rochester, United States, [2]Carnegie Institution for Science, Washington, United States, [3]Princeton University, Princeton, United States, [4]Lawrence Livermore National Laboratory, Livermore, United States

Outer Planets and Exoplanets 1, July 26, 2023, 10:15–12:15

SiO2 is one of the most widely studied materials at high-energy-density conditions because of its use as a standard in shock experiments and because of its geophysical importance. SiO2 is considered an archetype for the silicates that dominate terrestrial mantles so measuring its structure at the relevant pressures and temperatures is important to understanding rocky exoplanets. In this work, we quasi-isentropically (ramp) compressed SiO2 to ~400 GPa and probed its phase using in situ X-ray diffraction at the Omega laser facility. Both fused silica and novaculite, a microcrystalline quartz, were studied. Funding for this research was provided by the Centre for Matter at Atomic Pressures (CMAP), a National Science Foundation (NSF) Physics Frontiers Centre, under Award PHY2020249.

Correlating Atomic Structure and Macroscopic Properties at High-pressures and Temperatures through a Large Volume Press Program at HPCAT

Rostislav Hrubiak[1], Guoyin Shen[1], Curtis Kenney-Benson[1], Eric Rod[1], Changyong Park[1], Arun Bommannavar[1], Megan Mouser[2], Tyler Eastmond[1], Innocent Ezenwa[1], Maddury Somayazulu[1], Nenad Velisavljevic[3]

[1]X-ray Science Division, Argonne National Laboratory, Lemont, United States, [2]Earth and Planets Laboratory, Carnegie Institution for Science, Washington , United States, [3]Lawrence Livermore National Laboratory, Physics Division, Livermore, United States

Facility Development 2, July 27, 2023, 14:00–16:00

A large volume press at HPCAT allows for multiple experiment types that are not possible with smaller-volume devices like the diamond anvil cell. The program consists of a Paris-Edinburgh (PE) press integrated with a multitude of X-ray , electrical, optical, and ultrasonic techniques for in-situ synthesis and characterisation at high-pressure and high-temperature conditions. The larger sample volume enables in-situ investigations of the relationship between the atomic structure and resulting macroscopic properties at high P-T conditions. The established characterisation techniques include energy-dispersive X-ray diffraction, liquid/amorphous atomic structure factor determination, ultrasound echo, falling sphere viscometry, monochromatic X-ray absorption mapping, phase contrast radiography, and specialty sample cells with electrical probes.

Moreover, the beamline is undergoing a major redesign to coincide with the APS-U upgrade, resulting in even greater capabilities. The upgraded beamline will feature higher resolution X-ray tomography, optimised amorphous structure factor determination, and ultrasound measurement with online data analysis. Thermal transport measurements and electrical resistance/impedance measurements will also be integrated into the beamline, allowing for comprehensive characterisation of samples. A new anvil design will increase the pressure range of the beamline. The energy dispersive detector will be upgraded, and multi-element detector capabilities will be included. These advancements, together with the improved beamline optics, will significantly reduce the exposure time needed for data collection, allowing for faster experiments and higher throughput. The beamline's expanded capabilities and scientific examples will be presented.

Water & amorphous ice: using X-rays to map the phase diagram

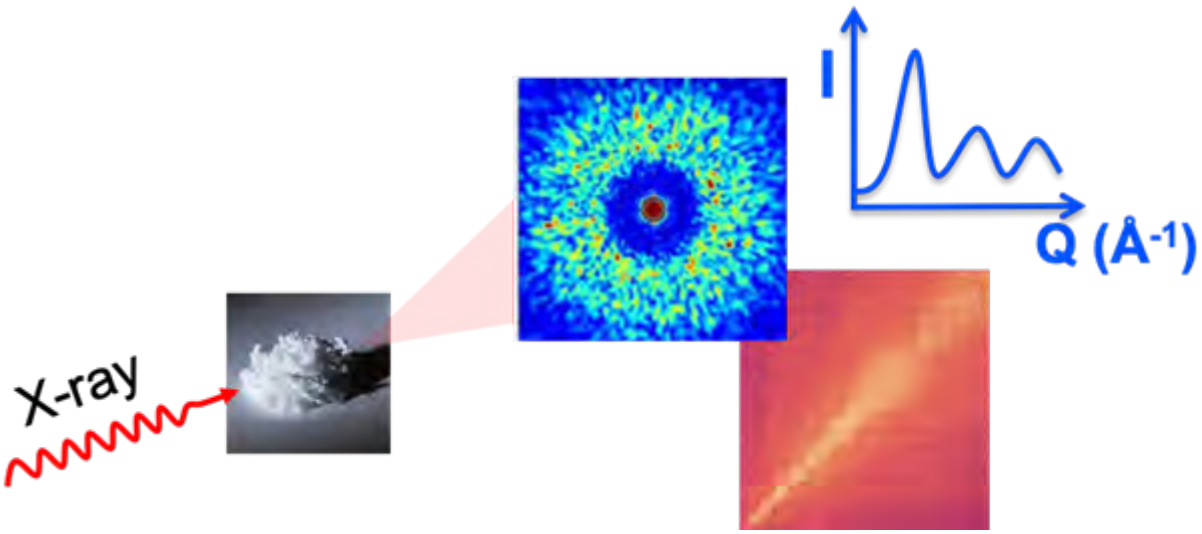
Katrin Amann-Winkel[1,2,3]
[1] Max Planck Institute for Polymer Research, Mainz, Germany, [2]Johannes Gutenberg University Mainz, Mainz, Germany, [3]Stockholm University, Stockholm , Sweden

Ice, Water and Clathrates, July 24, 2023, 10:15–12:15

Water is ubiquitous and the most important liquid for life on earth. Although the water molecule is seemingly simple, various macroscopic properties of water are most anomalous, such as the density maximum at 4 °C or the divergence of the heat capacity upon cooling. The fundamental origin of these anomalies is yet to be fully understood. Computer-simulations suggest the anomalous behaviour of ambient and supercooled water to be explained by a two-state model of water. An important role in this ongoing debate plays the amorphous forms of water [1]. Since the discovery of two distinct amorphous states of ice with different density (high- and low-density amorphous ice, HDA and LDA) it has been discussed whether and how this phenomenon of polyamorphism at high-pressuresis connected to the occurrence of two distinct liquid phases (HDL and LDL) [2].

X-ray scattering experiments on both supercooled water and amorphous ice are of major importance for our understanding of water. In my talk I will give an overview about recent experiments on amorphous ices [3-5]. We studied the glass transition in HDA using X-ray photon correlation spectroscopy (XPCS) at ambient and elevated pressure by using a diamond anvil cell. Further, we applied pump-probe experiments on amorphous ice at X-ray free electron laser facilities. This allowed us to investigate the ultrafast transition between HDL and LDL, and reversely, at elevated temperature and pressure. Our experimental results are consistent with a picture of two different states of water.

[1] K. Amann-Winkel et al., Rev. Mod. Phys. 88, 0110002 (2016)
[2] P. Gallo, et al., Chem. Rev. 116, 7463-7500 (2016)
[3] K.H. Kim, et al., SCIENCE, 370, 6519, 978 (2020)
[4] M. Ladd-Parada, et al., Environ. Sci.: Atmos., 2, 1314 (2022)
[5] K. Amann-Winkel et al., Nat. Comm., 14, 442 (2023)



Crossover from “gas-like” to “liquid-like” molecular diffusion in a simple supercritical fluid

Umbertoluca Ranieri[1,2], Ferdinando Formisano[3,4], Federico Gorelli[5,6], Mario Santoro[5,6], Michael Marek Koza[4], Livia Bove[2,7,8]

[1]CSEC, University of Edinburgh, Edinburgh, United Kingdom, [2]Dipartimento di Fisica, Università di Roma La Sapienza, Roma, Italy, [3]CNR-IOM & INSIDE @ ILL c/o Operative Group in Grenoble (OGG), Grenoble, France, [4]Institut Laue-Langevin, Grenoble, France, [5]Consiglio Nazionale delle Ricerche, Istituto Nazionale di Ottica, CNR-INO, Sesto Fiorentino, Italy, [6]European Laboratory for Nonlinear Spectroscopy, LENS, Sesto Fiorentino, Italy, [7]Laboratory of Quantum Magnetism, Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland, [8]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, UMR CNRS 7590, Paris, France

Other Molecular Systems, July 27, 2023, 10:15–12:15

The long standing – and continuing – interest in the pressure and temperature dependence of the physical properties of supercritical matter has provided us with a broad spectrum of experimental and theoretical data on “simple” supercritical fluids under pressure. This knowledge is important for planetary modelling (for example, for chemical transport at subduction zones) and fundamental physics as well as industrial applications (where supercritical fluids are widely employed in the food, petrochemical, waste, and pharmaceutical industries). However, many open questions remain.

In the last decade, there has been a vivid debate in the literature on whether the supercritical region can be divided into two domains that, although not connected by a first-order singularity, would be reminiscent of the subcritical gas and liquid regions. A “gas-like” to “liquid-like” crossover in the anomalous dispersion of the sound velocity [1,2], observation of a pseudo-boiling phenomenon [3], and a change in density fluctuations correlations [4] have been reported to occur when crossing the so-called Widom line upon compression of supercritical fluid samples. Other studies [5-8] have investigated how the Frenkel line, i.e. the line along which the structural relaxation time equals the shortest period of transverse oscillations of the particles (atoms or molecules) within the system, separates a “gas-like” diffusive behaviour of the supercritical fluid at low pressures from a somehow “solid-like” (rigid) behaviour at high-pressure s.

We recently performed quasi-elastic neutron scattering (QENS) measurements of the molecular diffusion in supercritical fluid methane as a function of pressure along the 200 K isotherm (corresponding to 1.05 times the critical temperature) [9]. The experiments were performed at the IN6-SHARP spectrometer installed at the Institut Laue-Langevin in Grenoble, France. Along the thermodynamic path we followed, we could cross both the Widom and the Frenkel line. We observe a clear crossover in the self-dynamic structure factor of the sample from a gas-like to a liquid-like signal upon compression. Concurrently, a sharp decrease in the pressure dependence of the translational diffusion coefficient takes place. To our knowledge, the present work represents the first to employ the QENS technique to investigate a supercritical fluid sample in the vicinity of its critical point.

[1] G.G. Simeoni et al., Nature Phys. 6, 503–507 (2010)
[2] T. Bryk et al., Phys. Rev. E 90, 042301 (2014)
[3] F. Maxim et al., Nature Comm. 10, 4114 (2019)
[4] E.A. Ploetz and E.A. Smith, J. Phys. Chem. B 123, 6554 (2019)
[5] V.V. Brazhkin et al., Phys. Rev. E 85, 031203 (2012)
[6] D. Bolmatov et al., Nature Comm. 4, 2331 (2013)
[7] C. Prescher et al., Phys. Rev. B 95, 134114 (2017)
[8] J.E. Proctor et al., J. Phys. Chem. Lett. 10, 6584–6589 (2019)
[9] U. Ranieri et al., submitted

Multigrain X-ray Diffraction for the Study of Deformation and Phase Transformation Microstructures at Deep Mantle Pressures and Temperatures

Sébastien Merkel[1], Matthias Krug[2], Estelle Ledoux[1], Jeffrey-Philipp Gay[1], Julien Chantel[1], Sergio Speziale[3], Carmen Sanchez-Valle[2]
[1]Univ Lille, France, Lille, France, [2]University of Münster, Münster, Germany, [3]Deutsches GeoForschungsZentrum GFZ, Potsdam, Germany

Facility Development 2, July 27, 2023, 14:00–16:00

Multigrain X-ray crystallography allows tracking the orientations of several hundreds of grains simultaneously during dynamical processes such as plastic deformation, phase transformation, or simply changes in pressure and temperature. The method is applicable to diamond anvil cell experiments at synchrotron beamlines, both at ambient temperature or high temperature, using either laser or resistive heating techniques.

In the course of the joint ANR-DFG TIMEleSS project, we relied on multigrain X-ray crystallography to track the orientations of minerals undergoing phase transformations and plastic deformation at conditions relevant for the Earth's mantle.

We streamlined the use of multigrain crystallography in diamond anvil cell experiments, for which we wrote a thorough online manual, which is now available to the community at http://multigrain.texture.rocks/ and a set of dedicated python tools, to help with specifics of diamond anvil cell experiments and post-processing of the experimental results, all available at https://github.com/FABLE-3DXRD/TIMEleSS.

We also addressed several transformation and deformation processes relevant to the Earth mantle, such as the coesite-stishovite phase transition and its potential relation to the X-discontinuity at 300 km depth in the Earth mantle [1], synthesis and deformation of wadsleyite, for the mantle transition zone [2], and transformation and deformation in a pyrolitic composition past the 660 km discontinuity [3]. With this work, we demonstrate that the method can be used to obtain relevant microstructural results at the pressures and temperatures of a mantle geotherm, and how they are useful for the interpretation of seismic observables.

In this presentation, I will highlight the main features and capabilities of multigrain X-ray diffraction in the diamond anvil cell and demonstrate how, for instance, one can track the orientations of several hundred grains of 3 different crystal phases studied simultaneously in the diamond anvil cell. I will then show results relevant for a pyrolitic composition in the Earth's lower mantle, how microstrostructures are formed upon synthesis at 660 km depth, how microstrostructures are then affected by further sample plastic deformation, and how pressure affects the plasticity of bridgmanite at lower mantle conditions.

Finally, I will also discuss how the technique offers a range of new opportunities for high-pressure research, well beyond the field of geosciences.

[1] Krug, M., Saki, M., Ledoux, E., Gay, J.P., Chantel, J., Pakhomova, A., Husband, R., Rohrbach, A., Klemme, S., Thomas, C., Merkel, S. & Sanchez-Valle, C. (2022) Geochem. Geophys. Geosyst. 23 doi: 10.1029/2022gc010544
[2] Ledoux, E., Krug, M., Gay, J.P., Chantel, J., Hilairet, N., Bykov, M., Bykova, E., Aprilis, G., Svitlyk, V., Garbarino, G., Guignot, N. Sanchez-Valle, C., Speziale, S. & Merkel, S. (2023) Amer. Mineral. In revision.
[3] Gay, J.P., Ledoux, E., Krug, M., Chantel, J., Pakhomova, A., Liermann, H.-P., Sanchez-Valle C. & Merkel, S. (2023) Earth Planet. Sci. Lett. 604 118015 doi: 10.1016/j.epsl.2023.118015

The study was financed by the bilateral ANR-DFG TIMEleSS project (ANR-17-CE31-0025; TH 1530/18-1; SA 2585/3-1; SP1216/8-1) and the bilateral PROCOPE-PPP program (PHC 40555PC; DAAD 57390184).

A substituted La-based 556 K Tc superhydride superconductor

Stanley Tozer[1], Toni Helm[2], Muhtar Ahtar[6], Konstantin Glazyrin[3], Morgan Oliff[1], Vaughan Williams[1], Yue Meng[8], Ravhi Kumar[6], Gaston Gabarino[7], Markus König[10], Rus Hemley[5], William Coniglio[1], Neal Ashcroft[9], Maddury Somayazulu[8], Audrey Grockowiak[4]

[1]National High Magnetic Field Laboratory, Tallahassee, United States, [2]Dresden High Magnetic Field Laboratory (HLD-EMFL), Dresden, Germany, [3]DESY (Deutsches Elektronen Synchrotron), Hamburg, Germany, [4]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW), Dresden, Germany, [5]Department of Physics, University of Illinois Chicago, Chicago, United States, [6]Department of Chemistry, University of Illinois Chicago, Chicago, United States, [7]European Synchrotron Radiation Facility (ESRF), Grenoble, France, [8]HPCAT, X-ray Science Division, Argonne National Laboratory, Lemont, United States, [9]Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, United States, [10]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Hydrides 2, July 24, 2023, 16:30–18:30

The recent finding of superconductivity at room temperature and above presents scientists and engineers with opportunities to make significant scientific, environmental, and societal advances. These pioneering discoveries built on Onnes' serendipitous 1911 discovery of zero resistance in elemental mercury at 4.2 K followed by discrete jumps in superconducting transition timeline as scientists synthesised more complex systems. Bednorz and Müller pushed the record to 30 K in 1986, publishing in Zeitschrift für Physik B due to what many felt were unsubstantiated claims. Chu, et al. quickly tripled that with the discovery of YBCO with an unfathomable Tc of 93 K. Simple rules and observations guided these discoveries, but in the background was a 1968 prediction by Ashcroft of room temperature superconductivity in atomic metallic hydrogen which required pressures unattainable in the laboratory environment of that day. After years of struggling, experimentalists were presented with an intriguing alternate means to achieve room temperature superconductivity using pressures approaching 200 GPa to drive hydrogen into a metal host at levels far in excess of the valence limit. H3S, proposed by computational theorists in 2015, was verified experimentally within days by Eremets and his colleagues. Four years on, LaH10 , synthesised by Somayazulu and verified by Eremets, et al at 180 GPa advanced to within 30 K of room temperature.

We have synthesised a distorted La-based superhydride that had an initial superconducting transition temperature of 294 K after laser synthesis which, when subjected to thermal cycling, morphed into a higher order system with an onset Tc of 556 K. X-ray data confirms our finding and shows that the superconductor is in close proximity to the Focused Ion Beam (FIBed) Pt electrodes. The X-ray and electrical resistivity data support one another with regard to the pressure measured, the materials present, and the inhomogeneous nature of the synthesis that resulted in a broad multi-phase transition and a non-zero background below Tc. These two features can be shown to be related to the use of ammonia borane (AB) as the hydrogen source and pressure medium as seen in many studies. Much work remains to be done to address a multitude of challenges in the superhydrides such as batch-to-batch variations, inhomogeneous growth, non-hydrostatic pressures, sample size, and a strong Tc(P). A multi-probe approach to validate this discovery and advance our understanding of the underlying physics will be discussed.

[1] A.D. Grockowiak, et al, "Hot Hydride Superconductivity Above 550 K", Frontiers in Electronic Materials 2, (2022). DOI: 10.3389/femat.2022.837651

High-pressure Plastic Phases of water and water-ammonia mixtures

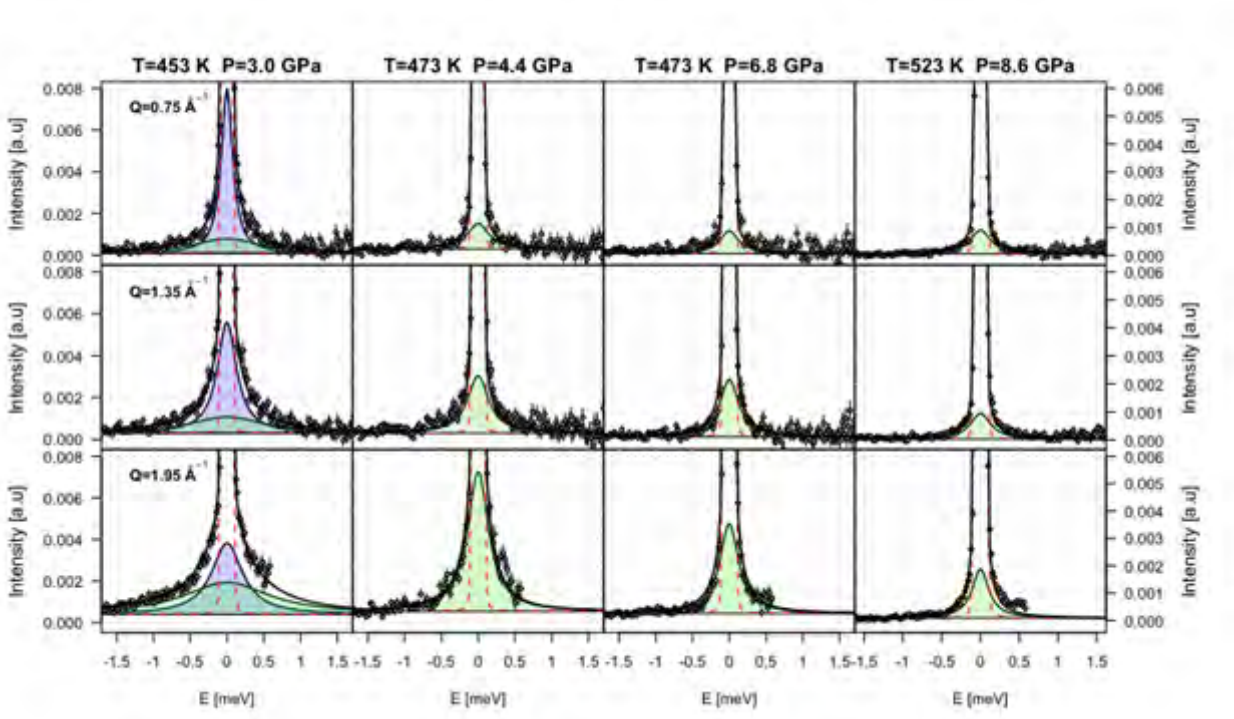
Maria Rescigno[1,3], Umbertoluca Ranieri[4], Stephan Klotz[2], Sandra Ninet[2], Frédéric Datchi[2], Richard Gaal[3], Livia Eleonora Bove[1,2,3]

[1]Sapienza, Rome, RM, Italy, [2]IMPMC, Paris, France, [3]EPFL, Lausanne, Switzerland, [4]University of Edinburgh, Edinburgh, United Kingdom

Molecular Compounds, July 25, 2023, 10:15–12:15

The 'ice giants' Uranus and Neptune, as well as some of their moons and many Neptune-like exoplanets, are mainly composed of mixtures of three molecular ices: water, ammonia and methane. All these molecular crystals show plastic phases. For methane [1] and ammonia [2] these phases are already known experimentally, while for water and ammonia hydrates only numerical simulations exist [3,4]. From the dynamical point of view the plastic phase is an intermediate phase between a liquid and a crystal: molecules are held tightly in an ordered structure but can rotate as in a liquid state. We will present the characterisation of the plastic phases of water [5] and of ammonia monohydrate [6] by high-pressure quasi elastic neutron scattering (HP-QENS) experiments performed at ILL, Grenoble.

[1] W. Press, Journal of Chemical Physics 56, 2597 (1972)
[2] S. Ninet, F. Datchi, and A. M. Saitta, PRL 108, 165702 (2012)
[3] J. L. Aragones and C. Vega, Journal of Chemical Physics 130, 244504 (2009)
[4] V. N. Robinson and A. Hermann, J. Phys.: Condens. Matter 32 184004 (14pp) (2020)
[5] M. Rescigno, U. Ranieri, M. M. Koza, S. Klotz, R. Gaal, J. Ollivier, J. Teixeira, L.E. Bove, submitted (2023).
[6] H. Zhang, F. Datchi, L. Andriambariarijaona, M. Rescigno, L. E. Bove, S. Klotz, S. Ninet, J. Phys. Chem. Lett., 14, 9, 2301–2307 (2023)



Magnetic detection under high-pressuresusing designed silicon vacancy centres in silicon carbide

Mrs Xiaodi Liu[1], Ms Lin Liu[1], Mr Eugene Gregoryanz[2]
[1]Institute of Solid-State Physics, Hefei Institutes of Physical Science, CAS, Hefei, China, [2]Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom

Instrumentation and Techniques 2, July 27, 2023, 10:15–12:15

Pressure-induced magnetic phase transitions are attracting interest as a means to detect superconducting behaviour at high-pressuresin diamond anvil cells, but determining the local magnetic properties of samples is a challenge due to the small volumes of sample chambers. Optically detected magnetic resonance of nitrogen vacancy centres in diamond has recently been used for the in-situ detection of pressure-induced phase transitions. However, owing to their four orientation axes and temperature-dependent zero-field splitting, interpreting these optically detected magnetic resonance spectra remains challenging. Here we study the optical and spin properties of implanted silicon vacancy defects in 4H-silicon carbide that exhibit single-axis and temperature-independent zero-field splitting. Using this technique, we observe the magnetic phase transition of Nd2Fe14B at about 7 GPa and map the critical temperature–pressure phase diagram of the superconductor YBa2Cu3O6.6. These results highlight the potential of silicon vacancy-based quantum sensors for in situ magnetic detection at high-pressure s. Based on this technique, the recently claimed near-ambient superconductivity in N-doped lutetium hydride would be discussed.

Inversion of the temperature dependence of thermal conductivity of hcp iron under high-pressure

Dr. Akira Hasegawa[1], **Dr. Kenji Ohta**[1], Dr. Takashi Yagi[2], Prof. Kei Hirose[3], Dr. Yasuo Ohishi[4]
[1]Tokyo Institute Of Technology, Japan, [2]National Institute of Advanced Industrial Science and Technology, Japan, [3]The University of Tokyo, Japan, [4]SPring-8, Japan Synchrotron Radiation Research Institute, Japan

Secular Evolution of the Earth, July 25, 2023, 10:15–12:15

Investigating how iron changes its thermal transport properties under extreme conditions, such as those found in the Earth’s core, is a major experimental challenge. Over the last decade, the thermal conductivity of the iron-based Earth's core and its thermal evolution have been controversial. One reason for this is the variability in the experimentally-obtained conductivity of iron at high-pressuresand temperatures. Here we present the experimental results of measuring the thermal conductivity of hexagonal-closed pack (hcp) iron over a wide pressure-temperature range up to 176 GPa and 2,900 K using the pulsed light heating thermoreflectance technique in a laser-heated diamond anvil cell. We found that the temperature derivative of the conductivity of hcp iron changes from negative to positive above 74 GPa, making hcp iron highly conductive at the conditions corresponding to the Earth’s core. Iron is the first example of a phenomenon where pressure changes the sign of the temperature derivative of the thermal conductivity of an isostructural metal.

High-pressure Synthesis and Physical Properties of New Functional Materials

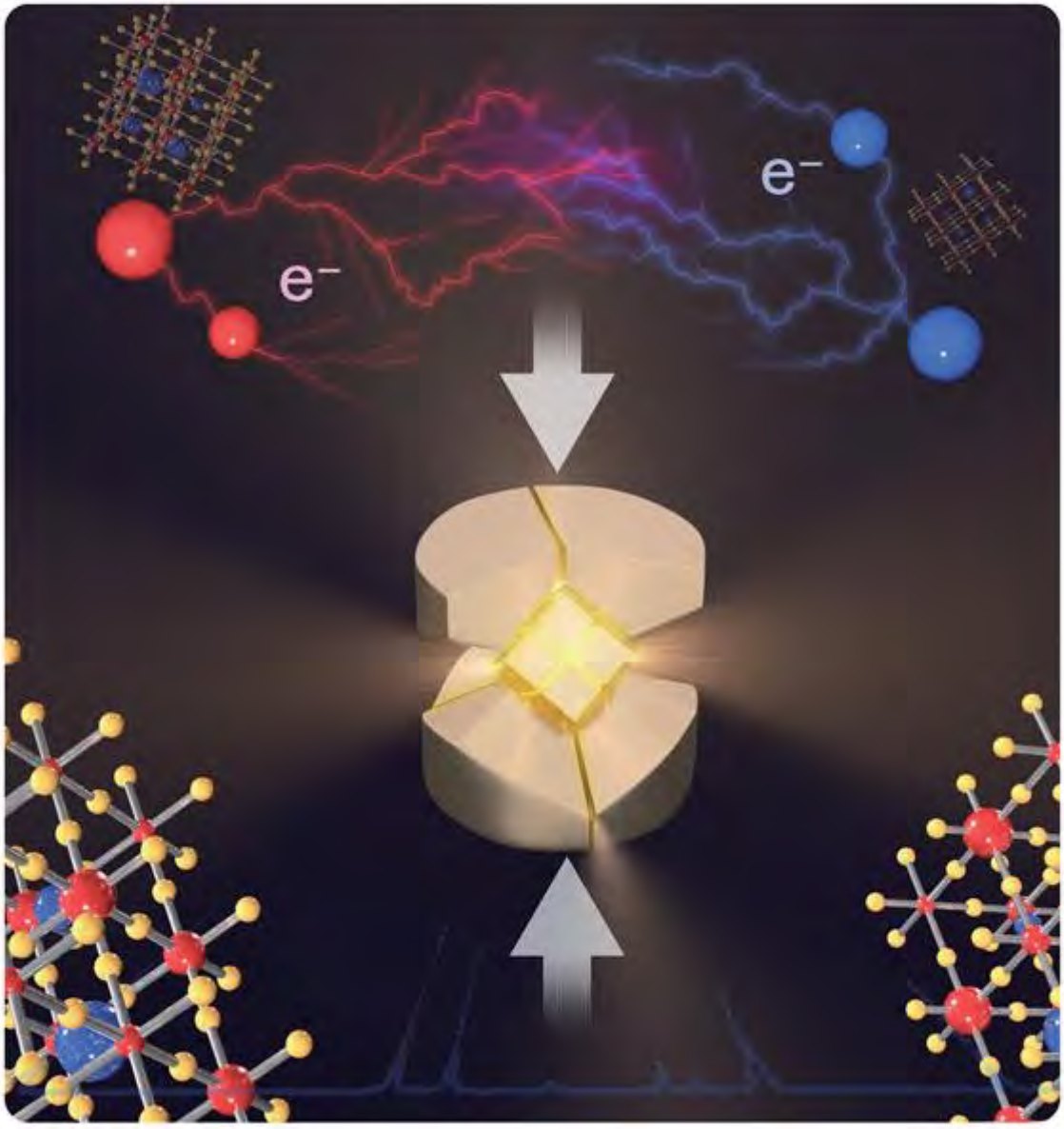
Professor Xiang Li[1]
[1]*Beijing Institute Of Technology, Beijing, China*

Synthesis and Properties of Novel Materials 2, July 26, 2023, 10:15–12:15

A great deal of interest has been focused on new functional materials, because there is a rich variety of intriguing phenomena such as multiferroicity, high-temperature superconductivity and colossal magnetoresistance due to strong correlations among lattice dynamics, charges, spins and orbitals. Pressure as one of the basic thermodynamic parameters influences crystal structures so as to control magnetic and transport properties. We have synthesised a series of new functional materials under high-pressure and studied their physical properties by fully comprehensive measurements, which helps to clarify a few fundamental questions and provide a roadmap for developing new functional materials.

cm CHEMISTRY OF MATERIALS

JANUARY 12, 2021 | VOLUME 33 | NUMBER 1 | pubs.acs.org/cm



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

ID27_II a unique beamline for science under extreme conditions

Mohamed Mezouar[1], Gaston Garbarino[1], Wolfgang Morgenroth[2], Anna Pakhomova[1], Bjorn Wehinger[1], Tomasz Poreba[1], Hermann Muhammad[1]
[1]European Synchrotron Radiation Facility, Grenoble, France, [2]Institut für Geowissenschaften, Universität Potsdam, Potsdam, Germany

Next Gen Synchrotrons, July 25, 2023, 14:00–16:00

We have built a new high-pressure X-ray diffraction, fluorescence and imaging beamline that take full advantage of the outstanding performance of the ESRF extremely brilliant source. The main objective is to perform the most challenging experiments under extreme pressure and temperature conditions that were not feasible before. The new beamline is composed of two optics hutches located in the experimental hall and a new experimental hutch housed on the High-Quality Slab (HQS) of the ESRF-EBS. The main characteristics of the new beamline are:

- 120 meters-long instrument. This is essential for nano-focusing experiments while keeping the maximum space around the pressure cells for bulky sample environments.
- Tunable energy from 15-65 keV in “pink” or monochromatic beam modes. The expected gain in photon flux is two orders of magnitude in monochromatic mode and three orders of magnitude in “pink” beam mode.
- “Pink” beam operation for time-resolved XRD, XRF and XRI down to the microsecond time scale using double-multilayer mirrors (DMM) as primary optics.
- Monochromatic operation for high resolution nano- and micro-XRD using a Si(111) double-crystal monochromator (DCM).
- Variable focal spot size from 0.25x0.3 µm2 to 2x2 µm2 (VxH at FWHM). This is achieved using three sets of KirkPatrick-Baez (KB) mirrors located in the experimental hutch and operating at different X-ray energies and working distances.

The experimental hutch is a thermally stabilised ($\Delta T<0.1$ K) “pink” beam hutch. It holds:

- A nano-positioning system including 3 translations (XYZ) and a rotation for nano-fluorescence and nano-diffraction experiments in diamond anvil cells (DAC).
- A micro-positioning goniometer for low and high temperature diamond anvil cell XRD, XRF and XRI experiments.
- A heavy-duty (load > 100 kg) goniometer for Paris-Edinburgh press (PEP) set-ups and other heavy equipment.

In this presentation, we will present the main features of this new instrument and provide recent research examples.

Static and dynamic high-pressure opportunities at ESRF XAS beamlines BM23 and ID24

Dr Olivier Mathon[1], Dr Jean-Alexis Hernandez, Dr Kirill A. Lomachenko, Dr Angelika D. Rosa, Dr Nicolas Sévelin Radiguet, Dr Raffaella Torchio
[1]ESRF, Grenoble, France

Facility Development 1, July 24, 2023, 16:30–18:30

BM23 and ID24 are two ESRF beamlines dedicated to X-ray Absorption Spectroscopy (XAS). Study of matter under extreme conditions of pressure, temperature and magnetic field is a core activity. Taking advantage of the performances of the newly developed Extremely Brilliant Source of the ESRF (ESRF-EBS), these two beamlines were fully reconstructed and optimised for extreme conditions activities.

BM23 is a multipurpose EXAFS beamline based on a new dipole wiggler source developed for ESRF-EBS. The beamline is designed to perform high quality EXAFS measurements on a large K-range (K > 20 $Å^{-1}$). The beamline is equipped with a µXAS station allowing XAS measurements with a beam of 3x3 $µm^2$ FWHM with 10^9 ph/s. The µXAS station has been refurbished, allowing to accommodate with improved precision and stability heavy sample environment such has DAC cryostat for high-pressure operation down to 4K, resistively-heated DAC setup for operation up to 1300K and Paris-Edinburgh press.

ID24 is a XAS beamline based on an undulator source with two branches operating sequentially. ID24-ED operates in energy dispersive mode using a polychromator whereas ID24-DCM is based on a Double Crystal Monochromator.

ID24-ED is optimised for ultrafast XAS measurements down to the single bunch (100 ps). The accessible X-ray energy ranges from 5 keV to 28 keV. The two target experiments are the study of matter under high pulsed magnetic field (XAS and XMCD under pulsed field up to 30 Tesla, low temperature down to 2K and moderate pressure of few GPa) and the study of matter under laser induced dynamic compression, generated by the High-Power Laser Facility (HPLF). The HPLF laser delivers on ID24-ED, a 75J laser beam at 1053nm with square or profileable temporal shapes between 4 and 15 ns. The laser beam is focused on the sample generating dynamic compression up to several hundreds of GPa and temperatures of several thousands of Kelvin. An online line-VISAR system with two interferometers is available for shock characterisation. A Streaked-Optical Pyrometer (SOP) is planned to be available at the end of 2023.

ID24-DCM is a high brilliance XAS beamline based on a next generation scanning Double Crystal Monochromator (DCM). This instrument gives access to a wide X-ray energy range from 5 to 45 keV and beamline combines a high flux up to 10^{13} ph/s from an undulator source with a highly focused X-ray beam down to 700x700 nm^2 FWHM. The new DCM developed by the ESRF allows to collect XAS spectra in continuous mode in a few second with unprecedented beam position and energy stability. The beamline is equipped with a unique microXAS/microXES setup and a LH-DAC setup. A Pilatus 1M detector is available for complementary XRD measurements. This combination of characteristics is particularly useful to study matter under static HP/HT conditions to probe ultra-high-pressure (above 200 GPa) or diluted systems at conditions relevant to geoscience.

This large range of opportunities of extreme conditions probed by XAS offers applications in the fields of fundamental science, materials science, Earth's and Planetary science and Plasma physics.

Electronic and Dynamical Properties and Polymorphism in the Solid and Liquid Phases of Compressed Sodium

Mr. Yuan Liu[1,2], Prof. Hanyu Liu[1], Prof. John Tse[1,2]
[1]Key Laboratory of Material Simulation Methods & Software of Ministry of Education, Jilin University, Changchun, China, [2]University of Saskatchewan, Saskatoon, Canada

Computational Studies of Elements, July 26, 2023, 10:15–12:15

Elemental alkali metals exhibit remarkable structural transformations and anomalous melting behaviour upon compression. To unravel the factors for the unusual phenomena, we undertook a comprehensive theoretical study to characterise the electronic and structural properties of the solid and liquid phases from 0 to 180 GPa. Several new techniques were employed in the analysis. The screened ion potentials for different phases were evaluated from structure factors computed from first-principles molecular dynamics (MD) simulations. The examination of the intrinsic structures characterises the structures of the liquids. Structural stabilities of the solids at high temperatures were investigated from phonon dispersions, including higher-order anharmonic force constants, from the projection of the MD trajectories. Electron topological analysis of critical points reveals interactions between electrides in the interstitials of the solid phase help to stabilise the crystal structure and prevent close contact between the ions. This leads to the observed unusual melting behaviour between 50-160 GPa, where the liquid has a higher density than the solid. The successive structural transformations from FCC – cI16 – oP8 – tI19 are driven by softening of shear vibrations and the progressive formation of layered structures. Near melting, the atoms in the system become very mobile and exhibit concerted collective hopping motions. In tI19 with the guest-host structure, vibrations of the atoms in the channel are correlated but unlike the 1-D chain as suggested in Rb-IV.

Pressure induced phase transition, crystallisation, and negative linear compressibility in crystalline and non-crystalline selenium

Dr. Lisa Luhongwang Liu[1,3], Prof. Arthur Haozhe Liu[2]
[1]SHARPS, Shanghai, China, [2]HPSTAR, Beijing, China, [3]UIUC, Urbana, United States

Static Studies of Elements 2, July 26, 2023, 16:30–18:30

The behaviour of crystalline and non-crystalline materials under high-pressure extreme conditions attracted great deal of interest. Unusual behaviour, such as various types of negative linear compressibility (NLC) were reported but not fully understood. NLC is a rare phenomenon where a crystal expands along one direction under hydrostatic compression. In this presentation, both crystalline and non-crystalline selenium samples were in situ studied in diamond anvil cell (DAC) under high-pressure using synchrotron X-ray diffraction. Two types of NLC mechanism were found at various pressure regions, i. e. at around 10 GPa, and around 120 GPa, respectively, in this same elemental sample [1, 2]. By adjusting the preheating history of non-crystalline Se samples [3], we could capture early crystallisation process and reveal the physics behind the controversy previous results on this system.

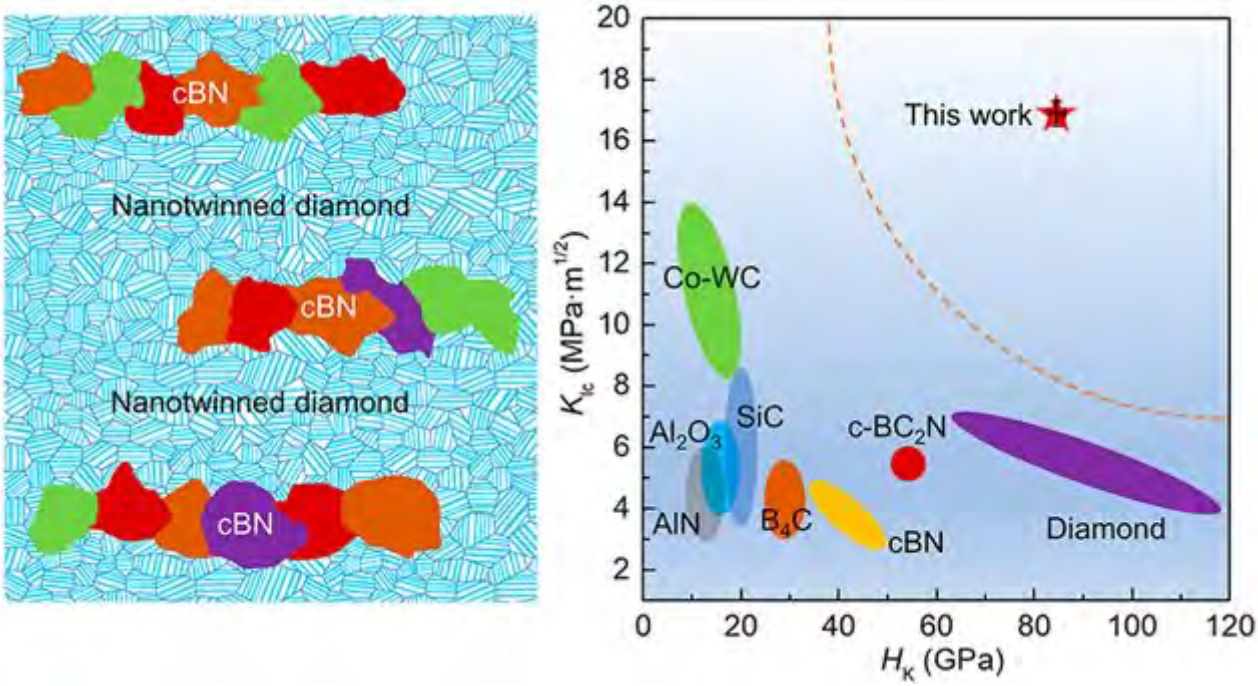
[1] Shuhua Yuan, Luhong Wang, Sheng-cai Zhu, Fuyang Liu, Dongzhou Zhang, Vitali B. Prakapenka, Sergey Tkachev, Haozhe Liu, Negative linear compressibility in Se at ultra-high-pressure above 120 GPa, IUCrJ, 9, 253, 2022.
[2] Kamil F. Dziubek, Negative linear compressibility at extreme pressure, IUCrJ, 9, 165, 2022.
[3] Shuhua Yuan, Luhong Wang, Fuyang Liu, Jay Bass, Yingzhe Li, Paul A. Ginsberg, Dongzhou Zhang, Vitali B. Prakapenka, Sergey Tkachev, Haozhe Liu, Early crystallisation of amorphous selenium under high-pressure studied by synchrotron XRD method, Journal of Physics: Condensed Matter, 10.1088/1361-648X/ acc8b0, 2023.

Heterogeneous Diamond-cBN Composites with Superb Toughness and Hardness

Prof. Bo Xu[1]
[1]Yanshan University, Qinhuangdao, China

Ceramics and Composites, July 24, 2023, 14:00–16:00

The traditional hardness–toughness trade-off poses a substantial challenge for the development of superhard materials. Due to strong covalent bonds and intrinsic brittleness, the full advantage of microstructure engineering for enhanced mechanical properties requires further exploration in superhard materials. Here heterogeneous diamond–cBN composites were synthesised from a carefully prepared precursor (hBN microflakes uniformly wrapped by onion carbon nanoparticles) through phase transitions under high-pressure and high temperature. The synthesised composites inherit the architecture of the precursors: cBN regions with an anisotropic profile that spans several micrometers laterally and several hundred nanometers in thickness are embedded in a nanograined diamond matrix with high-density nanotwins. A significantly high fracture toughness of 16.9 ± 0.8 MPa m1/2 is achieved, far beyond those of single-crystal diamond and cBN, without sacrificing hardness. A detailed TEM analysis revealed multiple toughening mechanisms closely related to the microstructure. This work sheds light on microstructure engineering in superhard materials for excellent mechanical properties.



High temperature conventional superconductivity

Dr Mikhail Eremets[1]
[1]*Max Planck Institute for Chemitry, Mainz, Germany*

Hydrides 4, July 26, 2023, 14:00–16:15

Superconductivity is a fascinating phenomenon. Although superconductivity was discovered in mercury in 1911, the theory, which explains its nature, was proposed only almost half a century later by J. Bardeen, L. N. Cooper and J. P. Schrieffer. The key ideas are the pairing of electrons and their Bose condensation. The theory does not limit in principle the critical temperature of superconductivity, allowing the existence of superconductors at room temperature and even higher. However, the lack of predictability in the BCS theory led to the fact that conventional superconductivity remained a low-temperature phenomenon for many decades. Only in 2015, the great potential of BCS theory was confirmed with the discovery of superconductivity at 203 K in hydrogen sulfide H3S under high-pressuresof about 150 GPa [1]. Shortly thereafter, superconductivity was found at nearly room temperatures of 250-260 K in LaH10 [2, 3] and 243 K in YH9 [4], also at high-pressure s. These materials with a high content of hydrogen, so-called “superhydrides”, can be considered as a close realisation of superconducting metallic hydrogen. The conventional BCS superconductivity in superhydrides has been well established by proving zero resistance, screening of magnetic field, trapped flux, the existence of persistence superconducting currents, isotope effect, IR reflection, X-ray diffraction studies of the structure, and the excellent agreement with the theory. In the present talk, I will emphasise our recent results on magnetic susceptibility and electronic transport spectroscopy measurements of hydrogen-rich superconductors. I will discuss in detail the further possible increase of the critical temperature of superconductivity to room temperature and higher at high-pressures and demonstrate new promising phases of hydrides occurring at extremely high-pressures of 400 GPa. Particular attention will be paid to the current progress in the field of high-temperature superconductivity at atmospheric and near-atmospheric pressures.

[1] Drozdov, A.P., et al., Conventional superconductivity at 203 K at high-pressures. Nature 2015. 525: p. 73.
[2] Drozdov, A.P., et al., Superconductivity at 250 K in lanthanum hydride under high-pressures Nature, 2019. 569: p. 528.
[3] Somayazulu, M., et al., Evidence for Superconductivity above 260 K in Lanthanum Superhydride at Megabar Pressures. Phys. Rev. Lett., 2019. 122: p. 027001.
[4] Kong, P.P., et al., Superconductivity up to 243 K in the yttrium-hydrogen system under high-pressure. Nat. Commun., 2021. 12: p. 5075.
[5] Minkov, V.S., et al., Magnetic field screening in hydrogen-rich high-temperature superconductors. Nature Communications, 2022. 13: p. 3194.

Universal diamond edge Raman scale to 0.5 terapascal: The implication to metallisation of hydrogen.

Dr Mikhail Eremets[1], Dr Vasily Minkov[1], Dr Panpan Kong[1], Dr Alexander Drozdov[1], DR Stella . Chariton[1], Dr Vitali Prakapenka[1]
[1]*Max Planck Institute for Chemitry, Mainz, Germany*

The recent progress in generating static pressures up to terapascal values opens opportunities for studying novel materials with unusual properties, such as metallisation of hydrogen1,2 and high temperature superconductivity6. However, an evaluation of pressure above ~0.3 terapascal is a challenge. We report a universal high-pressure scale up to ~0.5 terapascal, which is based on the shift of the Raman edge of stressed diamond anvils correlated with the equation of state of Au and does not require an additional pressure sensor. According to the new scale, the pressure values are substantially lower by 20% at ~0.5 terapascal compared to the extrapolation of the existing scales. We compared the available data of H2 at the highest static pressures. We showed that the onset of the proposed metallisation of molecular hydrogen reported by different groups is consistent when corrected with the new scale and can be compared with various theoretical predictions.

1 Eremets, M. I., Drozdov, A. P., Kong, P. P. & Wang, H. Semimetallic molecular hydrogen at pressure above 350 GPa. Nat. Phys. 15, 1246 (2019).
2 Loubeyre, P., Occelli, F. & Dumas, P. Synchrotron infrared spectroscopic evidence of the probable transition to metal hydrogen. Nature 577, 631 (2020).
3 Eremets, M. I. Megabar high-pressure cells for Raman measurements. J. Raman Spectroscopy 34, 515–518 (2003).
4 Akahama, Y. & Kawamura, H. Pressure calibration of diamond anvil Raman gauge to 310 GPa. J. Appl. Phys. 100, 043516 (2006).
5 M. I. Eremets, Troyan, I. A. & Drozdov, A. P. Low temperature phase diagram of hydrogen at pressures up to 380 GPa. A possible metallic phase at 360 GPa and 200 K. arXiv:1601.04479 (2016).
6 Drozdov, A. P., Eremets, M. I., Troyan, I. A., Ksenofontov, V. & Shylin, S. I. Conventional superconductivity at 203 K at high-pressures. Nature 525, 73 (2015).
7 Fratanduono, D. E. et al. Establishing gold and platinum standards to 1 terapascal using shockless compression. Science 372, 1063–1068 (2021).

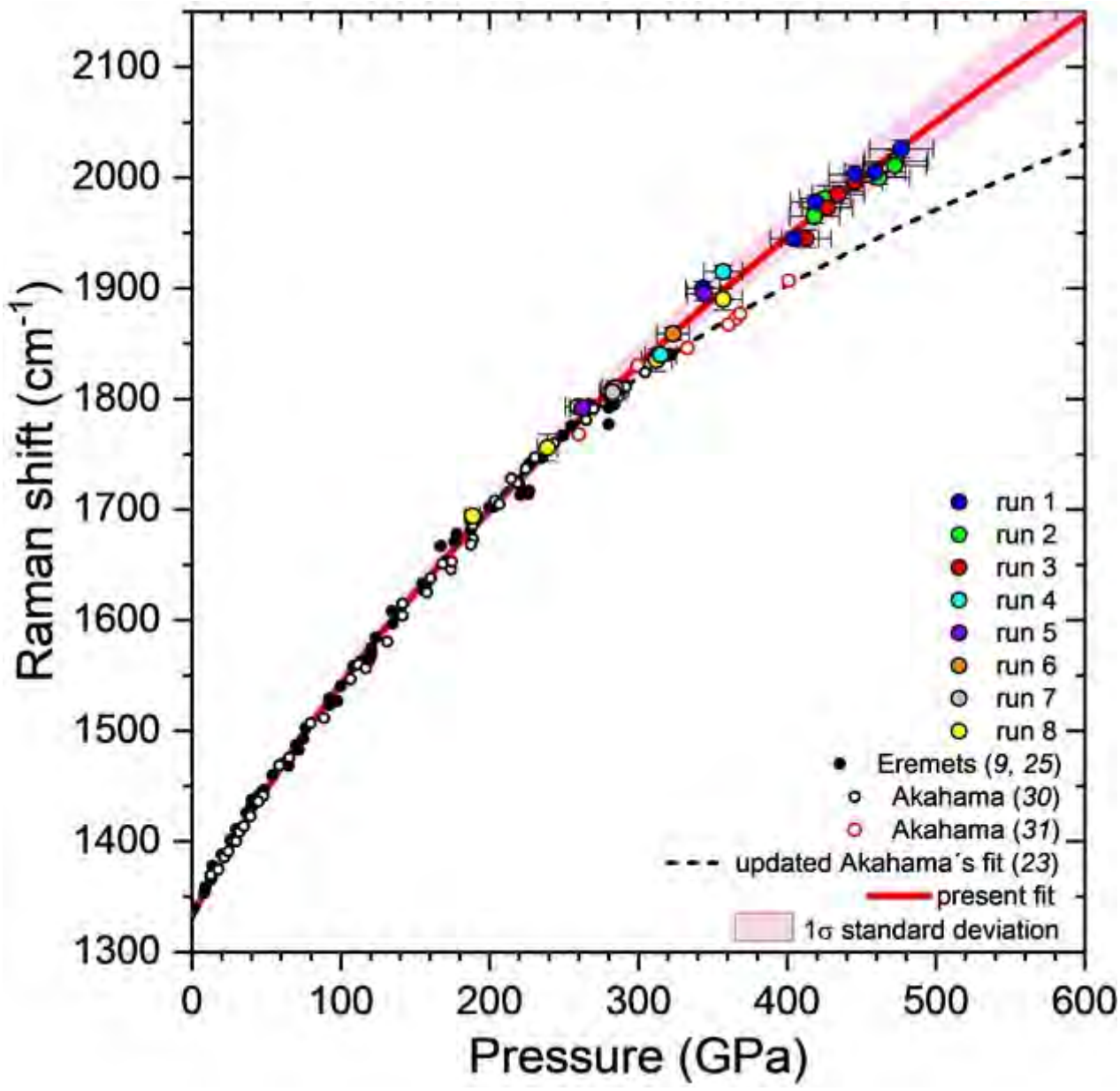


Figure 1. The universal diamond edge Raman scale. Large colourful circles correspond to the pressure dependence of the high-wavenumber Raman edge of the stressed diamond anvil measured in runs of the present study. The solid red curve fits the combined experimental data set, including the previous data measured below □300 GPa3-5. The black dotted curve is the updated diamond edge Raman scale of Akahama7 for the high-pressure range above 200 GPa.

High-precision room-temperature isotherm of Pt to over 400 GPa from ramp-compression experiments at the Z machine

Jean-Paul Davis[1], Justin Brown[1]
[1]*Sandia National Laboratories*, Albuquerque, United States*

Equation of Satate 1, July 26, 2023, 14:00–16:00

Experimental techniques for ramped dynamic compression have begun to fulfil their promise of precise absolute measurements of solid-phase compressibility to multi-megabar pressures, where isothermal diamond-anvil cell (DAC) techniques have limited pressure accuracy due to calibration standards that rely on theoretical equations of state to reduce shock data. One commonly used DAC standard is platinum (Pt), due to its phase stability, chemical inertness, and high X-ray scattering power. Detailed analysis of eleven measurements from experiments on Pt at the Z machine, with great care taken to quantify the propagation of uncertainties, has resulted in a new room-temperature isotherm Pt pressure scale to over 400 GPa with 1-sigma uncertainty of order 1% in pressure.

* Sandia National Labs is managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a subsidiary of Honeywell International, Inc., for the U.S. DOE NNSA under contract DE-NA0003525.

Applying methods of high-pressure crystallography in studies of high-pressure chemistry of metal borides

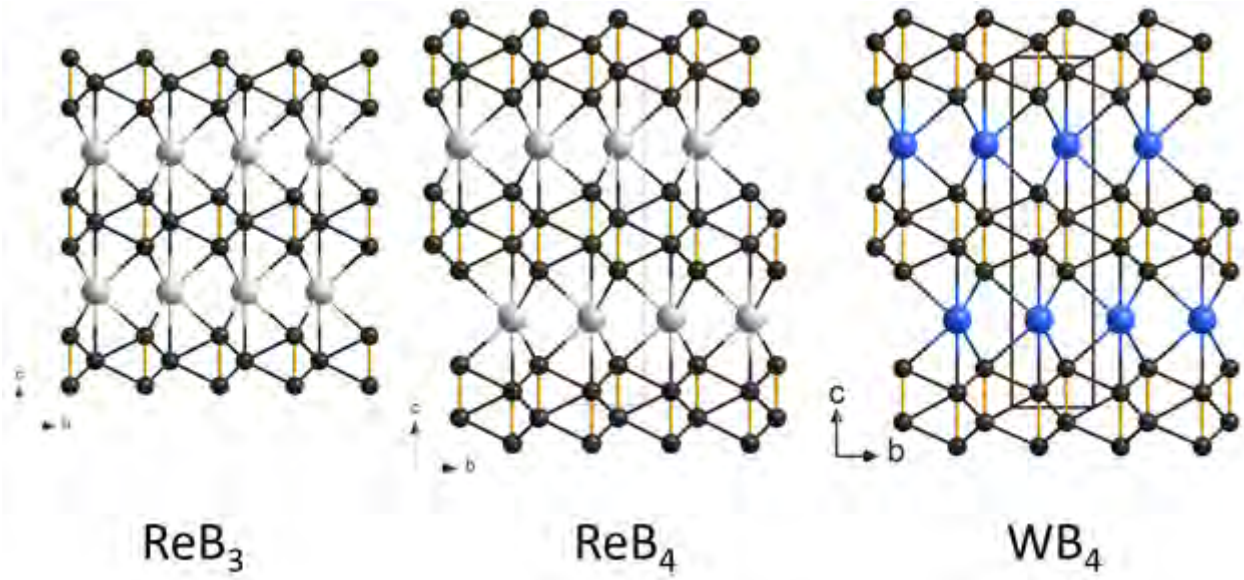
Dr. Elena Bykova[1,2], Dr. Erik Johansson[3], Dr. Maxim Bykov[4], Dr. Stella Chariton[5], Dr. Hongzhan Fei[2], Dr. Sergey V. Ovsyannikov[2], Ms. Alena Aslandukova[2], Dr. Stefan Gabel[6], Dr. Hendrik Holz[6], Dr. Benoit Merle[6], Dr. Björn Alling[3], Prof. Igor A. Abrikosov[3], Dr. Jesse S. Smith[7], Dr. Vitali B. Prakapenka[5], Prof. Tomoo Katsura[2], Prof. Natalia Dubrovinskaia[8], Dr. Alexander F. Goncharov[9], Prof. Leonid Dubrovinsky[2]

[1]FB11, Goethe-Universität Frankfurt, Frankfurt am Main, Germany, [2]Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, Germany, [3]Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden, [4]Institute of Inorganic Chemistry, University of Cologne, Cologne, Germany, [5]Centre for Advanced Radiation Sources, University of Chicago, Chicago, United States, [6]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany, [7]HPCAT, X-ray Science Division, Argonne National Laboratory, Argonne, United States, [8]Laboratory of Crystallography, University of Bayreuth, Bayreuth, Germany, [9]Earth and Planets Laboratory, Carnegie Institution for Science, Washington DC, United States

Nitrides, Borides and Carbides 2, July 25, 2023, 14:00–16:00

The materials with high hardness and low compressibility traditionally attract a great interest for industry as cutting and abrasive tools and components of protective coatings. A common approach to design such materials is to consider compounds that combine metals with high valence electron density and light elements (such as B, C, N) that form strong covalent bonds. Boron-rich transition metal borides with metal boron ratio ≥ 2 are often proposed as potential candidates for superconductive, hard and incompressible materials [1]. For example, hardness of rhenium diboride, ReB2, and tungsten tetraboride (WB4 or its derivatives WB4-x, WB4+x) according to some estimates [2,3] could exceed 40 GPa, that brings them to a class of superhard materials. Rhenium borides with boron content higher than in ReB2 have never been obtained experimentally, but theoretical studies suggest them to have similar mechanical properties with ReB2. Crystal structure of the stoichiometric WB4 phase still remains debatable to date. Applying extreme conditions, such as high-pressuresand high temperatures and/or huge temperature gradients, opens novel routes to metastable and kinetically hindered compounds. Here we have applied methods of single-crystal X-ray diffraction in laser-heating diamond anvil cells (DACs) in order to synthesise novel boron-rich borides of rhenium and tungsten, namely ReB3, ReB4 and stoichiometric WB4; characterise their crystal structure and compression behavior. We discuss their structural, mechanical and electronic properties derived from theoretical and experimental methods and compare them with the literature data.

[1] Akopov, G., Yeung, M.T. & Kaner, R.B. (2017). Adv. Mater. 29, 1604506.
[2] Chung, H.-Y. Y., Weinberger, M. B., Levine, J. B., Kavner, A., Yang, J.-M. M., Tolbert, S. H. & Kaner, R. B. (2007). Science. 316, 436–439.
[3] Gu, Q., Krauss, G. G. & Steurer, W. (2008). Adv. Mater. 20, 3620–3626



ReB_3 ReB_4 WB_4

Double Double to Double Perovskite Transformations in Quaternary Manganese Oxides

Kunlang Ji[1], Yao Yuan[1], Gessica T. Moyo[1], Clemens Ritter[2], J. Paul Attfield[1]
[1]University of Edinburgh, Edinburgh, United Kingdom, [2]Institut Laue-Langevin, GRENOBLE, France

Perovskites, July 27, 2023, 10:15–12:15

Perovskites ABO_3 are of great interest due to their large variety of electronic and magnetic properties. Their compositions can be modified to induce different cation orderings giving double perovskites $AA'B_2O_6$ or $A_2BB'O_6$, and even more complex double double perovskites ($AA'BB'O_6$) [1]. High-pressure methods are important for synthesising new materials exploring changes of structures and properties. Recently, by using high-pressure and high-temperature (HPHT) techniques, we reported a new type of double double perovskite derivatives (DDPv) where columnar ordering at A-site and rock-salt ordering at B site are combined [2].

Recently synthesised new Ca-based DDPv by our group members and one of the new rare earth-based series DDPv, $RMnMnTaO_6$ will be reviewed here. Large R cations in $RMnMnTaO_6$ (R = La-Sm) result in a DDPv structure with space group $P4_2/n$; whereas a disordered A-site DPv structure has been observed for the smaller R =Eu-Lu, with space group $P2_1/n$. By increasing the temperature, a structural transition from DDPv to DPv was observed for the very first time, confirming the structural phase boundary for the $RMnMnTaO_6$. [4]

Magnetic measurements show a ferrimagnetic ordering for the DDPv (R = La, Nd, Sm) and a ferromagnetic ordering for the DPv (R = Sm, Eu, Gd, Y, Lu). Two magnetic transitions with spin reorientation has been found for the DDPv Nd-compound.

The thermal transformation from (Fig. 1) of $AA'BB'O_6$ (first observed in $SmMnMnTaO_6$) double double perovskites, where both A and B sites have 1:1 cation order, to $(A_{0.5}A'_{0.5})_2BB'O_6$ double perovskites with fully disordered A/A' cations can be achieved in the new synthesised DDPv CaMnMnW06 as well [5]. This leads to a dramatic switch of magnetic properties from ferrimagnetic order in DDPv $CaMnMnWO_6$ to spin glass behaviour in the highly frustrated double perovskite polymorph. Comparison of double double and double perovskite polymorphs of other materials will enable effects of cation order and disorder on other properties such as ferroelectricity, conductivity and magnetoresistance to be explored.

[1] King, G., Woodward, P. M. (2010). J. Mater. Chem. 20, 5785.
[2] Solana-Madruga, E., Arévalo-López, Á. M., Dos Santos-García, A. J., Urones-Garrote, E., Ávila-Brande, D., Sáez-Puche, R. & Attfield, J. P. (2016). Angew. Chem. Int. Ed. 55, 9340.
[3] McNally, G. M., Arévalo-López, Á. M., Kearins, P., Orlandi, F., Manuel, P., & Attfield, J. P. (2017). Chem. Mater. 29, 8870.
[4] Ji, K., Yuan, Y., Moyo, G. T., Ritter, C. & Attfield, J. P. (2022). J. Solid State Chem. 313, 123329.
[5] Ji, K., Alharbi, K. N., Solana-Madruga, E., Moyo, G. T., Ritter, C., & Attfield, J. P. (2021). Angew. Chem. Int. Ed. 60, 22248.

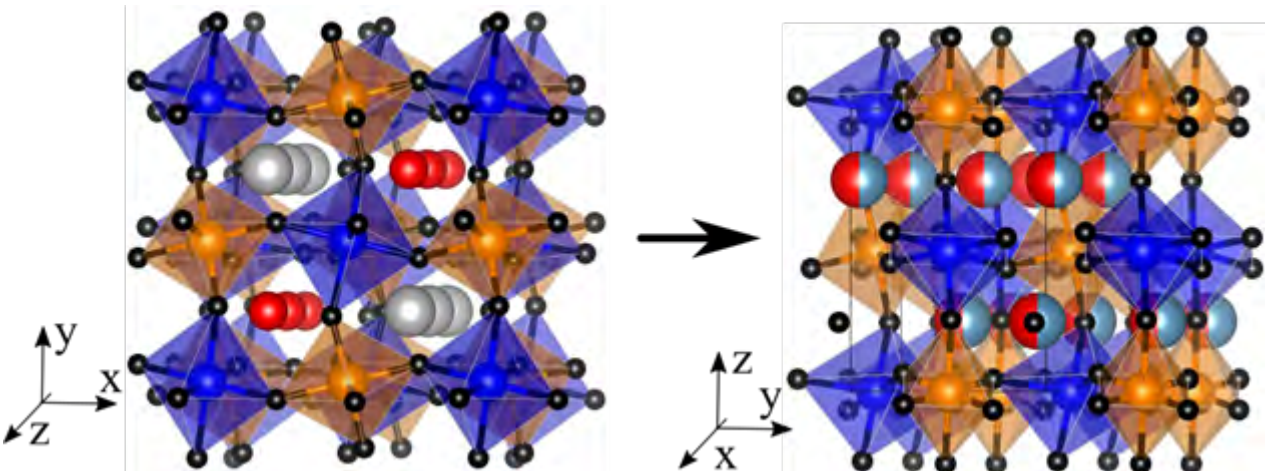


Fig. 1 Thermal transformation under pressure of AA'BB'O_6 to $(A_{0.5}A'_{0.5})_2$BB'O_6 DPv with complete A-site disorder.

Threshold distance of topochemical polymerisation

Kuo Li[1], Haiyan Zheng[1]
[1]*Centre for High-pressure Science and Technology Advanced Research, Beijing, China*

Chemical Bonding 2, July 24, 2023, 16:30–18:30

High-pressure is a robust force to drive unsaturated molecules to polymerise via topochemical reactions, and plenty of novel materials have been synthesised. By multiple crystallographic investigations including in situ high-pressure neutron diffraction and X-ray diffraction and theoretical calculations, we concluded the alkynes have an experiential threshold distance in the pressure-induced polymerisation, around 3.0 Å, and the aromatics probably have a similar threshold around 2.8 Å. To understand the threshold, we calculated the phonon spectrum of acetylene, and quantified the thermal displacement of carbon atoms at room temperature. We found that starting from the experiential critical structure the thermal vibration can push the carbon atoms to approach each other and overcome the energy barrier to polymerise. The experiential threshold distance is therefore related to the thermal vibrations and the transition state quantitatively, and other topochemical reaction can be understood following the same strategy.

Pressure driving novel superconductivity in chalcogenides

Kai Zhang, Limin Yan, **Wenge Yang**[1]
[1] *Centre for High-pressure Science and Technology Advanced Research (HPSTAR), Shanghai, 201203, P. R. China*

Novel Superconductors 2, July 27, 2023, 14:00–16:00

High-pressure has been utilised to compress the distance between atoms and enhance the density of materials. In return, the local and long-range ordering can be largely tuned, which leads emergent of novel transport properties. Here we focus on two unusually superconducting phenomena driven by density in chalcogenides. The ultrastable chalcogenide glass Sb2Se3 was subjected to hydrostatic pressure up to 80Gpa with monitoring of structural evolution by synchrotron X-ray diffraction and electronic transport properties under low temperature, we observed the emergent of superconductivity when the Sb2Se3 undergoes a low density amorphous (LDA) to high density amorphous (HDA) transition at 24 GPa. The superconducting critical temperature is enhanced when pressure induced crystallisation at 51 GPa. HAD phase, featured by metavalent bonding, plays a pivotal role in the delocalisation of electrons and the occurrence of superconductivity in the amorphous states [1]. Transition metal dichalcogenide (TMD) 4Hb-TaSe2 has two different layer configurations for alternating stacking 1T-TaSe2 and 1H-TaSe2. At ambient pressure, only the H-layer shows the superconductivity consistent with the 1T- and 2H-TaSe2 structure. Upon compression, surprisingly, the superconductivity competes with its intra-layered and adjacent-layer charge density wave (CDW)order, which results in substantially and continually boosted superconductivity. Upon total suppression of CDW, the superconductivity in the individual layer's responses differently to the charge transfer, and novel dual-layer superconductivity emerges when both CDW orders collapse. XRD experiments and DFT calculations show a quasi-2D to quasi-3D structure transition with enhanced charge transfer between T-layer and H-layer. The special competing relationship and dual-layer superconductivity revealed from the TaSe2 TMD for the first time provides crucial guidance for the application of devices based on Van Der Waals Heterogeneous structure and offer a new direction to deepen our understanding of this interesting class of TMDs. [2]

[1] Kai Zhang, Ming Xu, Matthias Wuttig, and Wenge Yang, Phys. Rev. Lett. 127, 127002 (2021)
[2] Limin Yan, Chi Ding, Jian Sun, Xin Wang and Wenge Yang, Nano Lett. 23, 2121 (2023).

Systematic analysis of relative compressibility of materials under compression

Dr. Christine Wu[1], Dave Young[1], Per Soderlind[1], Carrie Prisbrey[1], Wentinn Liao[2], Phil Sterne[1], Philip Myint[1], Zoe Long[1]

[1]Lawrence Livermore National Laboratory, Livermore , United States, [2]Univesity of California, Berkeley, United States

Compressibility of a material is a key physics requirement for the development of accurate equations of state. Over the last few decades, three techniques have contributed greatly to our understanding of how materials respond under compression: (1) static high-pressure techniques like diamond-anvil-cell (DAC), which measure the compressibility of a material relative to that of a pressure standard using X-ray diffraction; (2) dynamic ramp compression designed to mimic adiabats with recorded wave profiles, from which compressibility is inferred; and (3) direct prediction by ab initio electronic structure theory. In this work we present our examination of the consistency between results obtained from these three different techniques, with a focus on metals. In addition, we will report on our study of limiting behaviour under extreme compression using full potential DFT calculations within the framework of an atom-in-jellium model.

This work was carried out under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Tracking microstructures across phase transition in subducted basalt to illuminate the origin of seismic heterogeneities in the Earth's mid-mantle

Carmen Sanchez-valle[1], Matthias Krug[1], Estelle Ledoux[2], Jeff Gay[2], Julien Chantel[2], Sergio Speziale[3], Sebastien Merkel[2]

[1]Universität Münster, Münster, Germany, [2]Univ. Lille, Lille, France, [3]Deutsches GeoForschungsZentrum GFZ, Potsdam, Germany

Mantles of Terrestrial Planets, July 27, 2023, 14:00–16:00

Microstructures (i.e. distribution of phases, grain sizes and orientations, etc) induced by phase transitions and deformation in mantle minerals have important implications for the mechanical properties and thermal evolution of planetary mantles. Microstructures also affect the propagation of seismic waves (wave speed and anisotropy), which can be used to infer temperature and/or compositional heterogeneities in the Earth's interior. Here we present investigations of the microstructures developed in basaltic crust subducted into the lower mantle to elucidate the origin of seismic anomalies consistently reported at mid-mantle depths (950–1800 km depth) in the vicinity of subduction zones. We employed a combination of multigrain crystallography (MGC) and radial X-ray diffraction in diamond anvil cells to track phase transitions and textures to lower mantle pressures, 92 GPa (ca. 2700 km depth) along warm/hot slab geotherm conditions. First series of experiments were conducted in SiO2 stishovite, a major component of subducted basaltic crust, and demonstrate the effect of the starting material and /or pressure-temperature paths in the resulting textures. MGC analysis in multiphase basaltic assemblages successfully indexed grain-sizes and orientations simultaneously in hundreds of individual grains in all equilibrium phases. A primary result from the studies on multicomponent systems is the distinct microstructural behaviour of phases in basaltic crust, including SiO2 polymorphs, compared to the single-phase results, which reflect the effect of coexisting phases with different mechanical properties. Our experimental microstructures, combined with visco-plastic self-consistent modelling, allow identifying the deformation mechanisms of basaltic crust phases in the mid-mantle region. Further, we evaluate the effect of microstructures on the shear wave velocities and shear anisotropy of basaltic assemblages and constrain their seismic signature in the mid-mantle. Ultimately, we will discuss the implications for the interpretation of seismic anomalies in terms of geochemical heterogeneities in the mid-mantle region.

Converging to atomic pressures

D. Bishel, D. Polsin, M. Marshall, E. Smith, T.A. Suer, D. Chin, A. LaPierre, M. Ginnane, M. Signor, M. Huff, X. Gong, J.R. Rygg, **G.W. Collins**
[1]*University Of Rochester, Rochester, United States*

Equation of Satate 1, July 26, 2023, 14:00–16:00

How does matter behave at pressures to and beyond atomic pressures, ~30 TPa? Several experiments and theoretical works today are exploring matter at chemical pressures (incipient high energy density pressures ~100 GPa), revealing a rich new chemical landscape at such conditions. Scientists are however just beginning to explore the nature of matter near atomic pressures, conditions that alter the nature of atoms themselves. We will describe recent experimental techniques exploring this atomic pressure regime. Recent melt data to multi-TPa conditions reveal a crossover in melting temperatures between dielectric systems, which have high melting temperatures at ambient conditions (i.e. diamond, MgO) and metals (i.e. Fe), which have a comparatively lower melting temperature at ambient conditions. These results have impacted our understanding of the structure and evolution for a variety of compact astrophysical objects. We also show how electron screening, correlation and ionisation modify atomic orbitals and influence the resulting structural and thermodynamic behaviour of matter to 100's TPa conditions.

Distinct High-Pressure Responses of Halide Perovskites from Bulk to Low Dimension

Tingting Yin[1]
[1]*Nanyang Technology University, Singapore, Singapore*

Perovskites, July 27, 2023, 10:15–12:15

Hybrid organic-inorganic perovskites (HOIPs) are low-cost and highly efficient optoelectronic and photovoltaic materials for applications in solar cells, light emitting diodes (LEDs), and so on, which is correlated with their intrinsic structures. Now the hybrid perovskite families include three-dimensional (3D) (CH3NH3PbBr3), two-dimensional (2D) ((C4H9NH3)2(CH3NH3)n-1PbnI3n+1) and nanostructured ((CH3NH3PbBr3 nanoparticles) materials. Herein, well understanding the relationship between the crystal structures and the related functional properties of HOIP materials is essential to the application point of view. High-pressure up to gigapascal, offers a comprehensive way to study the structure-property correlation of solid materials in the atomic level, where both crystal structures and electronic properties are changed dramatically.

In this presentation, high-pressure induced dramatically inorganic and organic part changes in 2D HOIPs are comprehensively studied [1, 2], as shown in Figure 1. On the other hand, structural phase transition and morphology changes are also explored in 3D HOIP and their nanoparticles [3]. All the high-pressure-induced inorganic structural transition is resolved by in situ X-ray powder diffraction (XRD) measurements, morphology change is resolved by transmission electron microscopy (TEM), the correlated optical responses are investigated by absorption and photoluminescence spectroscopy. And the rotational isomerism is evidenced by the vibrational properties of the organic BA chain by Raman spectroscopy combined with the Ab initio calculations.

[1] T Yin, B Liu, J Yan, Y Fang, M Chen, WK Chong, S Jiang, J-L Kuo, J Fang, P L, S-H W, K-P Loh, T-C Sum, T J. White, and Z Xiang, J. Am. Chem. Soc. 141, 1235 (2019).
[2] Yin T, Yan H, Abdelwahab I, Lekina Y, Lü X, Yang W, Sun H, Leng K, Cai Y, Shen Z, Loh KP, Nat. Commun. 14, 411 (2023).
[3] T Yin, Y Fang, WK Chong, KT Ming, S Jiang, X Li, J-L Kuo, J Fang, T-C Sum, T J. White, J Yan, and Z Xiang, Adv. Mater. 30, 1705017 (2018).

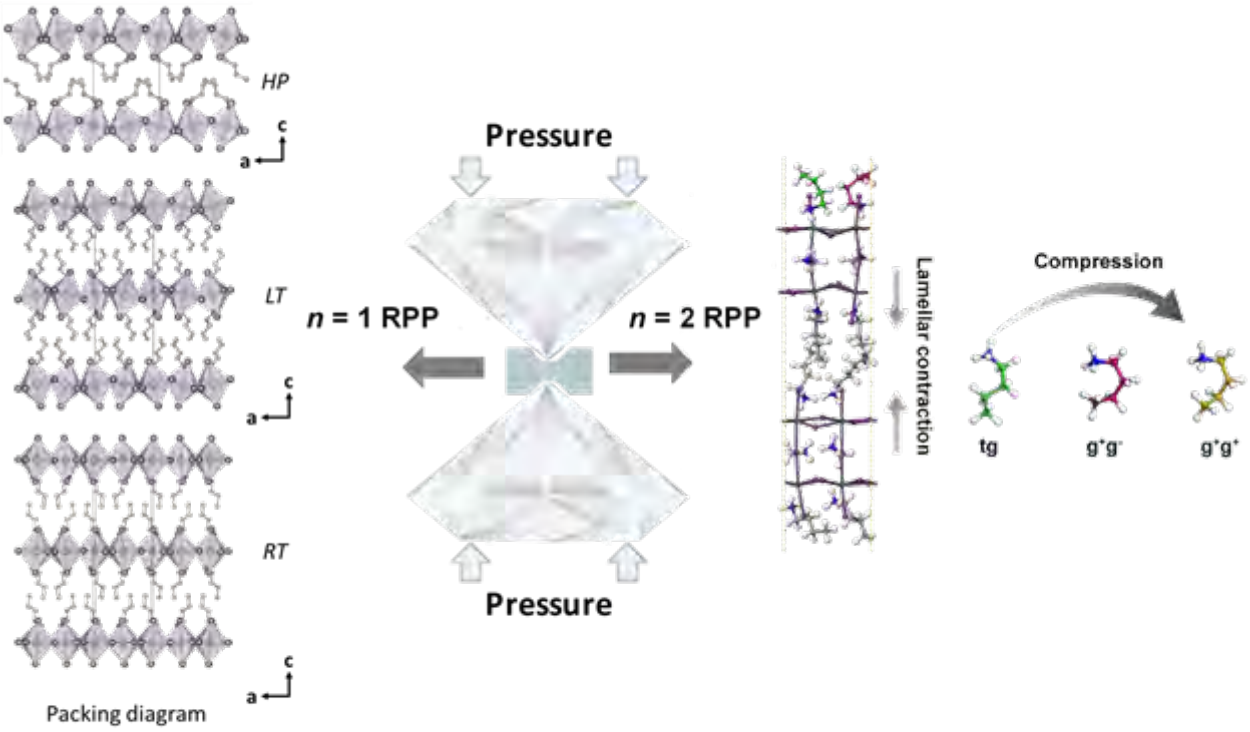


Figure 1. High pressure induced inorganic structural phase transitions in $n = 1$ RPP and organic rotational isomerism in $n = 2$ RPP.

Predicting the phase behaviours of high-pressure materials

Bingqing Cheng[1]
[1]*Institute of Science And Technology Austria, Austria*

Phase Diagrams – Molecular Systems, July 27, 2023, 14:00–16:00

Experimental synthesis and characterisation of high-pressure materials are extremely difficult, so first-principles methods based on quantum mechanics can play a crucial role. However, the high computational costs of these methods typically prevent rigorous predictions of macroscopic quantities at finite temperatures including the phase behaviours. In this talk, I will discuss how to enable such predictions by combining advanced statistical mechanics with data-driven machine learning interatomic potentials. As an example, we computed the low-pressure phase diagram of water from density functional theory at the hybrid level, accounting for thermal fluctuations, proton disordering and nuclear quantum effects. We then mapped the phase diagram of superionic water, which helps resolve the composition of ice giants. As a final example, we computed the pressure-temperature phase boundary where diamond can form from hydrocarbon mixtures with different atomic fractions of carbon. Notably, we find a depletion zone where diamond formation is thermodynamically favorable regardless of the carbon atomic fraction, due to a phase separation mechanism. The cooler condition of the interior of Neptune compared to Uranus means that the former is much more likely to contain the depletion zone, which may help explain the Uranus-Neptune dichotomy.

Ab-initio design of high-Tc conventional Superconductors: how far is room-temperature Superconductivity?

Lilia Boeri[1]
[1]*Physics Department, Sapienza Universita' Di Roma, Rome, Italy*

Hydrides 1, July 24, 2023, 10:15–12:15

The discovery of near-Room-Temperature Superconductivity in High-Pressure Superhydrides has revolution d the landscape of superconducting material research, establishing ab-initio calculations as the tool of choice for predicting superconducting properties and synthesis conditions of new superconductors. [1]

In this talk, I will give an overview of our recent efforts to design high-Tc conventional superconductors that can operate at ambient pressure[2] and to explore metastable phases of multinary phase diagrams and assess the kinetic stability of promising metastable phases[3]. At the end of the talk, I will also address recent claims of room temperature superconductivity at ambient pressure.[4]

[1] J. A. Flores-Livas, L. Boeri, A. Sanna, G. Profeta, R. Arita, M. Eremets, Physics Reports 856, 1-78 (2020).
[2] S. di Cataldo, W. Von der Linden, L. Boeri, NPJ Comp. Mat., 8, 2 (2022).
S. di Cataldo, C. Heil, W. von der Linden, and L. Boeri, Phys. Rev. B 104, L020511 (2021);
S. di Cataldo, S. Qulaghasi, G. B. Bachelet, L. Boeri, Phys. Rev. B 105, 064516 (2022);
S. di Cataldo and L. Boeri, Phys. Rev. B 107, L060501 (2023).
[3] S. Saha, S. di Cataldo, M. Amsler, W. von der Linden, and L. Boeri, Phys. Rev. B 102 024519 (2020); R. Lucrezi, S. di Cataldo, W. von der Linden, L. Boeri, C. Heil, NPJ Comp. Mat. 8, 119 (2022).
[4] P. P. Ferreira, L. J. Conway, A. Cucciari, S. Di Cataldo, F. Giannessi, E. Kogler, L. T. F. Eleno, C. J. Pickard, C. Heil and Lilia Boeri, cond-mat/2304.04447.

Design of Static High-pressure Experiments at Free Electron Lasers

R. Stewart Mcwilliams[1]
[1]*University Of Edinbrugh, United Kingdom*

Developments at XFELs & Lasers, July 24, 2023, 14:00–16:00

Use of X-ray free electron laser (XFEL) sources in high-pressure sciences is rapidly expanding beyond the field of dynamic compression to include static compression techniques, leading to a rapid growth of new possibilities for experimental study of matter at high-pressure, temperature, and rate. I will review our current understanding of XFEL techniques used in conjunction with static high-pressure investigations. Platforms for static high-pressure study developed at PAL-XFEL (Korea) and European XFEL (Germany) will be discussed with an emphasis on experimental design principles and methodologies, including numerical modelling of beam interactions, mitigation and control of 'diffract-and-destroy' beam effects, and currently accessible conditions of pressure, temperature, and timescale. This discussion will cover the recent work of several community-wide teams working at these facilities.

Mapping and accelerating stochastic explorations of dense matter

Prof Chris Pickard[1]
[1]*University of Cambridge, Cambridge, United Kingdom*

Computational Methods, July 25, 2023, 10:15–12:15

First principles methods for the prediction of the structures and chemistry of dense matter have delivered a powerful tool for computational exploration. While early studies focused on the exotic properties of relatively simple systems, typically the elements and binary compounds, much of the matter in the Universe is likely to be found in more complex mixtures.[1] At the same time, the promise of discovering materials with extreme properties relies on the ability of screen a wide variety of compounds.[2,3] I will reflect on why ab initio random structure searching (AIRSS) is particularly suited to these challenges, and the importance of visualising[4] and exploiting[5] the vast datasets we are now generating, to understand and accelerate structure search.

[1] Conway, Lewis J., Chris J. Pickard, and Andreas Hermann. "Rules of formation of H-C-N-O compounds at high-pressure and the fates of planetary ices", Proceedings of the National Academy of Sciences 118, no. 19 (2021).
[2] Lu, Ziheng, Bonan Zhu, Benjamin WB Shires, David O. Scanlon, and Chris J. Pickard. "Ab initio random structure searching for battery cathode materials", The Journal of Chemical Physics 154, no. 17: 174111 (2021).
[3] Shipley, Alice M., Michael J. Hutcheon, Richard J. Needs, and Chris J. Pickard. "High-throughput discovery of high-temperature conventional superconductors", Phys. Rev. B 104, 054501 (2021).
[4] Shires, Ben W.B., and Chris J. Pickard. "Visualising energy landscapes through manifold learning", Phys. Rev. X 11, 041026 (2021)
[5] Chris J. Pickard, “Ephemeral data derived potentials for random structure search”, Phys. Rev. B 106, 014102 (2022)

Pressure-based mapping of protein conformational landscapes

Dr. Catherine Royer[1]
[1]*Rensselaer Polytechnic Institute, Troy, United States*

Bio/Life Sciences and Soft Matter, July 26, 2023, 10:15–12:15

Much of biological regulation relies on very small changes in energetics, structure and dynamics. These transitions are encoded by the precise amino acid sequences of proteins which have evolved to function appropriately in a given environment. Even single amino acid substitutions in proteins can lead to profound functional outcomes, including many human diseases, increased viral infectivity and resistance of bacteria to antibiotics, to name a few. Most often, these effects are not due to differences in the proteins' ground state structures, but rather arise from altered populations of excited states. We have used pressure perturbation coupled with fluorescence, NMR, SAXS and computational approaches to describe protein excited states and to map protein configurational landscapes, structurally and energetically. We have character d the configurational dynamics on these landscapes as well using NMR relaxation approaches.

Metallisation of hydrogen through a semi-metallic state

Alexander Drozdov[1], Pan Pan Kong[1], Vasily Minkov[1], Mikhail Eremets[1]
[1]*Max-planck-institut Für Chemie, Mainz, Germany*

Hydrogen, July 25, 2023, 10:15–12:30

The previous measurements of electrical conductivity showed that hydrogen in the molecular phase III turns to metal, namely to semi-metallic state at pressures above ~350 GPa[123]. The present experiments confirmed and elucidated this metallisation. Hydrogen starts to conduct already at the pressure of ~300 GPa, where the temperature dependence of resistivity ρ(T) indicates the semiconducting behaviour. At ~330 GPa ρ(T) changes to a metallic behaviour. Hydrogen at this point is a poor metal with a high resistivity characteristic for semimetals, the resistivity strongly decreases with pressure. The Raman intensity changes accordingly, decreasing above ~300 GPa but the Raman signal is observed up to ~400 GPa where it disappears.
We established that metallic hydrogen lies in the (P, T) domain of phase III (phase C2/c), at the temperatures below phase IV(V). The results are in good agreement with the theoretical calculations for C2/c phase which describes the metallisation of molecular hydrogen through the closure of the indirect gap[4567].

[1] Eremets, M. I., Drozdov, A. P., Kong, P. P. & Wang, H. Semi-metallic molecular hydrogen at pressure above 350 GPa. Nat. Phys. 15, 1246 (2019).
[2] M. I. Eremets, Troyan, I. A. & Drozdov, A. P. Low temperature phase diagram of hydrogen at pressures up to 380 GPa. A possible metallic phase at 360 GPa and 200 K. arXiv:1601.04479 (2016).
[3] Eremets, M. I., Kong, P. P. & Drozdov, A. P. Metallisation of hydrogen. arXiv:2109.11104 (2021).
[4] Gorelov, V., Holzmann, M., Ceperley, D. M. & Pierleoni, C. Energy Gap Closure of Crystalline Molecular Hydrogen with Pressure. Phys. Rev. Lett. 124, 116401 (2020).
[5] Monacell, L., Errea, I., Calandra, M. & Mauri, F. Black metal hydrogen above 360 GPa driven by proton quantum fluctuations. Nat. Phys. 17, 63 (2021).
[6] Dogan, M., Oh, S. & Cohen, M. L. Observed metallisation of hydrogen interpreted as a band structure effect. J. Phys.: Condens. Matter 33, 03LT01 (2021).
[7] Dangic, Đ., L. Monacelli, Bianco, R., Mauri, F. & Errea, I. Large impact of phonon lineshapes on the superconductivity of solid hydrogen. arXiv:2303.07962v1 (2023).

Contributed Speaker Presentations

Superionicity of H- in LaH10 superhydride

Maelie Causse[1], PhD Gregory Geneste[1], PhD Paul Loubeyre[1]
[1]*CEA DAM, Bruyeres-le-Chatel, France*

Hydrides 3, July 25, 2023, 14:00–16:00

Computational studies have successfully predicted the dramatic uptake of hydrogen by metals under pressure leading to the formation of superhydrides. They can be viewed as additive volume alloys between metal hydrogen and a metal [1]. LaH10 exemplifies the properties of these novel H-rich compounds which form a novel class of superconducting materials, since it displays a very high superconducting critical temperature (Tc) of 250K [2,3].

We show here another remarkable property for superhydrides, namely H- superionicity[4].
In particular we will answer the following questions: can the H diffusion constant reach the high value needed for qualifying a superionic phase? If the fluid-like H atoms diffusion associated to a melting of the H sublattice and can LaH10 be stable under such conditions? How do the hydride ions (H-) conductivity in LaH10 compare to those of the recently discovered hydridic ionic conductors?

Superionic conductors are solid materials that display very high ionic conductivities, about 1 (Ω . cm)-1 and associated to a diffusion coefficient about D ~ 10-5 cm^2/s, as those typically found in molten salts [5]. Recently, the stability of a hydride (H-) superionic phase was predicted by ab initio molecular dynamics in sodium silicon hydride Na2SiH6 [6]. The current strategy to rational design of superhydrides at low pressure [7] could lead to a hydrogen energy material use of superionicity in superhydrides.

By means of ab initio molecular dynamics simulations in LaH10, an exceptionally high hydride (H-) diffusion coefficient is calculated at high temperature (D = 1.7 10-4 cm^2/s at 170GPa, 1500K, corresponding to an ionic conductivity of σ = 0.9 Scm-1). The connected path for the hydride ionic diffusion is disclosed, with the H-sublattice keeping its clathrate structure. LaH10 compound remains remarkably stable under temperature in its superionic phase up to a melting temperature similar to that of pure La. The conductivity properties of LaH10 are discussed in relation with the recently discovered family of compounds showing fast pure hydride ions transport. Superionicity in other hydrides is currently investigated and will be discussed.

[1] B. Guigue, A Marizy, and P. Loubeyre, Phy. Rev. B 102, 014107 (2020)
[2] M. Somayazulu, M. Ahart, A. K, Mishra, Z. M. Geballe, M. Baldini, Y. Meng, V. V. Struzhkin, and R. J. Hemley, Phy. Rev. Letters 122,027001 (2019)
[3] A. P. Drozdov, P. P. Kong, V. S. Minkov, S. P. Besedin, M. A Kuzovnikov, S. Mozaffari, D. A. Balicas, M. Tkacz and M. I. Eremets, Nature 569, 528 (2019)
[4] M. Caussé et al. Superionicity in LaH10 superhydride. PRB 107, L060301 (2023).
[5] J. Boyce and B. Huberman, Physics Reports 51,198 (1979)
[6] T. Liang, Z. Zhang, H. Yu, T. Cui, C. J. Pickard, D. Duan, and S. A. T. Redfern, The Journal of Physical Chemistry Letters 12,7166 (2021)
[7] Z. Zhang, T. Cui, M. J. Hutcheon, A. M. Shipley, H. Song, M. Du, V. Z. Kresin, D. Duan, C. J. Pickard and Y. Yao, Phys. Rev. Letters 128, 047001 (2022)

Molecular Dynamics to Explore the Role of Temperature, Water, and Porosity in Dynamic Shock Compression of SiO2

Dr. J. Matthew Lane[1], Kyle Cochrane[1], Jean-Paul Davis[1], Alisha N. Clark[2], Tracy J. Vogler[1]
[1]Sandia National Laboratories, United States, [2]University of Colorado Boulder, United States

Computational Methods, July 25, 2023, 10:15–12:15

Silica compression over a range of conditions can be important to understanding space and planetary impacts. We review our recent simulation work which uses classical molecular dynamics to investigate the effect of initial temperature and water content on the Hugoniot response of shock compressed silica. We have found that the initial temperature strongly influences the porous silica shock response in a relatively narrow pressure range (1-3 GPa). Outside this range the effect was negligible. We attribute this effect to thermal softening mechanisms in the compaction regime. In the lower pressure elastic regime and higher pressure fully compressed regime the final Hugoniot state depends only weaking on initial temperatures over a range from 77 to 1000K. Further, we explore the surprisingly small role that ~1 wt% of water/ hydroxide appear to play in silica dynamic response at moderate pressure, and discuss likely mechanisms. Appropriate interatomic potentials will be discussed for these two problems.

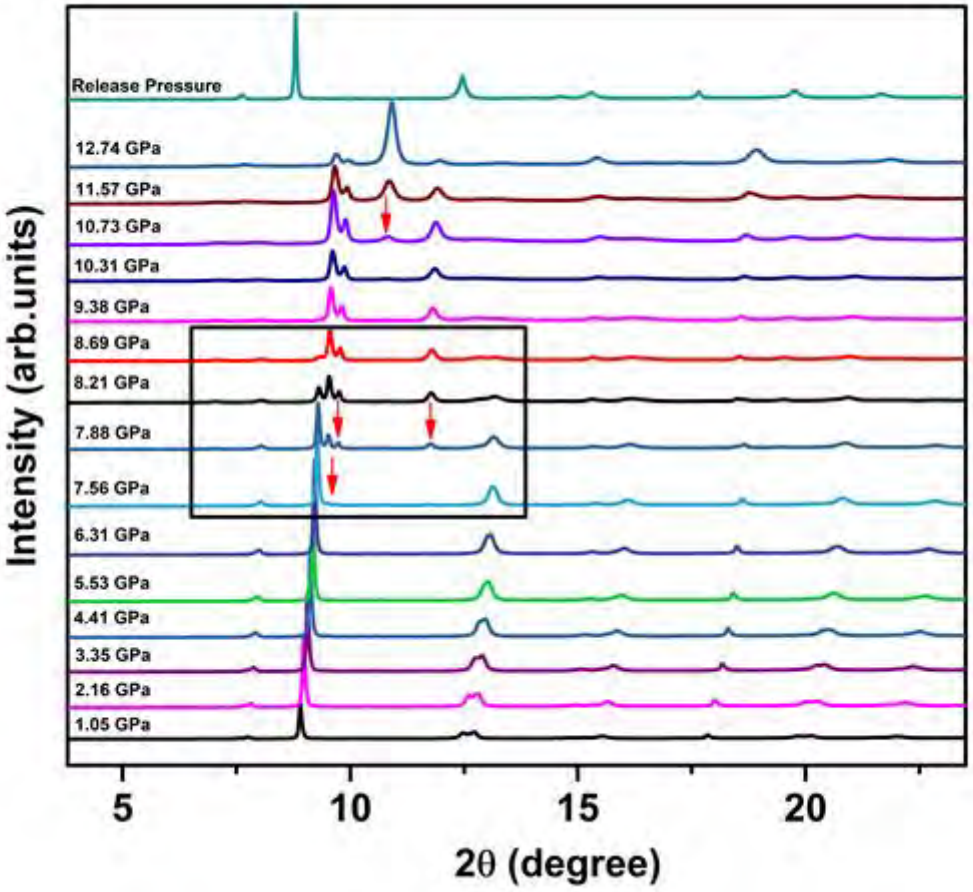
Pressure-induced phase transitions in 3D topological insulator TlBiTe2

Ms. Anjana Joseph[1], Dr. Ashutosh Kumar Singh[1], Dr. Boby Joseph[2], Dr. Irshad K.A[2], Dr. Rajaji Vincent[3], Prof. Chandrabhas Narayana[1]
[1]Jncasr, Bangalore, India, [2] Elettra Sincrotrone, Basovizza, Italy, [3]Institute of Light and Matter, 69100 Villeurbanne, France

Electronic Transitions 1, July 26, 2023, 16:30–18:30

Pressure (strain) offers a solid ground for the fundamental understanding of topological quantum phase transitions (TQPT) in strong spin-orbit coupling systems and for tuning the materials to get enhancement in properties like thermoelectric performance, for technological applications [1]. In this context, Thallium based III-V-VI_2 ternary chalcogenides compounds (III = Tl, V = Sb, Bi, VI = Te, Se, and S), especially $TlBiX_2$ (X = S, Se, Te) family of materials have been of particular interest due to their multiple TQPTs. The compounds $TlBiS_2$ (Eg = 0.42 eV), $TlBiSe_2$ (Eg = 0.28 eV), and $TlBiTe_2$ (Eg = 0.11 eV) crystallise in rhombohedral structure (SG: $R\bar{3}m$) and there is a strong interlayer coupling between the layers making their structure 3D [2]. Recent high-pressure Raman spectroscopic studies combined with X-ray diffraction and first-principles calculations on $TlBiS_2$ have shown its evolution to topological insulating and topological crystalline phases at 0.5 GPa and 1.8 GPa, respectively [3]. $TlBiS_2$ also shows TQPT under the chemical substitution of Se at the S site [4]. But $TlBiSe_2$ and $TlBiTe_2$ are 3D topological insulators at ambient conditions due to high spin-orbit coupling and lower band gap [5]. $TlBiTe_2$ has the least band gap among these materials and hence relatively small external pressure can drive it to topologically nontrivial phases. Here we report, detailed high-pressure Raman spectroscopy and Synchrotron X-ray diffraction (XPRESS, Elettra) studies on polycrystalline $TlBiTe_2$, exploring the pressure-induced topological, electronic, and structural phase transitions. From the phonon anomalies of A1g and Eg modes under hydrostatic pressure, we understand the unusual electron-phonon coupling associated with the TQPT. The pressure dependence of unit cell parameters was fitted and analyzed using Murnaghan equation of state to obtain the linear compressibility of the axes and the bulk modulus of the system. The X-ray diffraction results show the structural transition from rhombohedral to monoclinic phase starting at 7.5 GPa with the coexistence of phases over some pressure range and another possible transition at 10.7 GPa. The structural transition is reversible upon pressure release as observed from both synchrotron X-ray diffraction and Raman scattering measurements. In this study, we have also done a comparative analysis of the phonon and structural behavior of the $TlBiX_2$ (X = S, Se, Te) family of materials and tried to unify the understanding of their pressure-induced phenomena.

[1] L.-C. Chen et al., Nat. Materials 18 (12), 1321-1326 (2019).
[2] Q. Zhang et al., Sci. Rep. 5, 8379 (2015)
[3] V. Rajaji et al., Phys. Rev.B. 99 (18), 184109 (2019)
[4] T. Sato et al., Nat. Phys. 7, 840 (2011)
[5] Y. L. Chen et al., Phys. Rev. Letters. 105 (26), 266401 (2010)


Release Pressure
12.74 GPa
11.57 GPa
10.73 GPa
10.31 GPa
9.38 GPa
8.69 GPa
8.21 GPa
7.88 GPa
7.56 GPa
6.31 GPa
5.53 GPa
4.41 GPa
3.35 GPa
2.16 GPa
1.05 GPa
Intensity (arb.units)
5
10
15
20
2θ (degree)

Probing the unusual superconductivity of UTe2 with high pressure

Mr Daniel Braithwaite[1], Mr Michal Vališka[1,2], Mr William Knafo[3], Mr Gérard Lapertot[1], Mr Georg Knebel[1]

[1]University Grenoble Alpes, Grenoble INP, CEA, IRIG-PHELIQS, Grenoble, France, [2]Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Prague, Czech Republic, [3]Laboratoire National des Champs Magnétiques Intenses, UPR 3228, CNRS-UPS-INSA-UGA, Toulouse, France

Novel Superconductors 1, July 27, 2023, 10:15–12:15

The unconventional superconductivity in the strongly correlated system UTe2 displays a plethora of fascinating properties [1,2]. Its behaviour in magnetic field is striking, as the upper critical field, HC2, reaches values over 60T[3,4], of the same order of magnitude as the high-Tc superconductors, whereas the superconducting critical temperature of UTe2 is only 2K. Moreover, the extremely anisotropic and unusual shape of HC2 reveals unique features: re-entrant superconductivity in high field, a reinforcement of the superconducting pairing strength with field, and a field induced change of the superconducting order parameter, and possibly even of the underlying mechanism for superconductivity [5]. However, the microscopic mechanisms leading to these phenomena are not yet known.

As in many strongly correlated electron systems, high pressure is an extremely effective parameter in UTe2 to tune the microscopic interactions, significantly modifying the macroscopic properties. This brings insight into understanding the striking phenomena described above as well as leading to new discoveries in this material.

We will present results on UTe2 under high pressure using various experimental techniques. The application of pressure enhances superconductivity by a factor two. The combination of resistivity and specific heat measurements under pressure allowed us to discover a phase transition within the superconducting state between two different superconducting order parameters, and a magnetically ordered state at higher pressures [6]. We also address the challenge to characterise the effects of combined pressure and magnetic fields. A full investigation of this system requires magnetic field higher than the maximum available static magnetic fields. Here, we present an investigation of the electrical resistivity of UTe2 under pressure up to 3 GPa and pulsed magnetic fields up to 58T. We show that, near the critical pressure, a field-enhancement of superconductivity coincides with a boost of the effective mass related to the collapse of metamagnetic and critical fields [7]. These new elements improve our understanding of the interplay between magnetism and superconductivity, and the nature of these phases.

[1] D. Aoki et al., Journal of the Physical Society of Japan 88, 043702 (2019).
[2] S. Ran et al., Science 365, 684 (2019).
[3] G. Knebel et al., Journal of the Physical Society of Japan 88, 063707 (2019).
[4] S. Ran et al., Nat Phys 15, 1250 (2019).
[5] A. Rosuel et al., 2022), p. arXiv:2205.04524.
[6] D. Braithwaite et al., Communications Physics 2, 147 (2019).
[7] M. Vališka et al., Physical Review B 104, 214507 (2021).

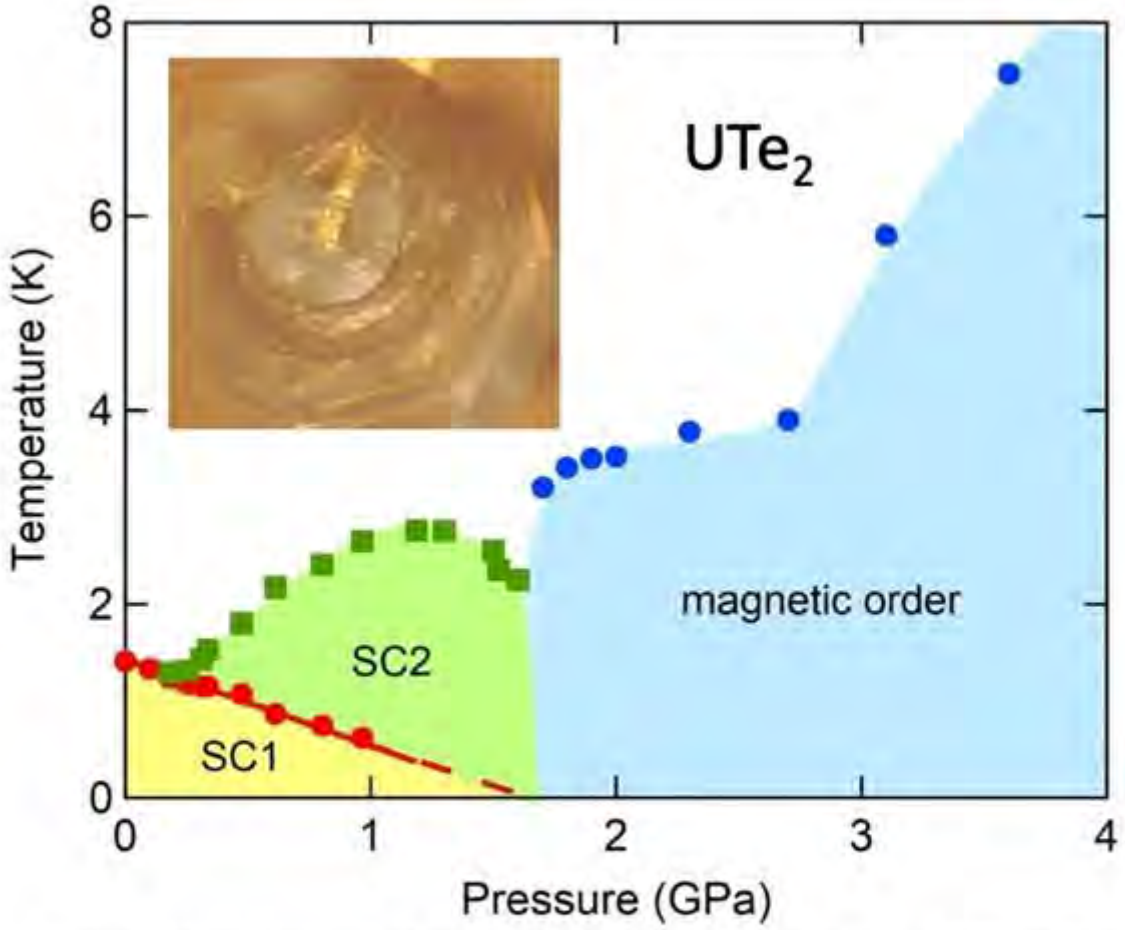


Figure 1. Phase diagram of superconductivity and magnetism of UTe_2 under pressure determined from calorimetry measurments in a diamond anvil cell (DAC). Inset shows the pressurized DAC with a Au:AuFe thermocouple bonded to the sample for calorimetry measurements. SC1 and SC2 are two distinct superconducting phases.

Developments in measuring collective excitations using inelastic Neutron Scattering under pressures up to 8kbar

Bernet Meijer[2], Shurong Yuan[2], Richard Dixey[2], Mark Kibble[1], Chris Goodway[1], Dr Anthony Phillips[2], **Dr Helen Walker**[1]

[1]ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, United Kingdom, [2]Queen Mary University London, London, United Kingdom

Facility Development 1, July 24, 2023, 16:30–18:30

While high pressure has long been a parameter of interest to people investigating the dynamics of materials, the use of pressure cells for Inelastic Neutron Scattering (INS) has not been fully exploited due to difficulties with the signal-to-noise ratio as a result of there being more cell in the neutron beam than sample, and the inherent weakness of the INS signal. This led to a SINE2020 project specifically aimed at developing pressure cells optimised for INS, which produced new low background high transmission gas cells manufactured from TAV6 (90 wt% Ti, 6 wt% Al & 4 wt% V) [1]. In this presentation I will present the first published experimental results using these cells, to demonstrate their powerful capabilities.

Today the most commonly used cooling technology is based on vapour compression, which uses 20-25% of global energy consumption and produces 10% of environmentally harmful emissions. Of these emissions two-thirds are indirect emissions from electricity use, and one-third are direct emissions originating from the leakage of greenhouse gases thousands of times more potent than CO_2. Furthermore, the demand for air conditioning is predicted to dramatically increase in the coming decades in emerging economies, leading to more environmental damage and a vicious cycle driving the demand for more cooling. It is therefore essential to search for new technologies.

Stating the obvious, solids do not leak. Therefore, if we could exploit endothermic phase transitions in solids, we would immediately eradicate the direct emissions. Calorics are solid-state materials which exhibit a large entropy change in response to an external field, where, if the material is thermally isolated, this leads to a change in temperature which can be the basis for a cooling cycle. Barocalorics, in which the external field is hydrostatic pressure, have shown the greatest potential for cost-effective deployment since they are often based on abundant cheap materials and have demonstrated Carnot efficiencies up to 82%.

A large number of different barocalorics have been discovered [2], but less work has focussed on understanding the barocaloric effect on the atomic scale. We have therefore been working to explore the structure and dynamics of a number of different barocaloric materials using neutron scattering, which has required the use of high-pressure measurements. We have shown that the vibrational dynamics are key to understanding the barocaloric effect in Ammonium Sulfate, instead of the commonly predicted configurational origin [3]. Meanwhile, we have identified adamatane as a good barocaloric and explored the effects of disorder on the phonon spectrum in a single crystal [4].

[1] Kibble et al., Journal of Neutron Research, 21 105 (2019)
[2] Boldrin, Applied Physics Letters, 118 170502 (2021)
[3] Yuan et al., Advanced Functional Materials, 2207717 (2022)
[4] Meijer et al., Phys. Chem. Chem. Phys., 10.1039/D2CP05412D (2023)

Exceptional phonon point versus free phonon coupling in Zn-based semiconductor mixed crystals under pressure

Alhaddad Toni[1], Shoker M.B.[1], Pagès O.[1], Torres V.J.B.[2], Postnikov A.V.[1], Polian A.[3,4], Hajj Hussein R.[1], Pradhan G.K.[5], Narayana C.[6], Nataf L.[4], Ravy S.[4], Itié J.-P.[4], Strzałkowski K.[7], Marasek A.[7], Firszt F.[7]

[1]1 Université de Lorraine, LCP-A2MC, ER 4632, Metz, France, [2]Departamento de Fisica and I3N, Universidade de Aveiro, Aveiro, Portugal, [3]IMPMC, Sorbonne Université — UMR CNRS 7590, Paris, France, [4]Synchrotron SOLEIL, L'Orme des Merisiers Saint-Aubin, Gif-sur-Yvette Cedex, France, [5]Department of Physics, KIIT Deemed to be University, Bhubaneswar, India, [6]JNCASR, Jakkur P.O. Bangalore, , India, [7]Institute of Physics, Nicolaus Copernicus University in Toruń, Toruń, Poland

Chemical Bonding 1, July 24, 2023, 14:00–16:00

The common zincblende-type A1-xBxC zincblende semiconductor mixed crystals exhibits two modes per bond in their Raman spectra, reflecting a sensitivity of bond vibrations to their local (A- or B-like) environment formalised within our percolation model [1]. In this work we explore how the Raman doublet of a bond can be used as a chemical probe to "see" how a mixed crystal behaves under pressure at the local scale in its native (zincblende) phase on approach to a structural transition; using Zn-based systems as a case study.

In fact, the Raman doublet appears to be reactive to pressure: either it closes (Zn1 xBexTe, Zn1 xCdxTe [2]) or it opens (Zn1 xCdxSe), depending on the hardening rates of the two environments under pressure [3]. Of special interest is the "closing" case, in which the two modes forced, into proximity by pressure, do mechanically couple. When a bond is so dominant that it forms a matrix-like continuum, its two submodes freely couple on crossing at the resonance, with an effective transfer of oscillator strength. Post resonance the two submodes stabilise into an inverted doublet shifted in block under pressure [4,2]. When a bond achieves lower content and merely self-connects via (finite/infinite) treelike chains, the coupling is undermined by overdamping of the in-chain stretching until a «phonon exceptional point» is achieved at the resonance, corresponding to a virtual decoupling by overdamping of the two oscillators forming the Raman doublet. In this case, only the out-of-chain vibrations «survive» the resonance, the in-chain ones are «killed» [3,4].

The discussion of the high-pressure Raman spectra is supported by ab initio (AIMPRO/SIESTA) Raman / phonon calculations and by determination of the pressure domain of the native zincblende phase by high-pressure X-ray diffraction at the SOLEIL synchrotron.

[1] O. Pages et al., Phys. Rev. B 77, 125208 (2009).
[2] T. Alhaddad et al., J. Appl. Phys. 133, 065701 (2023).
[3] M.B. Shoker et al., Sci. Rep. 10, 19803 (2020).
[4] M.B. Shoker et al., Sci. Rep. 12, 753 (2022).

Observation of superconducting gap in Carbonaceous Sulfur Hydride

Hiranya Pasan Vindana Wadhurawa Mudiyanselage[1], Elliot Snider[2], Sasanka Munasinghe[2], Nathan Dasenbrock-Gammon[1], Ray McBride[2], Sachith Dissanayake[2], Ranga Dias[1,2]
[1]Department of Physics and Astronomy, University of Rochester, Rochester, United States,
[2]Department of Mechanical Engineering, University of Rochester, Rochester, United States

Hydrides 4, July 26, 2023, 14:00–16:15

In last decade hydrogen rich materials have been in the spotlight for reaching high temperature superconductivity. Extensive experimental work such as conductivity, magnetic susceptibility and magnetic field measurements have been carried out on these hydrides, but little effort has focused on the superconducting energy gap. Hydrides are predicted to be conventional superconductors, so their superconducting gap follows BCS theory. In this work, we report magnetic susceptibility measurements using a double frequency technique and far IR spectroscopy measurements on a Carbonaceous Sulphur Hydride (CSH) sample. The maximum critical temperature was observed as 260 K based on the magnetic susceptibility. For the same sample, far IR spectroscopy performed for 70-200 meV energy realm and the results reveal an absorption at lower energies below the transition temperature which is an indication for the superconducting gap in CSH, which suggests the conventional mechanism for superconductivity in CSH.

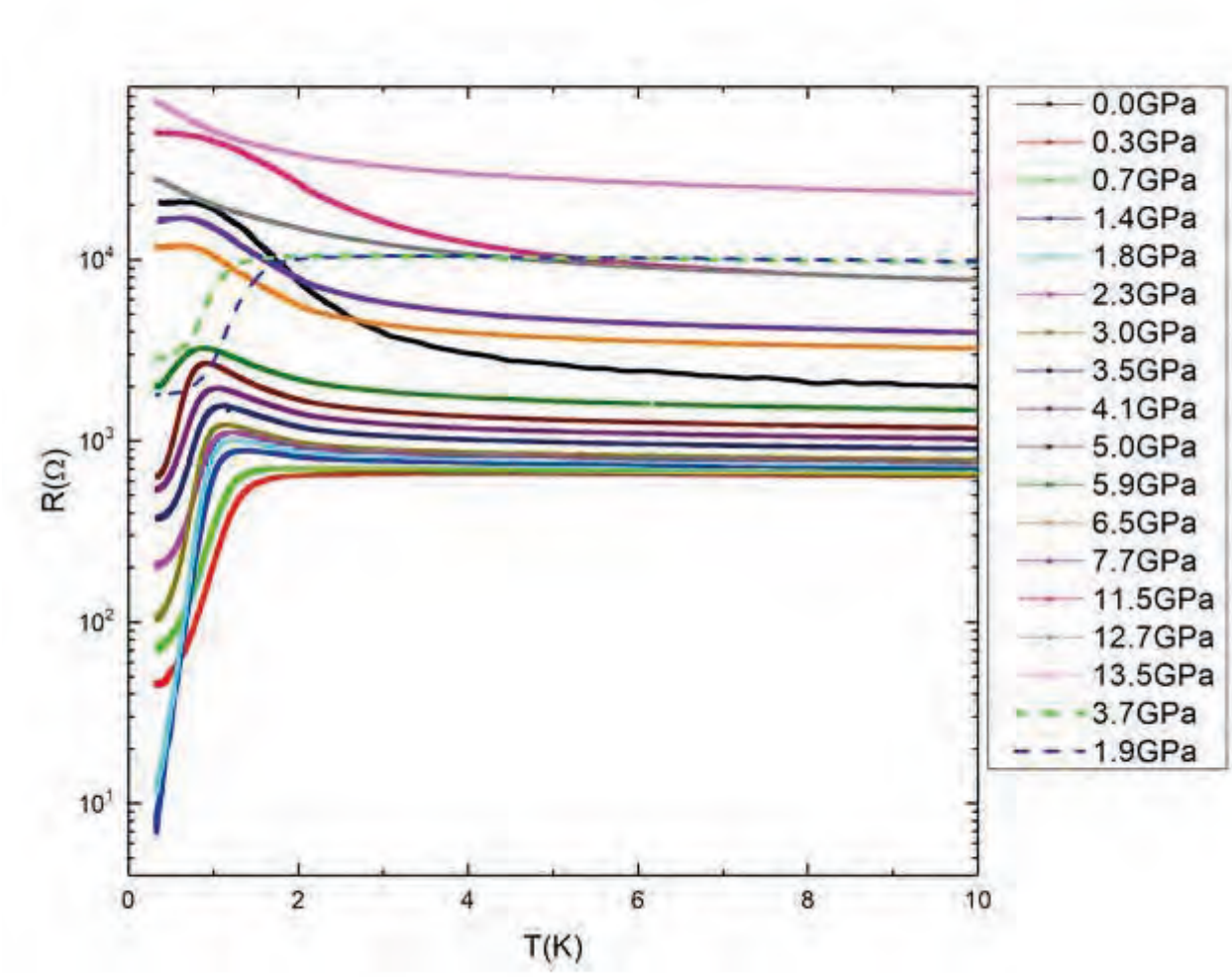
The Pressure Driven Superconductor-Insulator-Transition in 2D Films

Mr Roy Cohen, Professor Aviad Frydman, Mr Mark Nikolaevsky
[1]Bar – Ilan University, Ramat Gan, Israel

Electronic Transitions 2, July 25, 2023, 14:00–16:00

The Superconductor Insulator Transition (SIT) in 2D films has been in the front of condensed-matter research for the past few decades. The SIT is a quantum phase transition which occurs at zero temperature and is thus driven by quantum fluctuations and controlled by a non-thermal tuning parameter. So far, several tuning parameters have been used to drive the transition, such as thickness, external magnetic field, degree of disorder etc. We explore a new tuning parameter – hydrostatic pressure. For this we fabricate thin films of amorphous Indium Oxide directly on a diamond and apply pressure on the samples by using a diamond anvil cell, a device that can apply pressure up to 100 GPa.

We find that for pressures up to 1.5 GPa, superconductivity is improved, and the critical temperature increases with increasing Pressure. Applying higher pressure suppresses superconductivity and drives the films into the insulating state. These results imply two competing effects of the pressure on the superconductivity of thin films. Furthermore, we find that the pressure induced insulator may be of different nature than the disordered induced insulator. In my talk I will discuss the implications of the pressure induced SIT and the nature of the insulating phase in these films.



Swift heavy ion irradiation of bismuth nanowire networks pressurised in diamond anvil cells

Christopher Schröck[1,2], Ioannis Tzifas[1], Lkhamsuren Bayarjargal[2], Kay-Obbe Voss[1], Ina Schubert[1], Michael F.P. Wagner[1], Wilfried Sigle[3], Isabel Armstrong-Cowell[1], Christina Trautmann[1,4], Bjoern Winkler[2], Maria Eugenia Toimil-Molares[1]

[1]GSI Helmholtz Center for Heavy Ion Research GmbH, Darmstadt, Germany, [2]Institute of Geosciences, Goethe-University Frankfurt, Frankfurt am Main, Germany, [3]Max-Planck Institute for Solid State Research, Stuttgart, Germany, [4]Department of Materials- and Geosciences, Technical University of Darmstadt, Darmstadt, Germany

Nanoscale Systems, July 24, 2023, 16:30–18:30

The simultaneous exposure of materials to multiple extreme conditions is a field of increasing interest in modern high pressure (HP) research. Concomitantly applying HP using diamond anvil cells (DACs) and irradiation with swift heavy ions (SHI) of GeV energies represents a unique approach, that has been pioneered at GSI Helmholtz Centre Darmstadt. Ground-breaking experiments revealed new effects such as the generation of new phases far from thermodynamic equilibrium or the stabilization of HP phases at ambient conditions [1,2].

Our experimental activities aim at studying size-effects of GeV-ion-induced phase transitions under high pressure. As a material of interest, we selected bismuth (Bi), due to its complex and well-characterised HP phase diagram [3] (Fig. 1) and its sensitivity to SHI irradiation [4]. Bi-nanowire networks (Bi-NWNWs) with a diameter of 35 nm were fabricated by electrodeposition in etched ion-track membranes [5] and irradiated at HP using 238-U ions of up to 100 GeV kinetic energy. Ion-induced effects were investigated applying in situ Raman spectroscopy, and additionally characterised by synchrotron-XRD after the irradiation. Here, we will discuss the impact of ion-irradiation on the HP-behaviour of Bi-NWNWs and bulk Bi.

The authors gratefully acknowledge funding and beamtime provided by the GSI Helmholtz Centre, as well as support during the synchrotron beamtime at PETRA-III, DESY (Hamburg, Germany, proposal I-20220591).

[1] Glasmacher, U.A. et al., PHYS REV LETT, 96(19), (2006), p. 195701
[2] Lang, M. et al., NAT MAT, 8(10), (2009), p. 793
[3] Ono, S. et al., HIGH PRESSURE RES, 38(4), (2018), p. 414
[4] Dufour, C. et al., J PHYS-CONDENS MAT, 5(26), (1993), p. 4573
[5] Wagner, M.F.P. et al., ADV. ELECTRON. MATER., 7(3), (2021), p. 2001069

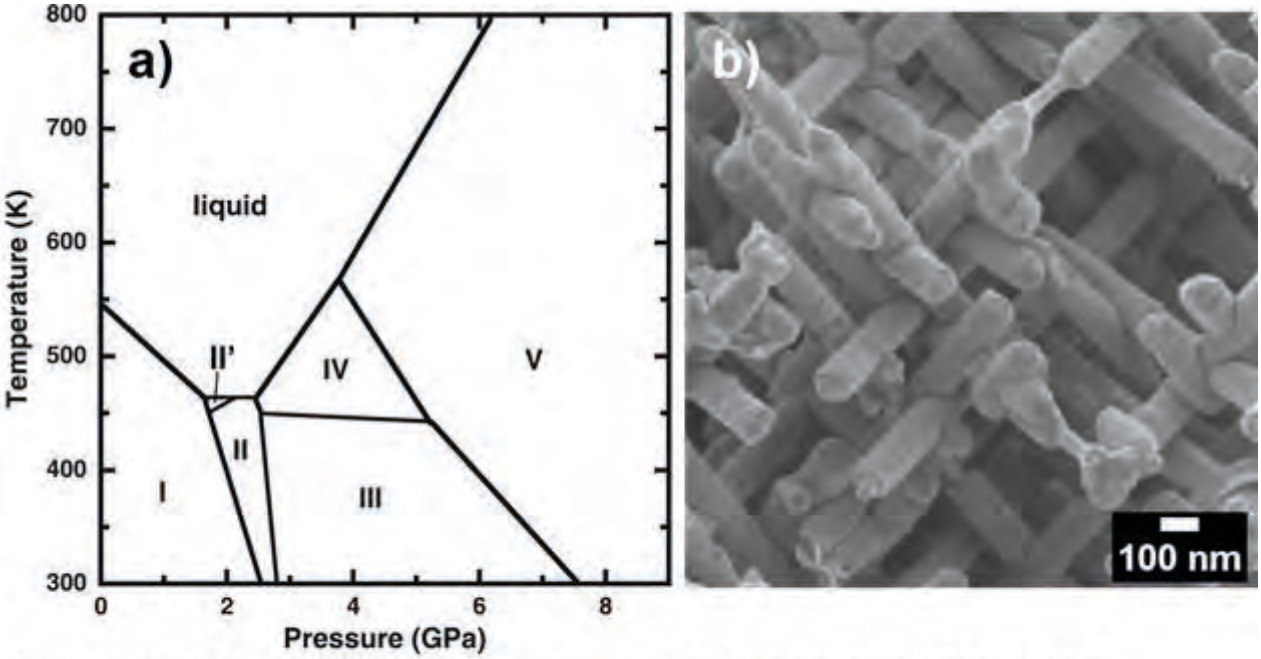


Figure 1: a) Equilibrium phase diagram of bulk-Bi (adapted from [3]), b) pristine Bi-NWNW (own work)

Colourful systematic in the phase-diagrams of the elements

Wilfried B. Holzapfel[1]
[1]*University Paderborn, Paderborn, Germany*

Computational Studies of Elements, July 26, 2023, 10:15–12:15

Colourful phase-diagrams of the elements provide a better basis for the discussion of structural systematics under pressure. The overview of 2016 (figure 1)[Ho13,HC16] will be updated with a detailed inspection into the different physical background in the individual groups of the periodic table.

[1] [Ho13] http://www.mog-group.de/Elemente/en/under_high_pressure.html
[2] [HC16] https://www.epubli.com/shop/modern-alchemy-and-the-philosophers-stone-9783741869334

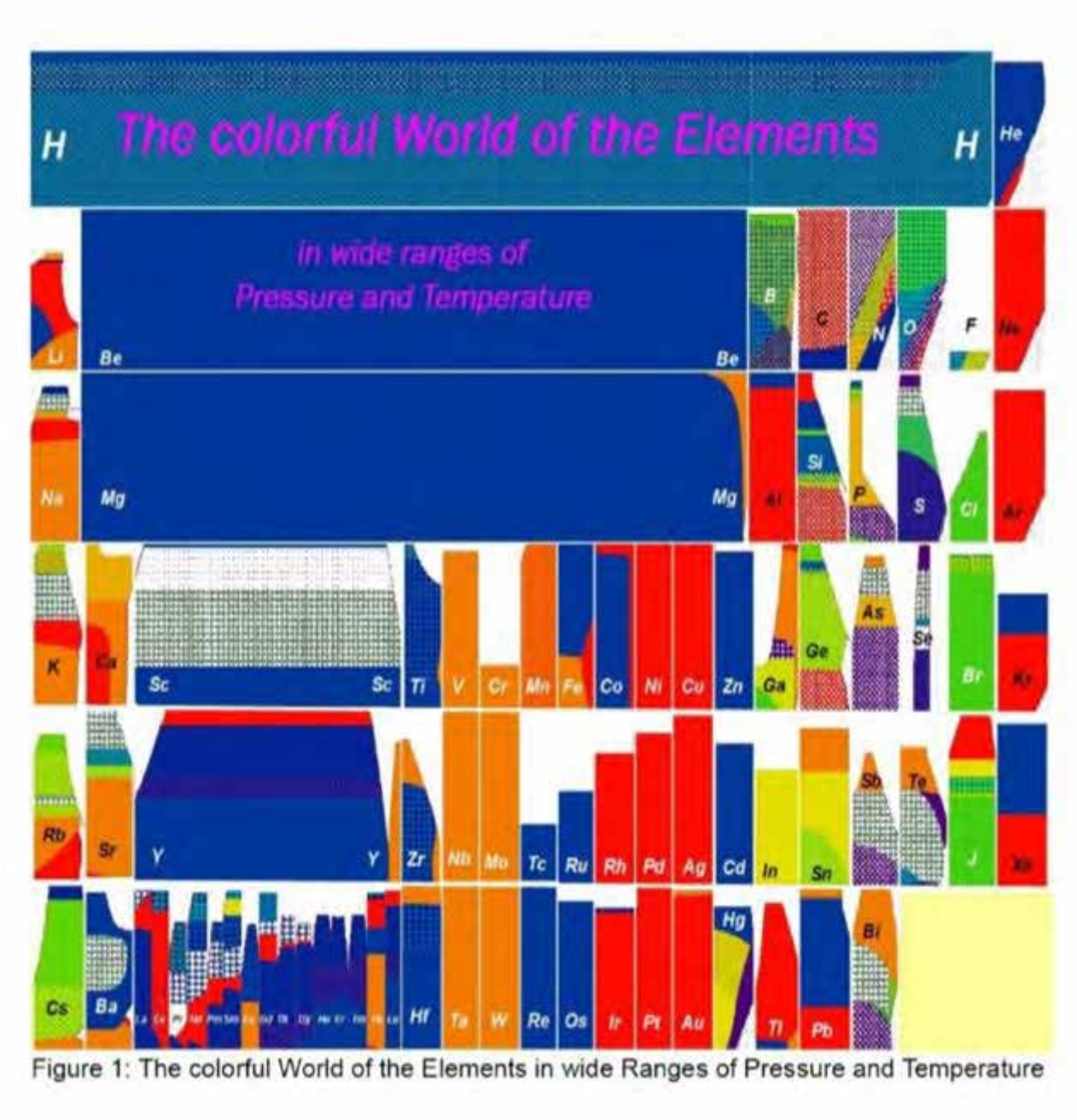


Figure 1: The colorful World of the Elements in wide Ranges of Pressure and Temperature

Pressure-induced phase transition in polymer brushes: thermodynamic predictions and structural studies

Mr. Leonardo Chiappisi[1]
[1]*Institut Laue-langevin, France*

Bio/Life Sciences and Soft Matter, July 26, 2023, 10:15–12:15

Polymers are key elements in modern material science, and, since the first polymer synthesis in 1907, tremendous progress in polymer chemistry were made. Today, an endless assortment of polymers – whose properties are adapted to specific needs – is available. In many cases, a thin polymer film, the coating, is sufficient to impart desired properties to the material. One of the most employed stimuli to tune phase transition in polymer coatings is temperature. Since the first reports of the thermo-responsive behaviour of poly(N-isopropylacrylamide) (PNIPAM) in an aqueous environment in the late sixties, PNIPAM has become the most studied model for non-ionic polymer systems. However, temperature is not the only physical parameter to tune the phase behaviour of polymeric systems. Pressure can be similarly used to control the phase behaviour of polymer solutions and thin films. Herein, we provide an extensive overview of the phase behaviour of end-grafted PNIPAM brushes as a function of pressure and temperature. The phase behaviour, extracted from the neutron reflectometry curves, is compared with the phase behaviour of semi-dilute solutions. Further, we show that the coexistence line as a function of pressure and temperature can be predicted assuming a two-state model – swollen and collapsed – knowing the different derivatives of the free energy of collapse as a function of pressure and temperature. These quantities can be precisely accessed using calorimetric and densitometric measurements. The results evidenced that the pressure-temperature phase behaviour of polymer solutions and coatings can be predicted from simple, laboratory-scale experiments, paving the way for the rational design of smart coatings with pressure and thermo-responsive behaviour.

Ref: Micciulla, S.; Gutfreund, P.; Kanduč, M.; Chiappisi, L. Pressure-Induced Phase Transitions of Nonionic Polymer Brushes. Macromolecules 2023, 56 (3), 1177–1188. https://doi.org/10.1021/acs.macromol.2c01979

Exploiting the reduction of Si melting temperature for the production of boron carbide-based composites under high pressure

Leonardo Resende[2,4], João Vítor dos Santos Ritter[3], **Altair Soria Pereira**[1,2,3]
[1]Instituto de Física, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil, [2]Programa de Pós-Graduação em Ciência dos Materiais, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil, [3]Escola de Engenharia, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil, [4]Engenharia Mecânica, Instituto de Ciências Agrárias e Tecnológicas. Universidade Federal de Rondonópolis, Rondonopolis, Brazil

Nitrides, Borides and Carbides 1, July 24, 2023, 14:00–16:00

The decrease in the Si melting temperature with increasing pressure enabled the production, using a one-step sintering process, of boron carbide-based ceramics composites with a particular combination of properties and microstructure. The sintered samples were obtained by high-pressure (7.7GPa) processing of a mixture of B4C+10 wt% Si powders at different sintering temperatures (800°C to 2000°C) and dwell times (5 or 30 min).

Highly-densified B4C-Si composites, for which Si is an effective binding phase, were produced by liquid phase sintering at 1000°C. Their microstructure is similar to those observed for some cermets and no significant grain growth was observed. The sample sintered at 7.7GPa/1000°C/ 30min had a Vickers Hardness (HV) of 19.64 ± 0.89 GPa and KIC of 5.95 ± 0.48 MPa.m1/2. Although no new phase resulting from the reaction of Si with boron carbide has been identified by XRD in the samples produced at 7.7 GPa/1000°C, significant changes were observed in the boron carbide lattice parameters. These structural changes are much more important than those induced in a pure B4C sample sintered at 2000°C and are associated with the observation, in SEM/BSE micrographs, of different shades of gray in boron carbide grains. Similar results for reaction bonded BxC-SiC-Si composites are associated to the dissolution in liquid silicon of B4C and free carbon and the consequent precipitation of a Si containing ternary boron carbide phase B12(B,Si,C)3, which competes with the precipitation of SiC particles. [1]

The observation of these structural changes in boron carbide without the simultaneous formation of SiC is probably due to B4C being brought into contact with liquid Si at a temperature significantly lower than that required in low pressure processing.

For samples processed at temperatures higher than 1000°C, the reaction between liquid Si and B4C caused the formation of SiC. The structural changes of boron carbide implied a much more abrupt change in the c/a ratio in the temperature range between 1200°C and 1500°C than observed at lower temperatures. It reached a value of 2.163 for a processing temperature of 1500°C, which was maintained up to the highest investigated temperature (2000°C). In turn, the unit cell volume increased by around 0.8% up to a processing temperature of 1000°C, but for higher temperatures no significant additional increase was observed.

No other phase was identified by XRD in the produced B4C-SiC composites. The best mechanical properties, HV=20.60 ± 1.24 GPa and KIC=5.83 ± 0.26 MPa.m1/2, were obtained for the sample sintered at 7.7 GPa/1500°C/5 min.

Even with the increase in apparent density as a function of increasing temperature and despite SiC being much harder than Si, the B4C-SiC sinters showed similar hardness and KIC in comparison to the B4C-Si sinters produced at 1000°C. The SiC formation prevents an efficient liquid phase sintering like that observed for the samples sintered at 1000°C, and other mechanisms, typical of solid-state sintering, must play an important role for advanced sintering stages to be achieved.

[1] S. Hayun, A. Weizmann, M.P. Dariel, N. Frage, Int. J. Appl. Ceram. Technol. 6 (2009) 492–500. https://doi.org/10.1111/j.1744-7402.2008.02290.x.

Non-Fermi-liquid behaviour of superhydrides

Dr. Dmitrii Semenok[1], Dr. Di Zhou[1], Dr. Thomas Meier[1]
[1] *Center for High Pressure Science and Technology Advanced Research, Beijing, China*

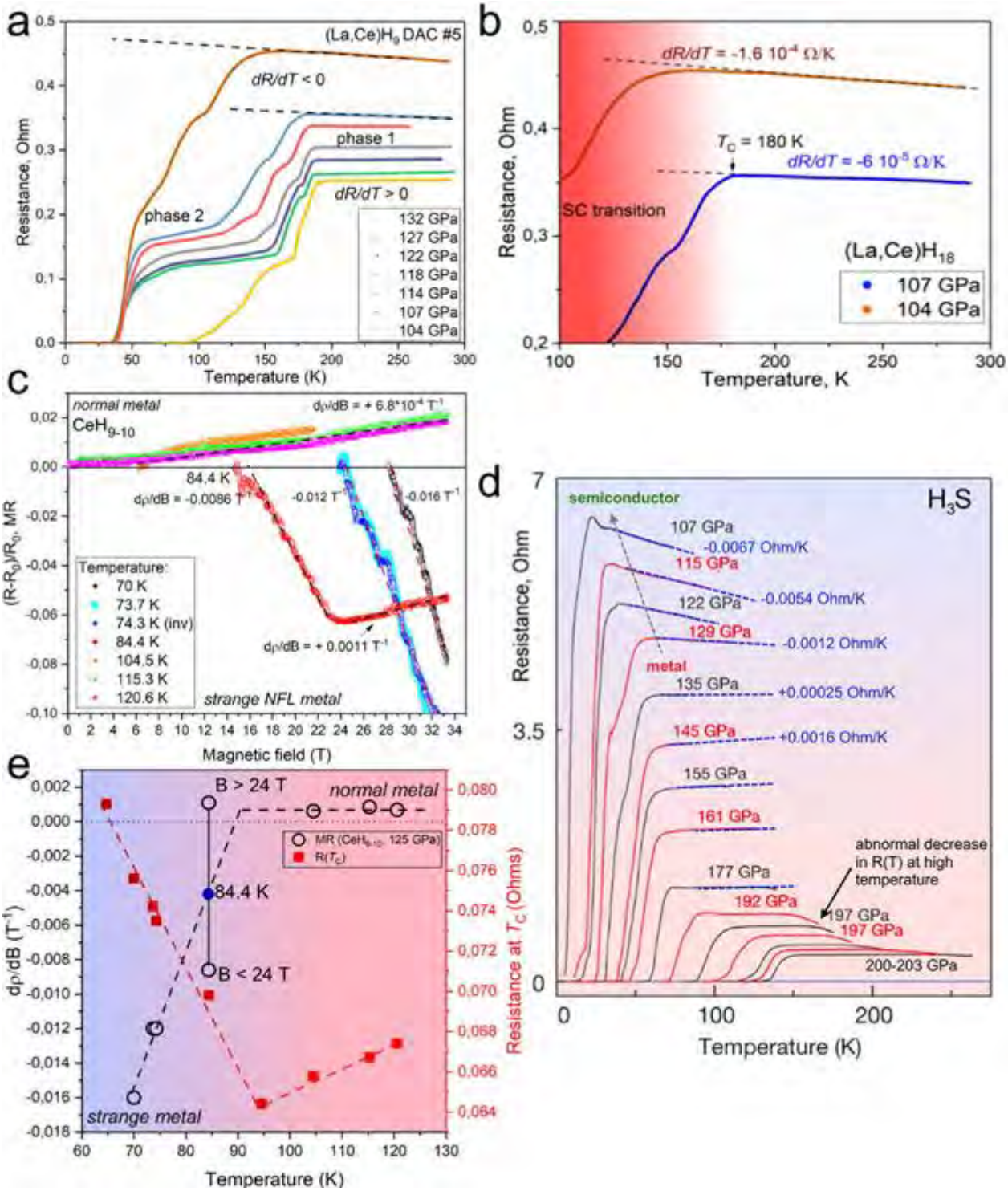
Hydrides 4, July 26, 2023, 14:00–16:15

Recent experiments in strong magnetic fields with cerium (CeH_9-CeH_{10}), tin (SnH_4, [1]), and lanthanum-neodymium ($(La,Nd)H_{10}$, [2]) polyhydrides have shown that the magnetoresistance (MR) and the temperature dependence of the electrical resistance in these materials exhibit anomalous behaviour at low temperatures. Samples of cerium hydrides exhibit negative B-linear magnetoresistance below 85 K, with a slope 20 times higher than positive MR above Tc. Electrical resistance of CeH_9-CeH_{10} below 90–95 K linearly increases with decreasing temperature, which is the opposite of what should be observed in ordinary metals. We managed to completely suppress superconductivity in cerium nonahydride CeH_9 and establish the experimental upper critical magnetic field Bc2(0) = 33-34 T. Bc2(T) of CeH_9 exhibits pronounced saturation at low temperatures, which is typical for Bardeen-Cooper-Schrieffer (BCS) superconductors.

SnH_4 at 170-190 GPa demonstrates unusual behaviour in magnetic fields: B-linear magnetoresistance and a linear temperature dependence of the upper critical magnetic field (Bc2 (0) = 14-16 T), which contradicts the Wertheimer–Helfand–Hohenberg model developed for conventional superconductors. Along with this, the temperature dependence of electrical resistance of fcc SnH_4 in normal resistivity state exhibits a deviation from what is expected for phonon-mediated scattering described by the Bloch-Grüneisen model [1].

The Hall coefficient of $(La,Nd)H_{10}$ sample at 200–250 K changes its sign [2]. At the same time, magnetoresistance becomes very small and even negative at 250 K. Both peculiarities are correlated with a kink in the temperature dependence of the electrical resistance (Tk ≈ 220 K). The anomalous behaviour of magnetoresistance, the Hall effect and electrical resistance at low temperatures in many polyhydrides (Figure 1) points to possible weak localization effects and non-Fermi-liquid properties of the non-superconducting state in these materials.

[1] I. Troyan, D. Semenok et al. “Non-Fermi-Liquid Behavior of Superconducting SnH_4”, ArXiv:2303.06339, 2023.
[2] D. Semenok et al. “Effect of Magnetic Impurities on Superconductivity in LaH_{10}”, Advanced Materials, 2022, 2204038.


a
(La,Ce)H9 DAC #5
dR/dT < 0
phase 1
phase 2
dR/dT > 0
132 GPa
127 GPa
122 GPa
118 GPa
114 GPa
107 GPa
104 GPa
Resistance, Ohm
Temperature (K)
b
dR/dT = -1.6 10-4 Ω/K
TC = 180 K
dR/dT = -6 10-5 Ω/K
SC transition
(La,Ce)H18
107 GPa
104 GPa
Resistance, Ohm
Temperature, K
c
normal metal
CeH9-10
dρ/dB = + 6.8*10-4 T-1
84.4 K
dρ/dB = -0.0086 T-1
-0.012 T-1
-0.016 T-1
dρ/dB = + 0.0011 T-1
Temperature:
70 K
73.7 K
74.3 K (inv)
84.4 K
104.5 K
115.3 K
120.6 K
strange NFL metal
(R-R0)/R0, MR
Magnetic field (T)
d
semiconductor
H3S
107 GPa
-0.0067 Ohm/K
115 GPa
122 GPa
-0.0054 Ohm/K
129 GPa
-0.0012 Ohm/K
metal
135 GPa
+0.00025 Ohm/K
145 GPa
+0.0016 Ohm/K
155 GPa
161 GPa
abnormal decrease
in R(T) at high
temperature
177 GPa
192 GPa
197 GPa
197 GPa
200-203 GPa
Resistance, Ohm
Temperature (K)
e
B > 24 T
normal metal
MR (CeH9-10, 125 GPa)
R(TC)
84.4 K
B < 24 T
strange metal
dρ/dB (T-1)
Resistance at TC (Ohms)
Temperature (K)

Is high-pressure an essential parameter for studying hydrogen-bonded materials? The case of monohydroxy alcohols.

Sebastian Pawlus
[1]*August Chełkowski Institute Of Physics, University of Silesia In Katowice, Chorzów, Poland*

Bio/Life Sciences and Soft Matter, July 26, 2023, 10:15–12:15

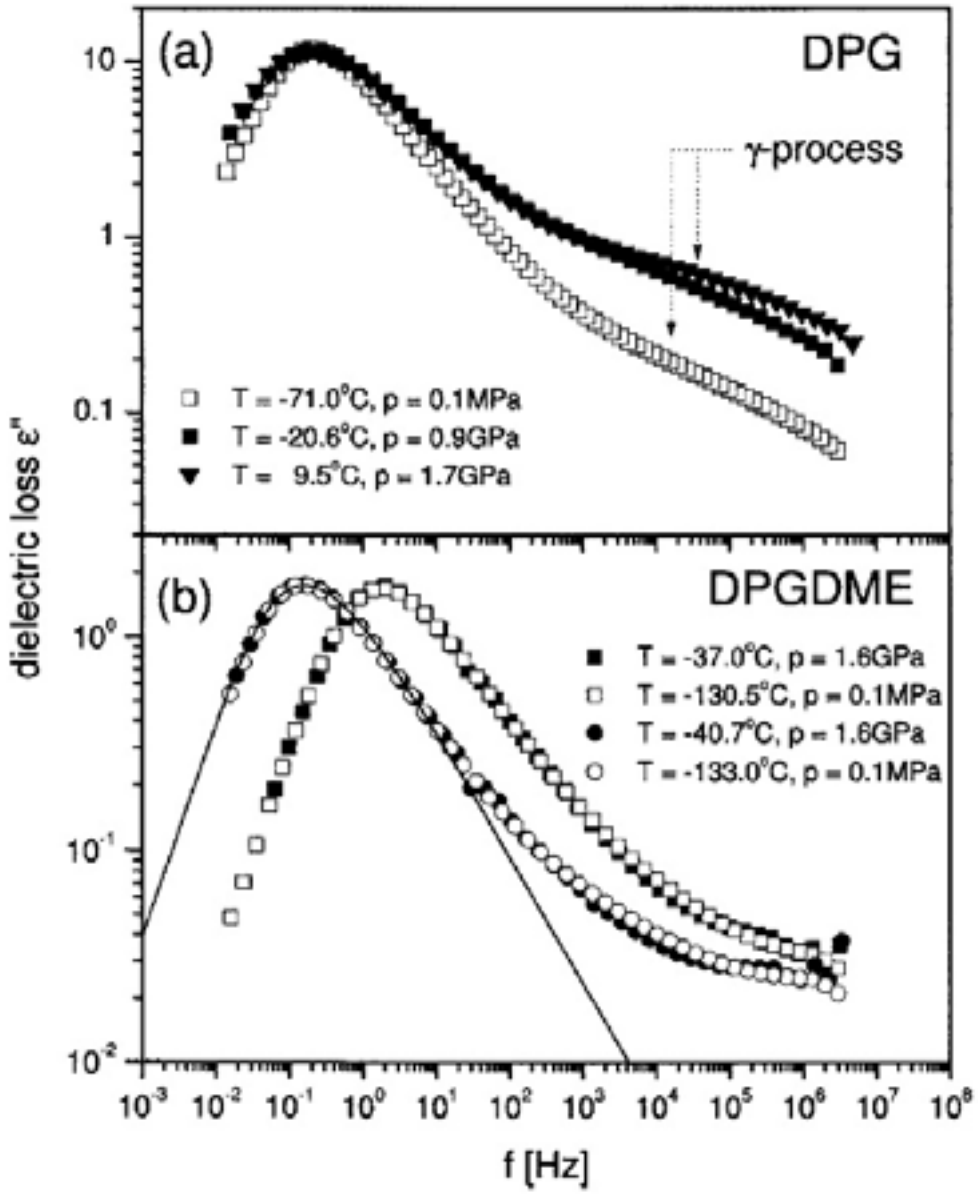
For our community, it is evident that pressure is as significant a parameter as the temperature in studies of the complex properties of various materials in the thermodynamic space. However, this statement remains obscure for many people unfamiliar with high-pressure studies. They still believe that investigations performed only at ambient pressure are sufficient for getting complete knowledge about the features of different materials.

Broadband dielectric spectroscopy is a handy experimental tool for studying dipole materials, especially glass formers, because it enables us to follow their relaxation dynamics in the time range of twelve or more decades. High-pressure investigations of H-bonded supercooled liquids exhibited that their properties, like steepness index and shape of the structural relaxation function, behave differently than, e.g., van der Waals materials.

For example, in the case of compressed dipropylene glycol (H-bonded liquid), the structural relaxation broadens compared to the unpressurised sample. In contrast, no broadening is observed for the methylated sample (van der Waals liquid) for different p-T conditions (i.e. so-called time-temperature-pressure superposition is observed) (see Figure 1 taken from J. Chem. Phys. 125, 144507 (2006); https://doi.org/10.1063/1.2354492). These differences are related to the existence of supramolecular structures developed via H-bonds. In the case of many monohydroxy alcohols, these structures are chain-like. Their presence is reflected as an additional, exponential process (called Debye relaxation), slower than the structural one, more or less visible on the dielectric spectra. It was already shown that increasing pressure modifies these supramolecular structures differently than decreasing temperature. These modifications are observed, as mentioned above, in differences in the relaxation dynamics of the associated material at different thermodynamic paths compared, e.g., for the same time scale of the relaxation processes.

However, for some persons, comparing results for different materials with different values of parameters like viscosity, glass temperature, or structural relaxation times at the same p-T conditions must be more convincing. They can state that comparisons make sense only if we compare materials with identical properties at the same starting thermodynamic conditions. Usually, it isn't easy to find materials that fulfill this criterion.

Fortunately, during this presentation, I will show results for phenyl monohydroxy alcohols that exhibit the same temperature behavior of relaxation dynamics at ambient pressure. Only at compression do differences between them become visible. It is a beautiful exemplification of the meaning of high-pressure studies as a necessary tool for understanding the properties of these alcohols in particular and any materials in general.


(a)
DPG
γ-process
T = -71.0°C, p = 0.1MPa
T = -20.6°C, p = 0.9GPa
T = 9.5°C, p = 1.7GPa
(b)
DPGDME
T = -37.0°C, p = 1.6GPa
T = -130.5°C, p = 0.1MPa
T = -40.7°C, p = 1.6GPa
T = -133.0°C, p = 0.1MPa
dielectric loss ε"
f [Hz]

High-pressure Raman scattering and X-ray diffraction study of the highly-mismatched ternary semiconductor alloy Cd1-xBexTe (x≤0.11)

Abdelmajid Elmahjoubi[1], Mohamad Baker Shoker[1], Olivier Pages[1], Andrei V. Postnikov[1], Vitor J. B. Torres[2], Alain Polian[3,4], Christophe Bellin[3], Keevin Beneut[3], Carole Gardiennet[5], Gwendal Kervern[5], Aotmane En Naciri[1], Laurent Broch[1], Jean-Paul Itie[4], Pascal Franchetti[1], Sébastien Diliberto[6], Stéphanie Michel[6], Ali Abouais[7,8], Karol Strzalkowski[7]

[1]LCP-A2MC, Université de Lorraine, F-57000 Metz, France, [2]Departamento de Fisica and i3N, Universidade de Aveiro, 3810 – 193 Aveiro, Portugal, [3]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université — 11 UMR CNRS 7590, F-75005 Paris, France, [4]Synchrotron SOLEIL, UR1, L'Orme des Merisiers Saint-Aubin, BP 48, F-91192 Gif-sur-Yvette Cedex, France, [5]Laboratoire de Cristallographie, Résonance Magnétique et Modélisations, Université de Lorraine, UMR CNRS 7036 , F-54506 Vandoeuvre-lès-Nancy, France, [6]Institut Jean Lamour, UMR 7198, CNRS, Université de Lorraine , F-57000 Metz, France , [7]Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, PL-87-100 Toruń, Poland, [8]National School of Applied Sciences, Engineering Science for Energy Lab, Chouaib Doukkali University of El Jadida , 24000 El Jadida, Morocco

Chemical Bonding 2, July 24, 2023, 16:30–18:30

The CdTe-BeTe ternary semiconductor alloy exhibits a large contrast between a short (d=2.40 Å) weakly ionic (fi=0.22) Be-Te bond and a long (d=2.81 Å) strongly ionic (fi=0.74) Cd-Te one (ref. [1]) resulting in a widely spaced vibrational mode. This makes the present alloy a benchmark to test the limits of the percolation model that distinguishes between bond vibrations in "same" and "alien" environments (two-phonon mode per bond) (ref. [2]). The percolation model further supports a classification of common semiconductor alloys depending on whether the bimodal pattern per bond converges or diverges under pressure, governed by the relative hardening rates of the same and alien environments under pressure. The large contrast in (Be-Te, Cd-Te) bond physical properties stimulates a broad examination as how the structural and optical properties are impacted by the alloy disorder in this system. To address the raised issues, we have combined high-pressure Raman scattering, high-pressure X-ray diffraction (HP-XRD) and spectroscopic ellipsometry, with ab initio calculations in support.

The Cd1-xBexTe crystals (x≤0.11), grown by the Bridgman method, adopt the zinc-blende structure and the lattice parameter varies linearly with x, like the main electronic transitions measured by spectroscopic ellipsometry. Solid-state nuclear magnetic resonance (NMR) has been utilised to identify the nature of the Cd/Be substitution in the alloy. The 125Te NMR signal has shown two peaks exhibiting a random substitution of the cations Cd and Be according to Bernoulli's law. As apparent in high-pressure X-ray diffractograms taken at the PSICHÉ beamline of SOLEIL synchrotron, the zincblende phase – subsequently studied by high-pressure Raman scattering – is preserved up to 5 GPa, with the following sequence of pressure-induced structural transitions: cubic-F43$\bar{m}$ (zinc-blende) ⟶ cubic-Fm3$\bar{m}$ (rock salt) at about 5 GPa and cubic-Fm3$\bar{m}$⟶ Orthorhomic Cmcm at about 16 GPa.

The bulk modulus (B0) of zincblende Cd0.89Be0.11Te determined from HP-XRD data, i.e., 41.67(8) GPa, is found to drop below the CdTe value, i.e., 43.7(1) GPa (ref. [3]). This markedly deviates from the linear B0 vs. x trend predicted by ab initio calculations, the sign of large anharmonic effects in the real crystal. Still, at the bond scale, the high-pressure Cd0.89Be0.11Te Raman spectra transiently reveal a bimodal phonon pattern per bond for the short/stiff Be-Te bond. The low-frequency mode corresponding to the Be-Te bond immersed in the Be-environment shifted faster under pressure catching up with the high-frequency mode due to the Be-Te bond immersed in the Cd-environment at about 3.5 GPa ,as discussed in the percolation model. The pressure-induced convergence of the Be-Te two Raman modes is independently predicted by ab initio calculations.

[1] Christensen, N. et al. Phys. Rev. B 36, 1032 (1987).
[2] Shoker, M. B. et al. Sci Rep 12, 753 (2022).
[3] McMahon, M. I. et al. Phys. Rev. B 48 (22), (1993).

Rapid Compression of Antimony in Dynamic Diamond Anvil Cells: Hunting the Phase Transitions

Emma Ehrenreich-Petersen[1], Earl O'Bannon[2], Daniel Campbell[2], Bernhard Massani[3], Rachel Husband[1], Stewart McWilliams[3], Hanns-Peter Liermann[1], Zsolt Jenei[2]
[1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany, [2]Lawrence Livermore National Laboratory, Livermore, United States, [3]University of Edinburgh, SoPA, CSEC, Edinburgh, United Kingdom

Static Studies of Elements 1, July 25, 2023, 14:00–16:00

Dynamic diamond anvil cell experiments provide information on the behaviour at high pressures using intermediate strain rates, i.e. strain rates between those generated in shock experiments and those achieved using conventional static diamond anvil cells. Therefore, this tool can be used as a unique probe to disclose hidden strain and compression rates, which reveal new information about the system in question. Here, elemental compounds are of momentous importance and can be particularly interesting for some systems due to the element's plethora of structural transitions observed under high pressures. One such compound, which has been studied in detail in both static and shock experiments, is antimony (Sb). However, there is a lack of results of the behaviour of the element at the intermediate rate between the two extremes. Therefore, in this study, we explore these strain rates and hunt down the multiple phase transitions in the element and expose how the transition pressures depend on the strain rate and reveal whether hidden phases are present.

New Polyhydride Superconductors

Prof. Changqing Jin[1]
[1]*Iopcas, Beijing, China*

Hydrides 1, July 24, 2023, 10:15–12:15

New polyhydrides superconductors are synthesised at high pressure high temperature using synergetic extreme conditions techniques basen on diamond anvil cell in combiantion with laser heating. The synthesised polyhydrides are founded to be superconductors at high pressures including calcium polyhydrides with Tc above 210K[1], the hafnium polyhydrides with Tc above 80K[2] the zircornium polyhydrides with Tc above 70K[3]. The priliminary properties of the supercondcutors will be presented.

[1] Z. W. Li, X. He, C. Q. Jin et al., "Superconductivity above 200K Observed in Superhydrides of Calcium", Nature Communications 13, 2863(2022);
[2] C. L. Zhang, X. He, C. Q. Jin et al., "Superconductivity above 80 K in polyhydrides of hafnium", Materials Today Physics 27, 100826(2022)
[3] C. L. Zhang, X. He, C. Q. Jin et al., "Superconductivity in Zirconium Polyhydrides with Tc above 70 K". Sci. Bull. 67, 907(2022)

Electronic Structure of Quantum Materials at High-Pressure

Yang Ding[1]
[1]*Center for High-pressure Science and Technology Advanced Research, Beijing 100094, China, Beijing, China*

Electronic Transitions 1, July 26, 2023, 16:30–18:30

Quantum materials, which primarily consist of electron correlated materials, topological insulators, and Dirac electron materials, are a seminal topic in condensed matter physics. High-pressure provides a unique way for tuning the emergency of quantum materials. We have recently focused on studying the electronic structure of strongly correlated materials at high pressure, such as rare earth metals and Mott insulators, using synchrotron in conjunction with optical spectroscopy, electrical transport, and theoretical calculations, and our findings have provided insights on how pressure tunes electronic states through the interplay of the spin-charge-orbit-lattice in these materials.

Extended X-ray Absorption Fine Structure (EXAFS) measurements in ramp compressed tantalum at the National Ignition Facility

Andrew Krygier[1], Hong Sio[1], Robert Rudd[1], Stanimir Bonev[1], Federica Coppari[1], Amy Coleman[1], Jon Eggert[1], Stanislav Stoupin[1], Yuan Ping[1]

[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Equation of State 2, July 27, 2023, 14:00–16:00

Dynamic compression is now a widespread technique for investigating material properties at extraordinary pressure, density, and temperature. However, there is a nearly complete lack of temperature measurements across the full scope of this field. As a result, thermal effects remain a large source of uncertainty in equation of state construction. Extended X-ray Absorption Fine Structure (EXAFS), which refers to modulations in the X-ray absorption spectra in the region just above an edge that arise from the photoelectron scattering off of neighbouring atoms, is a powerful diagnostic for characterizing material properties. EXAFS is particularly sensitive to density, temperature, and crystal structure in the range 100s-10000 K, where most materials form a solid at high pressure. Here we present results of several experiments at the National Ignition Facility (NIF) that measured EXAFS from tantalum ramp compressed up to several Mbar following different initial shock states. These measurements are made possible by the high flux X-ray source and high-fidelity laser pulse shaping available at the NIF, as well as the high-resolution X-ray spectrometer design. L-edge EXAFS, which is required for high atomic number materials, is particularly challenging due to intrinsically small amplitude EXAFS oscillations compared to K-edge. We discuss these results and prospects for this capability at NIF.

A large-volume high-pressure diamond anvil cell working under a magnetic field (BENMACON)

Prof Fernando Rodriguez[1], Dr Jesus González[1], Prof Diego Ferreño[1], Mr Jose Antonio Sainz-Aja[1], Mr Oscar Musitu[2], Dr Rodolfo San-Martín[3], Dr Estefania Abad[3], Prof Tetsuo Irifune[4]
[1]University of Cantabria, Santander, Spain, [2]Industrias Mecánicas de Precisión, INMEPRE, Vitoria, Spain, [3]ESS Bilbao, Bilbao, Spain, [4]Ehime University, Matsuyama, Japan

Instrumentation and Techniques 2, July 27, 2023, 10:15–12:15

We present a new large volume diamond anvil cell, named BENMACON, for the investigation of condensed matter systems under extreme pressure and temperature conditions in sample volumes of 1 mm^3. The cell is specially designed with an optical access for simultaneous spectroscopic measurements and imaging. This feature, together with its light weight and small size, makes it unique and extremely competitive for high pressure investigations carried out in home-based laboratories worldwide and at large neutron and synchrotron facilities, where large volume apparatus such as multi-anvil presses and Paris-Edinburgh cells [1-5] are optically blinded without optical access. This allows us to measure pressure in situ from the ruby luminescence R-lines, which is a well-known sensor for pressure and temperature (below about 150 K) [6].
We have developed two cell prototypes, one in steel and a lighter one in a non-magnetic titanium alloy for operation in a magnetic field. The design of the cells was optimised by a complete strain-stress analysis for different plate-anvil geometries and nanopolycrystalline (NPD) anvils [7] using finite element methods [8]. 8 mm-size NPD anvils were mounted on a Boehler-Almax type plate with open contact angles, using NiCoV steel plates instead of CW plates [9-11]. This feature enhances recent large volume press developments for neutron studies [11]. We will present first preliminary results of steel cell operation using steel gaskets and alcohol-water mixtures as pressure transmitting media and ruby for pressure sensing. Initial tests indicate that pressures in excess of 15 GPa can easily be achieved under a 7 ton load. The suitability of large NPD anvils for optical studies is also discussed [12].

We acknowledge the PRIUS Collaborative Project (2014–2022) for suitable NPD anvils. Financial support from the State Research Agency of Spain, Ministry of Science and Innovation, Projects PID2021-127656NB-I00 and MALTA-Consolider Team (RED2018-102612-T), Hazitek Gobierno Vasco ZL-2021/00893 and CDTI IDI-20220305 is acknowledged.

[1] D.J. Dunstan, I.L. Spain, J. Phys. E: Sci. Instrum. 22, 913 (1989)
[2] J.A. Xu and H.K. Mao, Science 290, 783 (2000)
[3] M. Guthrie, Lectures, Oak Ridge National Laboratory 2012 (unpublished results)
[4] J.M. Besson, R.J. Nelmes et al., Physica B: Condens. Matter 180-181, 907 (1992)
[5] N. Kawai, and S. Endo, Rev. Sci. Ins. 41, 1178 (1970)
[6] G. Shen, and other members of the IPPS task group (2020), High Press. Res. 40, 299 (2020)
[7] T. Irifune, A. Kurio, S. Sakamoto, T. Inoue, and H. Sumiya, Nature 421, 599 (2003)
[8] Software ANSYS, Static Structural module from ANSYS WORKBENCH
[9] R. Boehler, Rev. Sci. Instr. 77, 115103 (2006)
[10] R. Boehler, et al. High Press. Res. 33, 546 (2013)
[11] B. Haberl, J.J. Molaison, J.C. Neuefeind, L.L. Daemen and R. Boehler, High Press. Res.39, 426 (2019)
[12] J.A. Barreda-Argüeso, et al., High Press. Res. 40, 107 (2020)

The discovery of novel high-pressure yttrium nitrides in laser-heated diamond anvil cells using the Domain Auto Finder (DAFi) program

Andrey Aslandukov[1,2], Prof. Natalia Dubrovinskaia[2,3], Prof. Leonid Dubrovinsky[1]
[1]Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, Germany, [2]Material Physics and Technology at Extreme Conditions, Laboratory of Crystallography, University of Bayreuth, Bayreuth, Germany, [3]Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, Sweden

Nitrides, Borides and Carbides 2, July 25, 2023, 14:00–16:00

The laser-heated diamond anvil cell technique is the most powerful method for the synthesis of novel compounds under pressures up to 1000 GPa and temperatures up to 6000K. Laser heating of chemical precursors in a diamond anvil cell usually results in the crystallization of many tiny crystallites of one or several reaction products. Synchrotron singe-crystal X-ray diffraction (SCXRD) data analysis can be applied to determine the crystal structures of novel compounds. However, the superposition of numerous reflections originating from a large number of single-crystal domains of the same and/or different (especially unknown) phases precludes sorting out the reflections coming from individual domains which makes their automatic indexing impossible. Here we present the DAFi program [1] designed for the quick search of subsets of reflections from individual domains in the whole set of SCXRD data from seemingly polycrystalline samples and its application to study the Y-N system up to megabar pressures [2,3].

Chemical reactions between yttrium and nitrogen were realised in laser-heated diamond anvil cells at 50 GPa and 100 GPa and 2000-3000 K. Products of the reactions were analyzed using in situ high-pressure synchrotron SCXRD. The DAFi program enabled sorting out the sets of reflections of individual crystallites. Further SCXRD analysis revealed the crystal structures of three novel solids: Y_5N_{14} at 50 GPa, and YN_6 along with Y_2N_{11} at 100 GPa. The crystal structure of Y_5N_{14} contains three distinct types of nitrogen dimers (Fig. 1a). Crystal chemical analysis and ab initio calculations demonstrated that the dimers $[N_2]^{x-}$ are crystallographically and chemically non-equivalent and possess distinct non-integer formal charges (x) that make Y_5N_{14} unique among known dinitrides. The crystal structures of YN_6 and Y_2N_{11} (Fig. 1b,c) feature unique structural units—a previously unknown anionic N_{18} macrocycle and a polynitrogen double helix, respectively. Their discovery significantly extends the chemistry of polynitrides.

[1] Aslandukov, A., Aslandukov, M., Dubrovinskaia, N., Dubrovinsky, L. (2022). J. Appl. Crystallogr., 55(5), 1383-1391
[2] Aslandukov, A., Aslandukova, A., Laniel, D., Koemets, I., Fedotenko, T., Yuan, L., Steinle-Neumann, G., Glazyrin, K., Hanfland, M., Dubrovinsky, L., Dubrovinskaia, N. (2021). J. Phys. Chem. C., 125(32), 18077-18084.
[3] Aslandukov, A., Trybel, F., Aslandukova, A., Laniel, D., Fedotenko, T., Khandarkhaeva, S., Aprilis, G., Giacobbe, C., Bright, E.L., Abrikosov, I.A., Dubrovinsky, L., Dubrovinskaia, N. (2022). Angew. Chem., 61(34), e202207469.

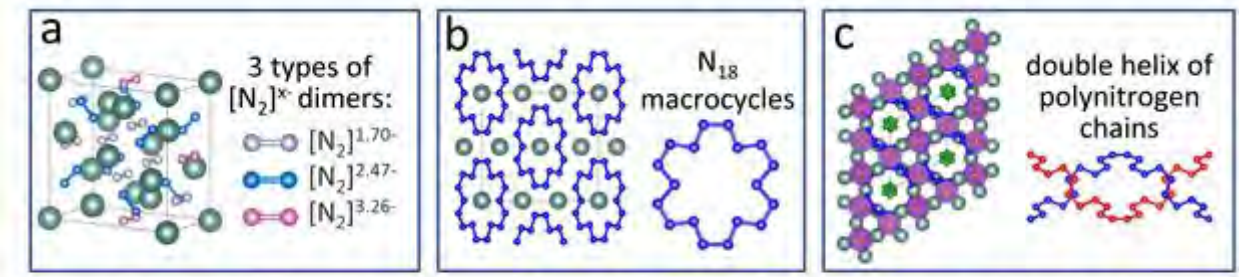


Figure 1. The crystal structures of (a) Y_5N_{14}, (b) YN_6, (c) Y_2N_{11}, and corresponding characteristic anionic nitrogen species. All Y atoms are greenish, other colors correspond to N atoms.

Monitoring gold nanoparticles at high pressure through in situ small-angle X-ray scattering

Camino Martín-Sánchez[1,2], Ana Sánchez-Iglesias[3], Jose Antonio Barreda Argüeso[1], Alain Polian[4], Luis M. Liz-Marzán[3,5], Fernando Rodríguez[1]

[1]MALTA Consolider, Departamento CITIMAC, Universidad de Cantabria, Santander, Spain, [2]Département de Chimie Physique, Université de Genève, Genève, Switzerland, [3]CIC biomaGUNE and CIBER-BBN, Donostia- San Sebastián, Spain, [4]Synchrotron SOLEIL, Gif-sur-Yvette, France, [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Nanoscale Systems, July 24, 2023, 16:30–18:30

In the last ten years, there has been significant progress in the use of noble metal nanoparticles for sensing in high-pressure experiments [1-10]. Particularly, those methods based on optical spectroscopy are very attractive, since they exploit the high sensitivity of surface plasmonic resonances (SPR) in gold nanoparticles (AuNP). The main driving mechanisms for the pressure-induced LSPR shifts are governed by two competing effects [4,5]: a redshift by the increase of refractive index of the surrounding medium (acting as pressure-transmitting medium), and the blueshift caused by the gold plasmon frequency due to increase in the conduction electron concentration.

Gold nanoparticle sensing assumes that AuNP remains dispersed (non-interacting) in the colloid along the pressurization process. In this way, gold nanorods (AuNR) provides a better sensitivity for refractive index sensing through their longitudinal SPR than gold nanospheres (AuNS) [6-8]. However, in contrast to AuNS, the optical extinction spectra of AuNR show abnormal behavior above the solidification pressure of the transmitting medium. This different behavior of AuNR and AuNS under non-hydrostatic high-pressure conditions has been attributed to either NP aggregation and/or NP deformation. Indeed, AuNR have a big tendency to aggregate and if this occurs SPR pressure shifts based on single-particle models are no longer valid.

Transmission electron microscopy (TEM) is the most powerful tool to get direct information on the structural changes undergone by the NP. However, in a high-pressure experiment using a diamond anvil cell (DAC), TEM images can be obtained only before and after the pressure treatment (in depressurised recovered AuNP) [10]. Thus, in situ characterization of metal NP colloids at given pressure and temperature conditions remains challenging when utilizing DAC.

In this work, we monitor the effects of non-hydrostatic high-pressure on the morphology and stability of AuNR and AuNS through small-angle X-ray scattering (SAXS). Although limited in reachable pressure due to current technical constraints, SAXS provides a powerful tool for the in situ observation of the form factor (nanoparticle) and the structure factor (interparticle correlation). Here, we demonstrate that under high-pressure conditions, AuNS remain isolated in both hydrostatic and non-hydrostatic regimes. In opposition, AuNR start to aggregate above the solidification pressure. This result unravels that diffusion of nanorods yielding aggregation takes place in the solid state of the solvent, an unprecedent phenomenon which cannot be evidenced by TEM using DACs but has been demonstrated by in situ SAXS measurements.

[1] Y. Bao et al. J. Appl. Phys. 2014, 115, 223503.
[2] Y. Bao et al. Appl. Phys. Lett. 2015, 107, 201909.
[3] X. Gu et al. Phys. Rev. Lett. 2018, 121, 056102.
[4] F. Medeghini et al. ACS Nano 2018, 12, 10310−10316.
[5] C. Martín-Sánchez et al. ACS Nano 2019, 13, 498-504.
[6] C. Martín-Sánchez et al. J. Phys. Chem. Lett. 2019, 10, 1587−1593.
[7] M. Runowski et al. Nanoscale 2019, 11, 8718−8726.
[8] C. Martín-Sánchez et al. J. Phys. Chem. C. 2020, 124, 8978−8983.
[9] K. A. Harkins et al. J. Phys. Chem. C 2021, 125, 27747−27752
[10] C. Martín-Sánchez et al. J. Phys. Chem. C. 2022, 126, 1982-1990.

Measuring viscoelasticity inside the laser-heated Diamond Anvil Cell: Time-resolved Synchrotron Mössbauer Source spectroscopy

Georgios Aprilis[1], Prof Dr Leonid Dubrovinsky[2], Dr Sergey Yaroslavtsev[1], Mr Xiang Li[3], Dr Kirsten Schulze[2], Ms Fariia Iasmin Akbar[2], Dr Stella Chariton[4], Mr Andrey Aslandukov[2,5], Ms Yuqing Yin[5,6], Dr Dominique Laniel[5,7], Mr Wenju Zhou[5], Dr Vitali Prakapenka[4], Dr Aleksandr Chumakov[1]

[1]ESRF – The European Synchrotron, Grenoble, France, [2]Bayerisches Geoinstitut, Universität Bayreuth , Bayreuth, Germany, [3]Institute for Mineralogy, University of Münster, Münster, Germany, [4]Center for Advanced Radiation Sources, University of Chicago, Chicago, United States, [5]Materials Physics & Technology at Extreme Conditions, Laboratory of Crystallography, Universität Bayreuth, Bayreuth, Germany, [6]State Key Laboratory of Crystal Materials, Shandong University, Jinan, China, [7]Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom

Instrumentation and Techniques 3, July 26, 2023, 14:00–16:00

While recent progress has been made in estimating the viscosity of minerals at conditions of the lower mantle, most of the studies do not include a direct measurement at both high pressure and temperature conditions. Estimations are deduced indirectly, by strain measurements at room temperature [1], modelling using homologous temperature scaling based on melting curves [2], ex situ compositional and textural analysis [3], or dislocation dynamics simulations [4]. The indirect determination introduces significant difficulties leading to large uncertainties in viscosity values. The newly developed detection scheme of the Nuclear Resonance Beamline (ID18) at the ESRF is used to perform fully time-resolved Synchrotron Mössbauer Source (SMS) [5] spectroscopy at high pressures, in combination with pulsed laser heating in Diamond Anvil cells (DACs) [6]. The experimental scheme allows the time-resolved observation of the Mössbauer absorption of the sample along the duration of the laser pulse and the estimation of its temperature on both heated surfaces using spectroradiometry as well as in bulk from the center shift of the Mössbauer spectra.

Pulse heating of an iron foil causes its displacement [7] and relaxation inside the pressure medium which is expressed as a dramatic change in the centre shift of the Mössbauer spectra, being the result of the doppler effect due to the movement of the foil relative to the Mössbauer source. Integrating the centre shift over time yields maximum displacements on the order of nanometers. The damping of the oscillation of the iron foil inside the surrounding pressure medium is related to the rheological properties of both the heat absorber (Fe foil) as well as the surrounding material (pressure medium). The strain rate that is necessary for the calculation of viscoelastic parameters can be directly derived from the heat absorber displacement inside the surrounding material, after correcting for the thermal pressure.

In this contribution, I would like to report the latest results in the progress of extracting the viscoelastic properties of laser heated samples inside the diamond anvil cell at pressure-temperature conditions of the lower mantle.

[1] H. Marquardt and L. Miyagi, Nature Geoscience 8, 311 (2015).
[2] J. Deng and K.K.M. Lee, Nature Communications 8, 1997 (2017).
[3] Z. Du, Dissertation, Yale University (2015).
[4] R. Reali et al., Physics of the Earth and Planetary Interiors 287, 65 (2019).
[5] V. Potapkin et al., Journal of synchrotron radiation 19, 559–569 (2012).
[6] G. Aprilis et al., Review of Scientific Instruments 88, 084501 (2017).
[7] F. Vagizov et al., Hyperfine Interactions 167, 917 (2006).

Influence of elastic anisotropy on measured sound velocities of cubic solids

Dr. Andreas Zerr[1], Dr. Feng Xu[2], Prof. Philippe Djemia[1], Prof. Yves Roussigné[1]
[1]Laboratoire des Sciences des Procédés et des Matériaux – CNRS, Villetaneuse, France, [2]School of Science, Wuhan University of Technology, Wuhan, China

Instrumentation and Techniques 4, July 26, 2023, 16:30–18:30

Pressure dependences of the longitudinal sound velocities, VL(P), single-crystal elastic moduli, Cij(P), and elastic anisotropy, described through the Zener anisotropy ratio $A=2C_{44}/(C_{11}-C_{12})=C_{44}/C'$, of three simple cubic solids, namely, sold argon, cubic H_2O ice and NaCl (B1-phase) were recently measured using the technique of the picosecond laser ultrasonics (ps-LU) [1-4]. These experiments revealed growing with pressure elastic anisotropy: A≈6 for argon at P=49 GPa, A≈6.5 for H_2O-ice VII at 62 GPa, A≈0.27 for NaCl-B1 at P=28 GPa. The latter manifested itself in diverging of the VL-extremes in single crystals corresponding, in cubic crystals, to the crystallographic directions <111> and <100>, while $VL_{111}>VL_{100}$ if A>1 and vice-versa if A<1. Moreover, the VLav(P) dependences measured for polycrystalline samples of these solids using Brillouin light scattering (BLS) e.g.[5-7] were found to approach VL_{110}(P), independent of the A(P) value, and to deviate from the VLH(P) dependences calculated applying the experimental Cij(P) and the Hill approximation. Here, we show that the latter inconsistency is caused by the elastic anisotropy and that the BLS provides overestimated longitudinal and transversal sound velocities of polycrystalline cubic solids, VLav(P) and VTav(P), respectively, if A>1 and underestimated VLav(P) and VTav(P) if A<1. However, the chance to recognise BLS-peaks of transversal waves in the polycrystalline solids decreases with increasing elastic anisotropy due to the peak broadening and splitting [3]. Distortion of the peaks of the longitudinal waves is less pronounced but still significant.

We evaluated the influence of such distortion on the aggregate shear modulus, Gav(P), derived from the VLav(P) and the bulk modulus, B(P), obtained from an EOS. For solid Ar at P=49 GPa, we found that Gav deviates from GH by ~50%. Furthermore, our LU- and BLS-measurements on polycrystalline γ-Ge_3N_4 having spinel structure [8] confirmed that the elastic anisotropy also influenced position and shape of the Rayleigh peak in the BLS measurements. In general, VRav is underestimated if A>1 and overestimated if A<1. Our evaluation of the influence of anisotropy on the BLS-peaks of γ-Ge_3N_4, with calculated A=2.1 [9], resulted in G underestimated by ~9% and B overestimated by ~29%.

However, similar limitations are relevant for any technique measuring sound velocities with probes having sizes comparable with those of the sample grains. The most reliable approach remains measurement of Cij(P) and extraction of the values of interest using the Hill (or similar) approximation. The ps-LU meets well this requirement at high pressures, also in excess of 100 GPa, because its high 3D-resolution makes use of single crystals unnecessary.

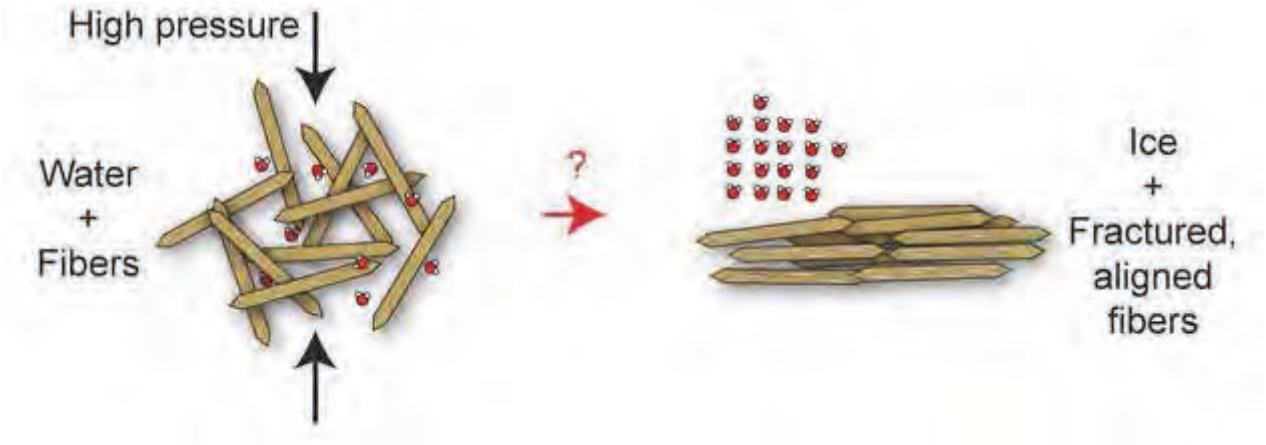
[1] Kuriakose M., et al., Phys. Rev. B 96, 134122 (2017)
[2] Raetz S., et al., Phys. Rev. B 99, 224102 (2019)
[3] Xu F., et al., J. Appl. Phys. 130, 035903 (2021)
[4] Xu F., et al., arXiv, 2209.10899 (2022)
[5] Ahart M., et al., J. Chem. Phys. 134, 124517 (2011)
[6] Grimsditch M., et al., Phys. Rev. B 33, 7192-7200 (1986)
[7] Campbell A.J. and Heinz D.L., Science 257, 66-68 (1992)
[8] Feldbach E., et al., Electron. Mater. Lett. 17, 315-323 (2021)
[9] Li C., et al., (submitted, 2023)

Effects of extreme hydrostatic pressure on the wood-pulp fibre cell wall structure

Rohan Ajit Kulkarni[1], Dr Fredrik Lundell[1], Dr Per Tomas Larsson[1], Dr Lars Wågberg[1], Dr Daniel Söderberg[1]
[1]KTH, Stockholm, Sweden

Bio/Life Sciences and Soft Matter, July 26, 2023, 10:15–12:15

Efficient routes for controlled modification of the wood-pulp fibre cell wall structure are attractive for obtaining increased accessibility to the fibre interior and enabling functionalization such as controlled drug delivery, interpenetrated networks, and selective removal of metal ions from aqueous mixtures to mention a few examples. By changing the physical state of water, it should be possible to significantly alter the structure of the wet fibre wall, providing the possibility to perform cell wall modifications under extreme conditions. To address this challenge, we have investigated the structural development of the wet softwood kraft pulp fibre wall under high pressure and high temperature (HPHT) conditions (up to 2 GPa and 100 °C). Characterisation has been performed to clarify the effects on the porosity and the accessibility of the fibre wall, before and after the HPHT treatment. Furthermore, changes in the crystalline structure have been identified, including in situ X-ray diffraction measurements at high pressures performed at the P02.2 Extreme Conditions Beamline at the DESY/Petra III synchrotron in Hamburg. These measurements have been complemented with Electron microscopy, X-ray diffraction, Small and wide-angle X-ray scattering, and Cross-polarised/magic angle spinning 13C-NMR. Key findings from the experiments show that extreme conditions cause changes in crystallinity, specific surface area, bound water content and surface morphology.



Extreme Zr-based synthetic phases for the safe disposal of nuclear waste

Volodymyr Svitlyk[1,2], Stephan Weiss[1], Christoph Hennig[1,2]
[1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Dresden, Germany, [2]Rossendorf Beamline (BM20), European Synchrotron Radiation Facility, Grenoble, France

Ceramics and Composites, July 24, 2023, 14:00–16:00

Nuclear energy is a key component in the world's energy mix, and as such, the safe management and disposal of nuclear waste is of utmost importance. One approach to managing nuclear waste is through the use of underground depositories for long-term storage. However, the safety of these depositories remains a concern, as the radioactivity of the waste poses a potential threat to human health and the environment for thousands of years. To address this concern, novel materials for immobilization of radiotoxic actinides are developed, such as Zr-based ceramics. These ceramics have been shown promising as potential hosts for long-term storage of tetravalent actinides. By using these materials, the goal is to reduce the risks associated with discharge of radiotoxic elements from nuclear waste storage and ensure the safety of future generations.

Placed underground for long-term storage (~10^6 years), phases containing radioactive elements are be exposed to elevated T and P. Depths of up to 15 km have been considered for these installations [1] where the corresponding values of T and P can reach 400˚C and 0.4 GPa, respectively. In this work we present synchrotron radiation diffraction experiments with in situ application of extreme T and P on phases intended for long-term immobilisation of tetravalent actinides.

Studied phases were Zr-based systems, synthetic and improved analogues of natural rocks. In particular, Y-stabilised ZrO2 (YSZ) was found to incorporate substantial amount of tetravalent actinides [2] and these phases exhibit excellent phase and structural stabilities when heated to elevated temperatures [3]. In addition, upon application of HP the cubic YSZ phase remained stable until 11 GPa [3]. However, the tetragonal YSZ phase showed transition towards higher symmetry at 9 GPa. Nevertheless, concentration of the incorporated tetravalent ions remained constant up to at least 12 GPa [3].

Studies on another family of compounds, derivatives of zircon ZrSiO4 mineral, will be presented as well. In this system phase diagram is severely influenced by synthetic procedure. Moreover, application of HP induces different responses for the corresponding phases. Specifically, Th-doped ZrSiO4 phases hydrothermally synthesised at low pH are found to be less stable than the corresponding phases synthesised at higher pH upon application of HP.

Corresponding phase and structural behavior will be illustrated in detail. Essential technical specifications of the BM20 ROBL station will be presented as well.

[1] L. Krall, T. McCartin, A. Macfarlane. Environ. Sci. Technol. 54 (2020) 629.
[2] V. Svitlyk, S. Weiss, C. Hennig. J. Am. Ceram. Soc., 105 (2022), 5975.
[3] V. Svitlyk, S. Weiss, C. Hennig. J. Am. Ceram. Soc., 105 (2022), 7831.

Structural, Vibrational and Electronic Behavior of Two GaGeTe Polytypes under Compression

Dr. Enrico Bandiello[1], Dr. Samuel Gallego-Parra[1], Dr. Akun Liang[2], Prof. Juan Ángel Sans[1], Prof. Vanesa Cuenca-Gotor[1], Dr. Estelina Lora da Silva[3], Prof. Rosario Vilaplana[1], Prof. Plácida Rodríguez-Hernández[4], Prof. Alfonso Muñoz[4], Mr. Daniel Díaz-Anichtchenko[2], Dr. Catalin Popescu[5], Dr. Frederico Gil Alabarse[6], Dr. Carlos Rudamás[7], Prof. Čestmír Drašar[8], Prof. Daniel Errandonea[2], Prof. Alfredo Segura[2], **Prof. Fransico Javier Manjón**[1]

[1]Universitat Politècnica de València, Valencia, Spain, [2]Universidad de Valencia, Valencia, Spain, [3]University of Porto, Porto, Portugal, [4]Universidad de La Laguna, La Laguna, Spain, [5]CELLS – ALBA Synchrotron Light Facility, Cerdanyola de Vallés (Barcelona), Spain, [6]Elettra Synchrotron, Basovizza (Trieste), Italy, [7]Universidad de El Salvador, San Salvador, El Salvador, [8]University of Pardubice, Pardubice, Czech Republic

Synthesis and Properties of Novel Materials 2, July 26, 2023, 10:15–12:15

GaGeTe is a layered topological semimetal that exists in at least two different polytypes: α-GaGeTe and β-GaGeTe. In this work, we conducted an extensive study of the structural, vibrational, and electronic features of these polytypes under ambient and high-pressure conditions.

X-ray diffraction reveals that the compressibility of α- and β-GaGeTe is anisotropic, and two-phase transitions occur under compression. The first transition occurs above 7 GPa, and the second one above 15 GPa, as also confirmed by Raman spectroscopy. Although the high-pressure phases above 7 GPa could not be directly confirmed, comparison with other chalcogenides and total-energy calculations enable us to propose possible high-pressure phases for both polytypes, which feature an increase in coordination for Ga and Ge atoms from 4 to 6. Above 15 GPa, both polytypes undergo a transition to a structure of higher symmetry, as evidenced by the simplification of X-ray patterns. This observation is consistent with previous studies on compounds such as GaTe, GaSe, and InSe, which exhibit rocksalt-like high-pressure structures. Furthermore, pressure-induced amorphization is observed for GaGeTe upon pressure release. We also calculate and discuss the equation of state for both polytypes.

Raman spectroscopy confirms the presence of the two-phase transitions. The first transition is indicated by changes in the pressure dependence of the Raman active modes, while the second transition is signaled by the disappearance of the Raman activity of the samples.

We find that both polytypes of GaGeTe are indirect semiconductors, with very small band gaps at room pressure. The electronic band structures of α-GaGeTe and β-GaGeTe and their pressure dependence exhibit similarities to III-VI semiconductors, such as GaTe, suggesting that the germanene-like sublayer induces a semimetallic character in both GaGeTe polytypes. Finally, we discuss the dependence of the band gap and topological properties of both polytypes.

High pressure studies in compounds with multicenter bonds

Prof. Dr. Francisco Javier Manjón[1], Dr. Hussien Helmy Hassan Osman[2,3]
[1]Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Universitat Politècnica de València, Valencia, Spain, [2]Instituto de Ciencia de Materiales, MALTA Consolider Team, Universitat de València, Valencia, Spain, [3]Chemistry Department, Faculty of Science, Helwan University, El Cairo, Egypt

Chemical Bonding 1, July 24, 2023, 14:00–16:00

Binary IV-VI and V2-VI3 compounds (also their related ternary IV-V2-VI4 compounds) can be divided into two clases: i) Those that are common semiconductors with relatively large bandgaps, whose atomic coordination (8-N) follows from the octet rule, and ii) those with very low bandgaps, whose atomic coordination does not follow from the octet rule. The later compounds exhibit an extraordinary property portfolio that makes them ideal for phase change materials (PCMs) in re-writable data storage in DVDs and BlueRays, phase change RAM memories, highly efficient thermoelectric systems, and also as topological materials [1-3].

In order to explain their exceptional properties, chemical bonding in PCMs of IV-VI and V2-VI3 families has recently been paid a great attention. Several bonding models, such as resonant bonding, electron-rich multicenter bonding, hypervalent bonding, and metavalent bonding, have been proposed to explain the unconventional type of bond present in PCMs that is intermediate between ionocovalent and metallic bonds, as recently reviewed by Jones [4]. He has concluded that all these models allow describing the same kind of unconventional bond from different perspectives and has proposed that the bonding of PCMs should be named electron-rich multicenter (ERM) bonding, because the existence of multicenter bonds was already postulated on the early days of quantum mechanics [5].

The lack of consensus regarding the notation of this unconventional type of bond is in part due to the few studied solids with this type of bond. In fact, multicenter bonds were not even mentioned by L. Pauling in his well-known book [6] because he likely thought it was a similar type of bond as that present in metals. This explains why this bond has been rediscovered several times along the last century under different notations. In this talk, we will present the poorly-known ERM bond, a more common interaction than previously thought, for Condensed Matter Scientists and will show results on several solid compounds with this kind of bond at high pressure that will help us to show how pressure can help us to understand this type of interaction and its associated properties.

Acknowledgments: This work is part of the Project MALTA Consolider Team network (RED2018-102612-T), financed by MINECO/AEI/10.13039/501100003329; by I+D+i project PID2019-106383GB-42, financed by MCIN/AEI/10.13039/501100011033; and by projects, PROMETEO CIPROM/2021/075 (GREENMAT) and MFA/2022/025 (ARCANGEL), financed by Generalitat Valenciana with "NextGenerationEU"/PRTR funds. H.H.O. acknowledges financial support from GREENMAT project.

[1] M. Wuttig and N. Yamada, Nature Materials 6, 824 (2007).
[2] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[3] I. T. Witting, T. C. Chasapis, F. Ricci, M. Peters, N. A. Heinz, G. Hautier, G. J. Snyder, Advanced Electronic Materials 5, 1800904 (2019).

Inner shell chemistry at extreme conditions

Professor Michael Pravica[1], Mr. Trimaan Malik[1], Dr. Narayan Appathurai[2], Dr. Al Rahemtulla[2], Dr. Beatriz Diaz *Moreno*[2]
[1]University Of Nevada Las Vegas, LAS VEGAS, United States, [2]Brockhouse Beamline, Canadian Light Source, University of Saskatchewan, Saskatoon, Canada

Chemical Bonding 1, July 24, 2023, 14:00–16:00

We have been seeking to verify predictions of certain heavy elements (e.g. Cs and Hg) that, when subjected to high pressure (>10 GPa) in an environment rich in molecular fluorine, will change their oxidation states, enabling inner shell electrons to bond with fluorine to form novel exotic compounds such as CsF3 (e.g. via CsF + F2 →CsF3) and HgF4 (via HgF2 + F2 →HgF4) [1]. It is thus necessary to develop a means to load fluorine with a reactant (e.g. Hg or Cs) and observe the predicted chemical reaction at high pressure. However, toxic fluorine, as the most electronegative element, is very challenging to load in a diamond anvil cell. It is thus no surprise that there is only one study of fluorine at high pressure that we are aware of [2]. We have managed to develop a method to release fluorine in situ inside a diamond anvil cell (DAC) by irradiating a fluorine-rich compound (e.g. C6F14 [3], KBF4 [4] and XeF2 [5]) with hard X-rays (which penetrate the diamonds), to break down the fluorine-bearing compound and release F2 (e.g. XeF2 + hv →Xe + F2). Thus, by mixing CsF or HgF2, (both easy-to-load solid powders at ambient conditions) with a fluorine-rich compound such as XeF2 (also a powder), we can produce molecular fluorine at will via X-ray irradiation inside a sealed DAC to be available for chemical reactions at high pressure.

Here, we report on two X-ray experiments at the Brockhouse beamline of the Canadian Light Source: (CsF + XeF2) and (HgF2+XeF2), respectively. In both cases, the samples, each loaded in an inert gas glove box and sealed at high pressure, were initially irradiated to release molecular fluorine in situ. Afterward, both samples were further pressurised, and X-ray diffraction patterns were recorded up to 40 GPa. Significant changes in X-ray diffraction patterns from both samples were observed above 10 GPa in both cases which suggest the possibility that fluorine reacted with the CsF and HgF2, respectively. Observations from the HgF2 experiment correlate with bonding changes observed with far-IR spectroscopy [5].

[1] M. Miao, J. Botana, M. Pravica, D. Sneed, C. Park, Japanese Journal of Applied Physics 56 05FA10 (2017).
[2] “Raman spectra and phase diagram of fluorine at pressures up to 6 GPa and temperatures between 10 and 320 K,” D. Schiferl, S. Kinkead, R.C. Hanson, D.A. Pinnick, J. Chem. Phys. 87(5) 3016-3021 (1987).
[3] “Novel method for producing molecular fluorine,” M. Pravica, D. Sneed, M. White and Y. Wang, Review of Scientific Instruments, 85, 086110 (2014).
[4] “A novel method to create molecular mixtures at high pressures: The case of fluorine and oxygen,” M. Pravica, M. White and Y. Wang, Shock Compression of Condensed Matter 2015-AIP Conference Proceedings, 1793, pp. 060030:1–4 (2017).
[5] “Fluorine chemistry at extreme conditions: possible synthesis of HgF4,” M. Pravica, S. Schyck, B. Harris, P. Cifligu, B. Billinghurst, Papers in Physics 11, 110001 (2019).

Fig. 1 (Left): An irradiated sample of C_6F_{14} (see green-yellow region in the center) as viewed between the diamonds with a microscope. (Right):After the sample was depressurized and released and the gasket material removed, a damage pit remained in the diamond surface etched by F_2 released during irradiation.

Fig. 2. Colored α-F_2 (left) 15GPa and (right) 44GPa with a novel Hg compound (possibly HgF_4) in the center formed via hard x-rays and pressure. Similar to O_2, F_2 is colored under pressure.

The synthesis and property study of ternary high-temperature superconducting polyhydride under high pressure

Guangtao Liu
[1]*Jilin University, Changchun, China*

Hydrides 4, July 26, 2023, 14:00–16:15

In the past decade, the discovery of SH3 and LaH10 with Tc exceeding 200 K ignited the enthusiasm of human beings to search for high-temperature superconductors under high pressure. No other recognised hydride with Tc higher than LaH10 has been obtained, although almost all binary hydrides with various stoichiometries have been theoretically and experimentally investigated. At present, the research focus has thus shifted to the ternary system with a higher degree of freedom, which may bring new opportunities for the search for room-temperature superconductor under high pressure. Recently, we successfully synthesised and characterised a series of ternary high-Tc hydrides near megabar pressure, such as (La,Ce)H9, providing clear experimental evidence of giant Tc enhancement. Our experimental results establish an important paradigm in search of new ternary or potential higher multinary high-Tc superhydrides via a suitable combination of metal elements.

Synthesis of single-bonded cubic AsN from the high-pressure and high-temperature chemical reaction of arsenic and nitrogen

Matteo Ceppatelli[1,2], Demetrio Scelta[1,2], Manuel Serrano-Ruiz[2], Kamil Dziubek[1], Marta Morana[3], Volodymyr Svitlyk[4], Gaston Garbarino[4], Tomasz Poręba[4], Mohamed Mezouar[4], Maurizio Peruzzini[2], Roberto Bini[1,2,5]

[1]LENS – European Laboratory for Non-linear Spectroscopy, Sesto Fiorentino (FI), Italy, [2]ICCOM-CNR, Institute of Chemistry of OrganoMetallic Compounds, National Research Council of Italy, Sesto Fiorentino (FI), Italy, [3]Dipartimento di Scienze della Terra, Università degli Studi di Firenze, Firenze (FI), Italy, [4]ESRF – European Synchrotron Radiation Facility, Grenoble, France, [5]Dipartimento di Chimica "Ugo Schiff", Università degli Studi di Firenze, Sesto Fiorentino (FI), Italy

Nitrides, Borides and Carbides 1, July 24, 2023, 14:00–16:00

Taking advantage of our results on phosphorus [1, 2], high-pressure (>25 GPa) and high-temperature (>1400 K) conditions, generated by a laser heated diamond anvil cell, have been successfully employed to induce a direct chemical reaction between As and N2, leading to the synthesis of crystalline arsenic nitride [3].

The analysis of single-crystal synchrotron X-ray diffraction data, acquired at different pressure points between 30 and 40 GPa, provides experimental evidence for the formation of a covalent compound of As and N, having AsN stoichiometry and adopting a crystalline structure belonging to cubic space group P213. In this structure each As atom is single-bonded to three N atoms and vice versa, with every pnictogen atom hosting an electron lone pair. Accordingly, the crystalline lattice of AsN consists of a three-dimensional network of alternating AsN3 and NAs3 trigonal pyramids, where only single As-N bonds are present. This atomic arrangement is responsible for the existence of high electron density regions in the unit cell of AsN, where the non-bonding electron lone pairs at the vertex of each trigonal pyramid repel each other by strong directional repulsive interactions.

The observation of characteristic structural motifs, identified as four different types of As4 tetrahedra, as well as cage and cavity structures made of condensed As3N3 rings, highlights the key role played by the directional repulsive interactions between non-bonding electron lone pairs in the stabilization of the crystalline structure of AsN. This occurrence is consistently supported by the pressure evolution of bond distances and angles. Additional powder XRD data indicate that at room temperature AsN persists on compression up to 50 GPa and on decompression down to at least 9.8 GPa, with recent spectroscopic data apparently confirming this behaviour. Implications of the discovery and characterizations of AsN concern fundamental aspects of pnictogens chemistry and the synthesis of innovative advanced materials.

Acknowledgements:
PHOSFUN “Phosphorene functionalization: a new platform for advanced multifunctional materials” (ERC-Advanced Grant No. 670173), Deep Carbon Observatory (DCO, Physics and Chemistry of Carbon at Extreme Conditions), “GreenPhos-alta pressione” (MUR-CNR), HP-PHOTOCHEM (Fondazione Cassa di Risparmio di Firenze), European Synchrotron Radiation Facility (ESRF).

[1] Ceppatelli, M., Scelta, D., Serrano-Ruiz, M., Dziubek, Garbarino, G., Jacobs, J., Mezouar, M., Bini, R. & Peruzzini, M. (2020). Nat. Commun. 11, 6125.
[2] Ceppatelli, M., Scelta, D., Serrano-Ruiz, M., Dziubek, K, Izquierdo-Ruiz, F., Recio, J.M., Svitlyk, V., Garbarino, G., Mezouar, M., Peruzzini, M., & Bini, R. (2022). Inorg. Chem. 61, 12165-12180.
[3] Ceppatelli, M., Scelta, D., Serrano-Ruiz, M., Dziubek, K, Morana, M., Svitlyk, V., Garbarino, G., Poręba, T., Mezouar, M., Peruzzini, M., & Bini, R. (2022). Angew. Chem. Int. Ed. 61, e202114191.

Calculation of metallic melt curves via the ab initio Z method

Shailesh Mehta[1]
[1]*AWE, Reading, United Kingdom*

Phase Diagrams – Metals, July 27, 2023, 10:15–12:15

Density functional theory is used to compute the melt curves of a selection of metals to high pressure via the Z method. The technique is first applied to Al to a pressure of 300 GPa and very good agreement is found with both experiment and previous theoretical calculations. Attention is then turned to Mg, for which the hcp-bcc-liquid triple point is located by calculation of the melt curves from both the bcc and hcp phases and excellent agreement is found with experiment. Finally, the melt curve of Ta, which has previously been the subject of some controversy, is computed. The present calculations are found to be in reasonable with the measurements of Dewaele et al. [PRL, 104, 25570 (2010)], which extend to 135 GPa However, above 150 GPa the calculated melt curve flattens considerably.

Magnetic field screening and magnetic flux trapping in hydrogen-rich high-temperature superconductors

Dr. Vasily S. Minkov[1], Dr. Mikhail Eremets[1], Dr. Vadim Ksenofontov[1], Dr. Sergey L. Budko[2], Dr. Fedor F. Balakirev[3], Dr. Evgeny F. Talantsev[4]

[1]Max-Planck-Institut für Chemie, Mainz, Germany, [2]Ames Laboratory, Iowa State University, Ames, United States, [3]Los Alamos National Laboratory, Los Alamos, United States, [4]M.N. Mikheev Institute of Metal Physics, Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russian Federation

Hydrides 3, July 25, 2023, 14:00–16:00

In the last few years, the superconducting transition temperature, Tc, of hydrogen-rich compounds has increased dramatically and is now approaching room temperature. However, experimental studies are severely limited by high-pressure conditions, and electrical transport measurements have long been the primary technique for detecting superconductivity in hydrides. Magnetic properties, one of the most important characteristics of a superconductor, have not been satisfactorily defined.

Here, we developed SQUID magnetometry for tiny superconducting samples pressurised under extreme high-pressure conditions in miniature non-magnetic diamond anvil cells. Using this technique, we studied magnetic field screening in Im-3m-H_3S and Fm-3m-LaH_{10} – the representative members of two families of high-temperature superconducting hydrides, which are characterised by covalent and ionic bonding between H and non-hydrogen atoms. We determined characteristic superconducting parameters, such as a lower critical field Hc1 and a London penetration depth λL. The small values of λL of approximately 20–40 nm indicate a high superfluid density in both hydrides. These compounds have the values of the Ginzburg-Landau parameter κ of approximately 10–20 and belong to the group of “moderate” type II superconductors, rather than being hard superconductors as would be intuitively expected from their high Tcs.

We also implemented the non-conventional protocol for magnetic measurements of superconductors in SQUID magnetometer and probed the trapped magnetic flux in H_3S and LaH_{10}. The specific behavior of the trapped flux generated under zero-field-cooled and field-cooled conditions unequivocally proved superconductivity in these materials. Contrary to traditional magnetic susceptibility measurements, a magnetic response from the trapped flux is almost not affected by the background signal of the bulky diamond anvil cell due to the absence of external magnetic fields. In addition, the trapped flux method allows one to determine Tc, critical currents and their temperature dependence, Hc1, λL, a full penetration field, pinning properties, and flux creep. We revealed that the absence of the pronounced Meissner effect in hydrides is associated with the strong pinning of vortices. The trapped flux approach can be a powerful tool for a routine screening of new superconducting materials at high pressures, and also for studying multiphase samples or samples having a low superconducting fraction at ambient pressure.

[1] V. S. Minkov, S. L. Bud'ko, F. F. Balakirev, V. B. Prakapenka, S. Chariton, R. J. Husband, H. P. Liermann, M. I. Eremets. Magnetic field screening in hydrogen-rich high-temperature superconductors Nat. Commun. 2022, 13, 3194.

[2] V. S. Minkov, V. Ksenofontov, S. L. Budko, E. F. Talantsev, M. I. Eremets. Trapped magnetic flux in hydrogen-rich high-temperature superconductors. Arxiv 2023, https://doi.org/10.48550/arXiv.2206.14108.

In situ X-ray diffraction of Al2O3 during laser compression and release

Anirudh Hari[1], Rohit Hari[1], Dr. Patrick Heighway[2], Dr. Raymond Smith[3], Professor Thomas Duffy[4], Dr. Saransh Singh[3], Professor Todd Hufnagel[1], Professor June Wicks[1]
[1]Johns Hopkins University, Cary, North Carolina, United States, [2]University of Oxford, Oxford, United Kingdom, [3]Lawrence Livermore National Laboratory, Livermore, United States, [4]Princeton University, Princeton, United States

Mantles of Terrestrial Planets, July 27, 2023, 14:00–16:00

Sapphire (Al2O3) is an important earth mineral notable for its high compressive strength and hardness. Static compression experiments on Al2O3 in the polycrystalline alumina form have found evidence of phase transformations from the α-corundum phase to a Rh2O3 (II)-type structure at ~80 GPa (Funamori & Jeanloz, 1997, Lin et al., 2004), and then to the post-perovskite structure at ~130 GPa (Oganov & Ono, 2005).

In this work, we describe laser-driven shock compression experiments on a-cut and c-cut sapphire to 150 GPa and polycrystalline alumina to 110 GPa conducted at the Matter in Extreme Conditions endstation of the Linac Coherent Light Source. Ultrafast X-ray pulses (50 fs, 1012 photons/pulse) were used to probe the lattice-level response as a function of time during and after shock propagation. VISAR velocimetry was used to measure free-surface particle velocity, from which pressure was calculated. Through in situ X-ray diffraction, we observe evidence of anisotropic strain and crystal break-up during and after compression. After release to ambient pressure, measured temperatures exceed those predicted by isentropic release, indicating plastic work heating. We will discuss the effect of crystal orientation on shock-induced phase transformation.

Neutron and X-ray Diffraction Study of Magnetic Ordering in Terbium at High-Pressures and Low-Temperatures

Matthew Clay[1], Raimundas Sereika[1], Wenli Bi[1], Logan Burnett[1], Cheng-Chien Chen[1], Yogesh Vohra[1]
[1]*University of Alabama at Birmingham, Birmingham, United States*

Magnetic Materials 2, July 26, 2023, 14:00–16:00

The application of pressure causes electron transfer from the extended s-band to a more compact d-band in lanthanides due to a relative rise in the energy of the s-band states with increasing pressure. This s-d electron transfer drives the structural phase transitions in lanthanides and leads to hcp→Sm-phase→dhcp→fcc→distorted-fcc phase transitions with increasing pressure. The changes in electronic structure driving structural phase transitions under pressure in lanthanides are well recognised; however, their role in the onset of magnetic ordering temperatures and magnetic structures is unknown. We have investigated magnetic ordering in heavy lanthanide Terbium (Tb) to high pressures of 50 GPa and low temperature of 20 K by neutron diffraction at the Spallation Neutron Source, Oak Ridge National Laboratory and by synchrotron X-ray diffraction at the Advanced Photon Source, Argonne National Laboratory. At ambient pressure in the hexagonal close packed (hcp) phase, Tb undergoes a transition at 230 K from a paramagnetic (PM) to an antiferromagnetically (AFM) ordered phase with the magnetic moments arranged in a helical structure in which the c-axis is the screw axis. With decreasing temperature below 220 K, the structure shifts to a ferromagnetic (FM) configuration. On application of pressure, the FM phase is suppressed, and an AFM ordering is observed in the alpha-Samarium (α-Sm) phase above 4 GPa (Kozlenko et al. Phys. Rev. Mater. 5, 034402, 2021). In this talk, we will focus on the magnetic ordering in higher pressure phases like the double hexagonal close-packed (dhcp above 16 GPa), distorted face-centred cubic (hR-24 above 29 GPa), and orthorhombic (oF16 above 53 GPa) phases. We observed the phenomenon of magnetostriction in the high-pressure phases of Tb where magnetic ordering at low temperatures give rise to subtle splitting in X-ray diffraction peaks. This allows us to obtain magnetic ordering temperatures at high pressures from the X-ray data and indicates that magnetic ordering temperature increases with increasing pressure and reaches 100 K at a pressure of 50 GPa. The magnetic ordering temperatures obtained from X-ray diffraction agree with neutron diffraction measurements where magnetic superlattice reflections are observed at the same magnetic ordering temperature as indicated by X-ray diffraction studies. The experimental studies have identified propagation vector q for various magnetic phases at high pressures and our theoretical effort is focused on calculation of the spin susceptibility $\chi(q, T)$ to identify the dominant spin fluctuations and the magnetic transition temperatures.

Raman study of supercritical fluid phase of hydrogen at room temperature

Prof. Nakayama Atsuko[1], Mr. Yuya Isurugi[2], Mr. Yuya Serizawa[3], Dr. Satoshi Nakano[4], Dr. Ayako Ohmura[5], Dr. Fumihiro Ishikawa[5]

[1]Faculty of Science and Engineering, Iwate University, Morioka, Japan, [2]Graduate School of Science and Technology, Niigata University, Niigata, Japan, [3]Graduate School of Arts and Science, Iwate University, Morioka, Japan, [4]National Institute for Materials Science (NIMS), Tsukuba, Japan, [5]Faculty of Science, Niigata University, Niigata, Japan

Hydrogen, July 25, 2023, 10:15–12:30

To utilise hydrogen effectively and safely in the future of clean energy, we must know the physical properties of fluid hydrogen at room temperature, however, we have a few information on it in the current phase diagram [1-3]. Recent study on supercritical fluid phase of hydrogen by Raman spectroscopy and X-ray diffraction revealed the change in the compressibility at 1 GPa [4]. The phenomena is explained to be affected by the enhancement of the intermolecular interaction based on the phase transition to liquid or solid. Such significant and interesting change are expected to occur even in the megapascal pressure range, however, the detailed phenomena are being overlooked.

In this study, rotational and vibrational spectra of supercritical fluid phase of hydrogen at room temperature were investigated by Raman spectroscopy under pressure. Rapid changes in Raman shifts and their hull widths of half maximums for the rotational and vibration-rotational modes were observed at the pressure around 0.56 GPa [5]. The peak analysis revealed that the ortho-para conversion started under pressure beyond 0.56 GPa. The anomalous pressure changes at 0.56 GPa are probably generated by the fluid-fluid phase transition which induces a change is the ration of equilibrium composition of ortho-para hydrogen.

[1] B. P. Stoicheff, Can. J. Phys. 35, 730 (1957).
[2] R. L. Mills, D. H. Liebebergm, J. C. Bronson, and L. C. Schmidt, J. Chem. Phys. 66, 3076 (1977).
[3] N. E. Moulton, G. H. Watson, W. B. Daniels, and D. M. Brown, Phys. Rev. A 37, 2475 (1988).
[4] Y. Akahama, R. Miyamoto, S. Nakano, S. Kawaguchi, N. Hirao, and Y. Ohishi, J. Appl. Phys. 128, 135901 (2020).
[5] A. Nakayama, Y. Isurugi, Y. Serizawa, S. Nakano, A. Ohmura, and F. Ishikawa, J. Phys. Soc. Jpn. 91, 093601 (2022).

Heavy Metals under Pressure and the Effect of Spin-Orbit Coupling

Mr Pascal Thomas Salzbrenner[1], Professor Chris Pickard[1,2]
[1]*Department of Materials Science and Metallurgy, University Of Cambridge, Cambridge, United Kingdom,*
[2]*Advanced Institute of Materials Research, Tohuku University, Sendai, Japan*

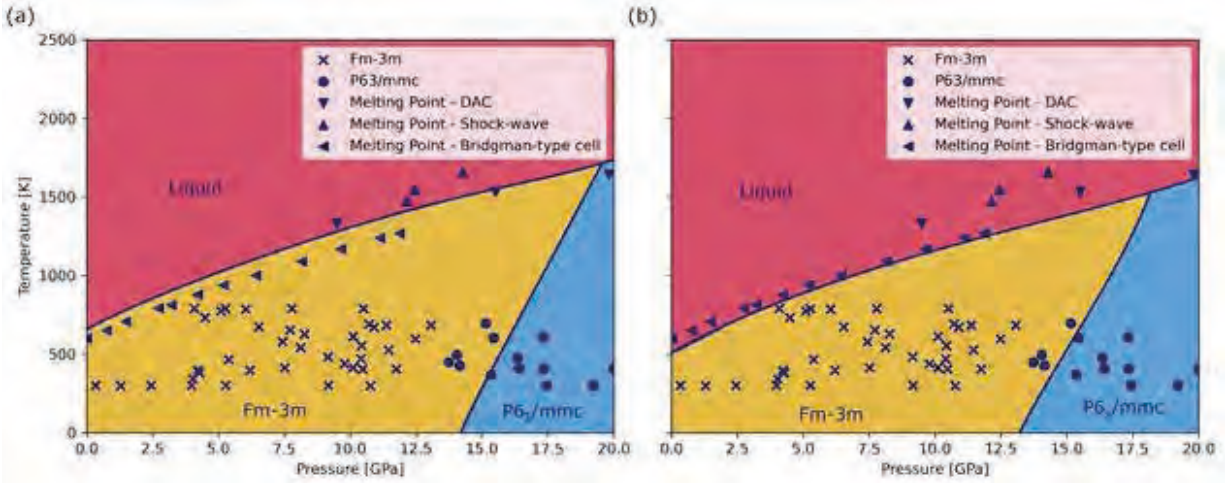
Phase Diagrams – Metals, July 27, 2023, 10:15–12:15

Density functional theory [1, 2] has been remarkably successful at describing the electronic structure and predicting the physical properties of a wide range of materials. This success is, at least in part, based on making sensible approximations which preserve much of the accuracy while reducing the computational expense. For instance, the relativistic spin-orbit coupling (SOC) is usually neglected, resulting in a speed-up of 1-2 orders of magnitude. Since SOC increases with increasing nuclear charge, this is usually justified for light elements. This has enabled applications which rely on DFT simulations of a large number of atoms, such as ab initio molecular dynamics (AIMD), as well as those relying on a large number of simulations of more moderately-sised systems. A prominent example of the latter is high-throughput first principles crystal structure prediction [3].

However, for heavier elements, SOC plays an important role in the electronic structure and hence in the energy landscape. As a result, accurate first-principles quality structure searches or AIMD have been practically out of reach for these materials. As a result, the pressure-temperature behaviour of the heavy metals is theoretically much more poorly understood than that of lighter elements. For polonium, for example, no ab initio phase diagram exists whatsoever.

Here, we rely on the ephemeral data-derived potentials (EDDPs) [4], a flavour of neural network interatomic potential, to learn the energy landscape including SOC from small-cell DFT calculations. These potentials are then used to carry out extensive structure searches and explicit melting MD calculations. Using this technique, we present the first ab initio phase diagram for lead including SOC, and the first phase diagram for polonium altogether. In both cases, we demonstrate that taking SOC into account is essential for improving agreement with experimental results.

[1] P. Hohenberg and W. Kohn, “Inhomogeneous electron gas,” Phys. Rev. 136, B864–B871 (1964).
[2] W. Kohn and L. J. Sham, “Self-consistent equations including exchange and correlation effects,” Phys. Rev. 140, A1133–A1138 (1965).
[3] C. J. Pickard and R. J. Needs, “Ab initio random structure searching,” Journal of Physics: Condensed Matter 23, 053201 (2011).
[4] C. J. Pickard, “Ephemeral data derived potentials for random structure search,” Phys. Rev. B 106, 014102 (2022).



Strain induced structural and electronic phase transitions in Transition metal dichalcogenides

Bishnupada Ghosh[1], Mrinmay Sahu[1], Debabrata Samanta[1], Pinku Saha[2], Goutam Dev Mukherjee[1]
[1]IISER Kolkata, Mohanpur, Nadia, 741246, India, [2]ETH Zurich, Zurich, 8092, Switzerland

Electronic Transitions 2, July 25, 2023, 14:00–16:00

Backgrounds: Transition metal dichalcogenides (TMDs) have been in the research forefront due to their rich structural, electronic, and optical properties. The application of pressure can modulate the structural and electronic properties through volume compression. In recent years strain engineering, controlling layer numbers, and the presence of impurities have been found to modify the band structure of these 2D materials leading to novel electronic properties. There have been theoretical and experimental reports that TMDs undergo semiconductor-to-metallic transition under high pressures [1-4]. Here we have studied the effect of strain on the structural as well as electronic properties of ReS2, MoTe2, and ZrSe2.

Methods: Strain in the materials is induced by the application of high pressure using a diamond anvil cell (DAC). To probe the pressure-induced changes in structural and electronic properties, X-ray diffraction measurements at synchrotron, Raman spectroscopy, low-temperature transport measurements as well as ab initio first-principles calculations using density-functional theory (DFT) is performed at high pressures.

Results and Discussion:
ReS2: High-pressure XRD data of ReS2 shows a structural transition from distorted 1T to distorted 1T' phase, above 6 GPa, followed by a lattice expansion of the new structure in the pressure range of 15–25 GPa. A softening in the Raman modes corresponding to the Re atoms is observed in the same pressure range [5].

MoTe2: Our high-pressure XRD study on 1T' MoTe2 shows a large compressibility below 8.4 GPa, which reduces drastically above 12.7 GPa. A sharp drop in resistivity up to 3.4 GPa followed by saturation at higher pressures is observed. First-principles DFT calculations at high pressure show an increase in DOS at EF till about 8 GPa followed by saturation. From stress calculations, the strain is found to be highest along the ab-plane which causes an enhancement of the metallic nature of the semi-metallic 1T' MoTe2 above 8 GPa [6].

ZrSe2: Whereas 1T ZrSe2 undergoes a pressure-induced gradual structural phase transition, which starts around 5.9 GPa and completes around 14.8 GPa. The low-temperature and high-pressure resistivity measurements of the sample show an electronic phase transition from metallic to semiconducting nature above 5.1 GPa (Fig.1). The low-temperature resistivity data at all pressure values show an upturn which is possibly due to the Kondo anomaly in the sample due to the presence of additional Zr, which acts as the magnetic impurity. Though the observation of a pressure-induced metal-to-semiconductor transition is rarely reported, due to the increase in strain inside the material a small band gap opens up in the sample resulting in a pressure-induced metal-to-semiconductor transition [7].

[1] Nayak et al., Nano Lett. 15, 346 (2015).
[2] Chi et al., Phys. Rev. Lett. 113, 036802 (2014).
[3] Zhao et al., Nat.Commun. 6, 7312 (2015).
[4] Saha et al., J. Appl. Phys. 123, 204306 (2018).
[5] Saha et al., J. Appl. Phys. 128, 085904 (2020).
[6] Ghosh et al., Electron. Struct. 3, 045002 (2021).
[7] Ghosh et al., Phys. Rev. B 106, 104102 (2022).

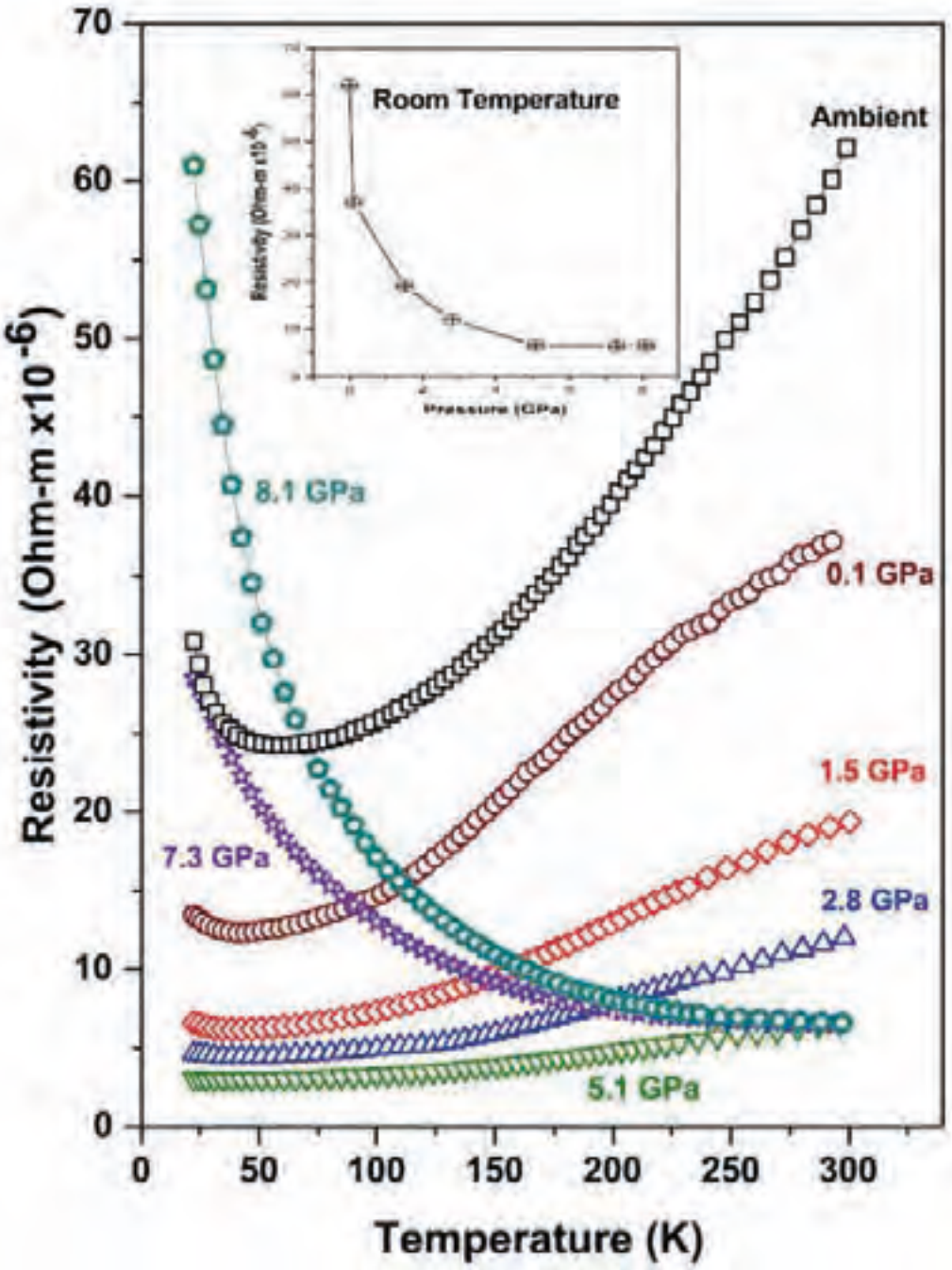


Fig.1: Temperature variation of resistivity of ZrSe2 at different pressure points

High-pressure Structural Stability of $Ni_3V_2O_8$ and $Co_3V_2O_8$: Raman and Infrared Spectroscopy (Ni, Co) and X-ray diffraction (Co) studies

Mr. Josu Sánchez-Martín[1], Julio Pellicer-Porres[1], Jordi Ibáñez-Insa[2], Robert Oliva[2], Catalin Popescu[3], Zhangzhen He[4], Akun Liang[1], Plácida Rodríguez-Hernández[5], Alfonso Muñoz[5], Daniel Errandonea[1]

[1]Departamento de Física Aplicada-ICMUV, Universidad de Valencia, Dr. Moliner 50, Burjassot, 46100, Spain, [2]Geosciences Barcelona (GEO3BCN), Spanish Council for Scientific Research (CSIC), Lluís Solé i Sabarís s/n, 08028 Barcelona, Spain, [3]CELLS-ALBA Synchrotron Light Facility, Cerdanyola del Vallès, 08290, Spain, [4]4 State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, China, [5]Departamento de Física, MALTA-Consolider Team, Instituto de Materiales y Nanotecnología, Universidad de La Laguna, San Cristóbal de La Laguna, E-38200, Spain

Multifunctional Materials, July 24, 2023, 10:15–12:15

$Ni_3V_2O_8$ and $Co_3V_2O_8$ orthovanadates have been studied for decades due to their rich magnetic polymorphism [1] and multiferroic properties [2]. They also present several industrial applications in nanostructured systems, such as the water splitting process, electrochemical energy storage [3], nitrogen fixation and glucose detection. $Ni_3V_2O_8$ have already been studied under high-pressure by means of powder XRD diffraction up to 23 GPa [4]. No phase transition has been found.

In this work we would like to complement previous studies performed in $Ni_3V_2O_8$ with new Raman experiments, and extend the research to a new compound, $Co_3V_2O_8$. We will analyse the results with the help of ab-initio calculations. Both compounds present a Kagomé staircase structure (Cmca) at ambient conditions and remain structurally stable up to 20 GPa. As there is a lack of information concerning the basic properties of these compounds, in a first step we have characterise the vibrations in ambient conditions. To this end, we have oriented single crystals to perform polarised Raman and Infrared measurements in ambient conditions, which we have interpreted thanks to DFT calculations. With the ambient pressure modes properly characterised, we have been able to follow the evolution of 24 (17) out of the 36 Raman active modes that powder $Ni_3V_2O_8$ ($Co_3V_2O_8$) presents up to 19.5(1) (20.3(1)) GPa. Raman experiments confirm that $Ni_3V_2O_8$ remains in the low-pressure phase in the studied pressure range. Co3V208 is also observed to be stable both by Raman and by XRD experiments. The analysis of the equation of state yields a bulk modulus of 122(1) GPa, which is slighty smaller than that of $Ni_3V_2O_8$ [139(3) GPa].

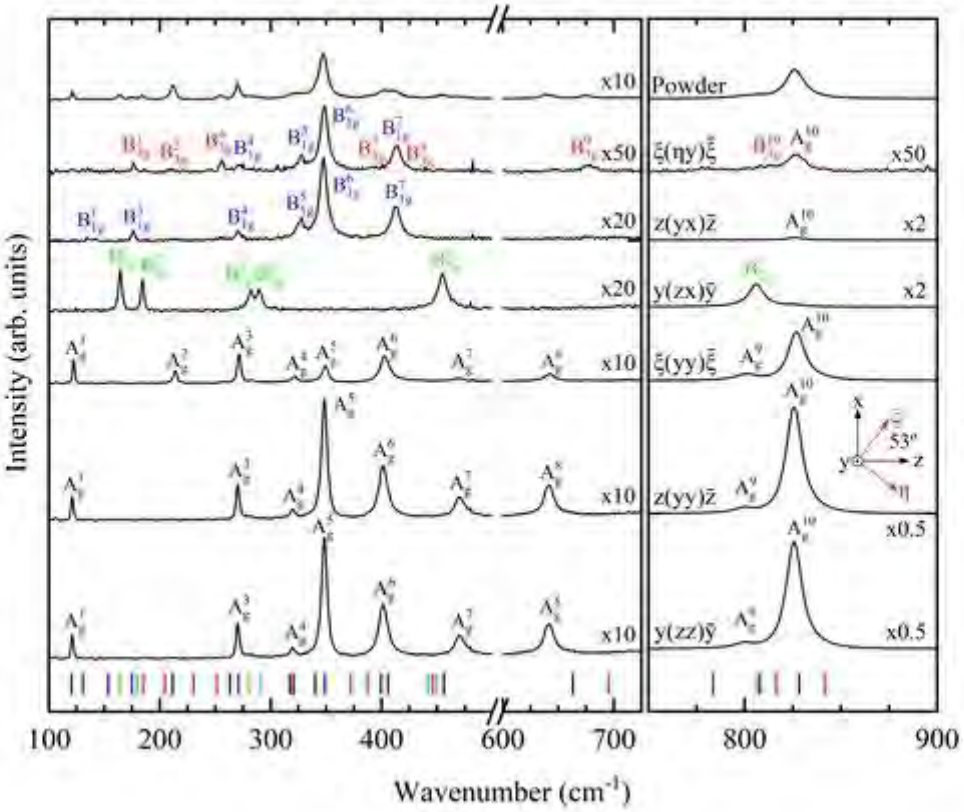
Comparing the results of both compounds, we observe that all modes increase in wavenumber with the pressure, and the pressure coefficients obtained experimentally are in a good agreement with the simulated ones. In addition, all modes in Ni orthovanadate are higher in wavenumber than the Co orthovanadate ones. This fact added to having a higher bulk modulus indicates that $Ni_3V_2O_8$ has a slightly pre-compressed structure compared with $Co_3V_2O_8$.

[1] Wilson, N.R.; Petrenko, O.A.; Balakrishnan, G. Magnetic phase diagrams of the Kagomé staircase compounds $Co_3V_2O_8$ and $Ni_3V_2O_8$. J. Phys.: Condens. Matter 2007, 19, 145257.

[2] Chaudhury, R.P.; Yen, F.; dela Cruz, C.R.; Lorenz, B.; Wang, Y.Q.; Sun, Y.Y.; Chu, C.W. Pressure-temperature phase diagram of multiferroic $Ni_3V_2O_8$. Phys. Rev. B Condens. Matter 2007, 75, 012407.

[3] Hosseini, H.; Shahrokhian, S. Advanced binder-free electrode based on core–shell nanostructures of mesoporous $Co_3V_2O_8$-$Ni_3V_2O_8$ thin layers@porous carbon nanofibers for high-performance and flexible all-solid-state supercapacitors. Chem. Eng. J. 2018, 341, 10–26.

[4] Diaz-Anichtchenko, D.; Turnbull, R.; Bandiello, E.; Anzellini, S.; Errandonea, D. High-Pressure Structural Behaviour and Equation of State of Kagome Staircase Compound, $Ni_3V_2O_8$. Crystals 2020, 10, 910.


Intensity (arb. units)
Wavenumber (cm^{-1})
100
200
300
400
600
700
800
900
x10
x50
x20
x20
x10
x10
x10
Powder
x50
ξ(ηy)ξ̄
x2
z(yx)z̄
x2
y(zx)ȳ
ξ(yy)ξ̄
z(yy)z̄
x0.5
y(zz)ȳ
x0.5
53°
x
y
z
η

Crystal Structure, Characterization and Luminescence Properties of Mn(4+)-Doped K3Nb2O4F5

Fabian Zimmerhofer[1], Klaus Wurst[1], Hubert Huppertz[1]
[1]*University of Innsbruck, Innsbruck, Austria*

Synthesis and Properties of Novel Materials 1, July 26, 2023, 14:00–16:00

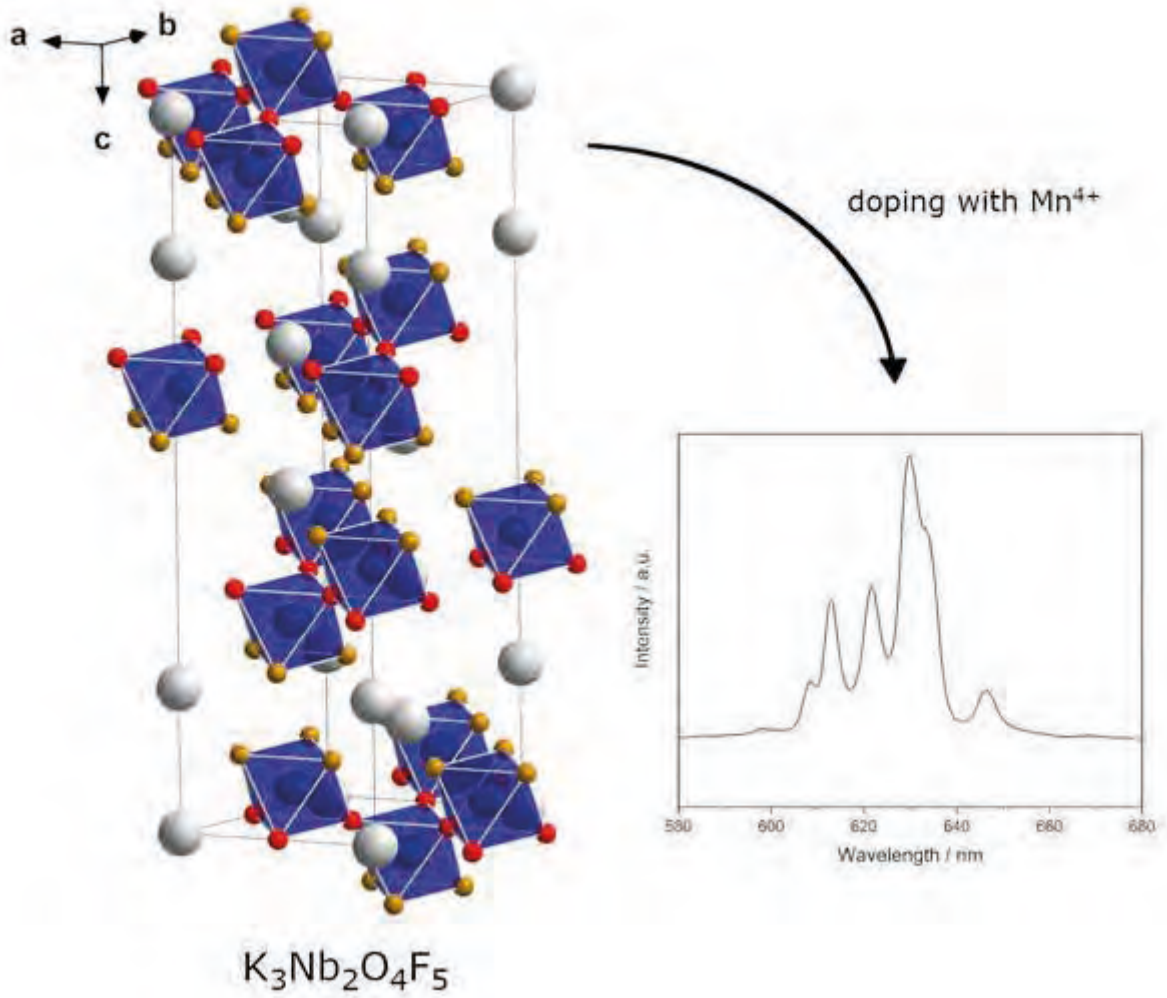
Fabian Zimmerhofer[a], Klaus Wurst[a], and Hubert Huppertz[a]

[a]Institute of General, Inorganic and Theoretical Chemistry, Universität Innsbruck, 6020 Innsbruck, Austria

For several years now, we have been investigating the substance classes of fluorides and fluoridooxidometallates and their potential application as Mn(4+)-activated red phosphor materials in solid state lighting.[1] By use of high-pressure/high-temperature methods, we were able to obtain single crystals of the hitherto unknown fluoridooxidoniobate $K_3Nb_2O_4F_5$. The compound crystallises in the trigonal space group $R\bar{3}m$ (no. 166) with a = 5.799(2), c = 21.371(4) Å, V = 622.4(4) Å^3 and Z = 3 at T = 299K exhibiting a structure type closely related to that of $Ba_2RbFe_2F_9$. The assignment of fluorine and oxygen to the anion positions is based on crystallographic data and the calculation of oxidation states via BLBS[2, 3] and CHARDI[4-6] methods. Further characterization via EDX spectroscopy was carried out, corroborating the ratio of K to Nb. Doping of the pale blue compound with Mn(4+) was achieved in a secondary step by ball-milling with K_2MnF_6, producing a pale pink powder. Upon excitation with UV/blue light, the powder exhibits red luminescence with an emission maximum at λmax = 630 nm. The early onset of heavy thermal quenching and the significant degradation of $K_3Nb_2O_4F_5$:Mn(4+) at temperatures below 150 °C, renders the new phosphor commercially unviable for application in LEDs.

DOI for the original research article: https://doi.org/10.1002/ejic.202200714

[1] Adachi S. ECS J. Solid State Sci. Technol. 2020, 9, 016001.
[2] N. E. Brese, M. O'Keeffe, Acta Crystallogr. Sect. B 1991, 47, 192–19.
[3] I. D. Brown, D. Altermatt, Acta Crystallogr. Sect. B 1985, 41, 244–24.
[4] R. Hoppe, S. Voigt, H. Glaum, J. Kissel, H. P. Müller, K. Bernet, J. Less-Common Met. 1989, 156, 105–122.
[5] M. Nespolo, Acta Crystallogr. Sect. B 2016, 72, 51–6.
[6] L. Pauling, J. Am. Chem.Soc. 1947, 69, 542–55.


a
b
c
doping with Mn4+
Intensity / a.u.
580
600
620
640
660
680
Wavelength / nm

$K_3Nb_2O_4F_5$

Fine-tuning the strategy XtalOpt + Gibbs2 codes. Application to thermoelectric compounds (AgCl, PbTe and CoSb3): Phase diagrams pT.

Hocine Chorfi[1], Ali Boultif[2], Hannane Maoudj[3], José. Manuel Récio[4], Ruth Franco de Uria[5], Miguel. Angel Salvado[6], Alvaro Labado[7]

[1]Brothrs Mentouri University (UMC), Constantine/Algeria, Constantine, Algeria, [2]Brothrs Mentouri University (UMC), Constantine, Algeria, [3]Brothrs Mentouri University (UMC), Constantine, Algeria, [4]Oviedo University, Oviedo, Spain, [5]Oviedo University, Oviedo, Spain, [6]Oviedo University, Oviedo, Spain, [7]Oviedo University, Oviedo, Spain

Computational Methods, July 25, 2023, 10:15–12:15

The ultimate objective of this work is the proposal of new materials with high thermoelectric performance. The success in its achievement is associated with the fulfilment of two intermediate objectives. The first is of a methodological nature and consists on the combination of prediction models of crystalline structures with strategies for chemical-quantum calculation of electronic, thermodynamic and transport properties (VASP/QE+newGIBBS). The second is of an applied nature. It seeks to obtain property-structure correlations from the computational exploration of regions of increasing pressures in the phase diagram of families of compounds with high value of the figure of merit (ZT) (AgCl, PbTe, CoSb3) and allowing stoichiometric variations.

The code XtalOpt is a computational tool that makes use of evolutionary algorithms for the prediction of crystal structures based solely on the composition of a material system. The number of atoms in the unit cell that handles. XtalOpt can reach a hundred. It has been created entirely of Prof. Eva Zurek. Its set up to couple it with the code GIBBS2 supposes a novel computational strategy in the search for stable structures in specific regions of the phase diagram, created in the group TCCMAT at the University of Oviedo.

In situ, high-pressure experiments using synchrotron white X-rays at the Large Volume Press end-station P61B, PETRA III, DESY

Dr. Robert Farla[1], Dr. Shrikant Bhat[1], Dr. Shuailing Ma[2], Dr. Adrien Néri[3], Mr. Lianjie Man[3], Dr. Artem Chanyshev[3], Dr. Kristina Spektor[1,4], Dr. Christian Lathe[1,5], Mr. Stefan Sonntag[1], Prof. Holger Kohlmann[4], Prof. Ulrich Häussermann[6], Prof. Tomoo Katsura[3]

[1]Deutsches Elektronen-synchrotron DESY, Hamburg, Germany, [2]Institute of High-Pressure Physics, School of Physical Scientific and Technology, Ningbo University, Ningbo, China, [3]Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, Germany, [4]Institute for Inorganic Chemistry, Leipzig University , Leipzig , Germany, [5]Department Geochemistry, Deutsches GeoForschungsZentrum (GFZ), Potsdam, Germany, [6]Department of Materials and Environmental Chemistry, Stockholm University, Stockholm, Sweden

Facility Development 2, July 27, 2023, 14:00–16:00

The 'Aster-15' Large Volume Press (LVP) is now installed and fully operational for user experiments on the high-energy wiggler end-station beamline P61B at PETRA III. High pressure and temperature (HPHT) conditions up to 30 GPa and 2300 K can be reached routinely to address problems in Earth / Materials sciences and Chemistry. For 50% availability of X-rays, the standard detector setup is used, featuring 2 Ge-detectors for energy-dispersive X-ray diffraction (ED XRD) at 30–160 keV, and a white-beam microscope for radiography [1]. Using various anvil-cell assembly designs, mm-sised polycrystalline samples can be investigated in the LVP to document chemical reactions and phase relations of materials in situ, as well as physical properties such as deviatoric stress, strain and ultrasonic wave velocities. A dedicated glovebox is available to prepare assemblies in a controlled atmosphere for sensitive materials, such as nitrides and hydrides.

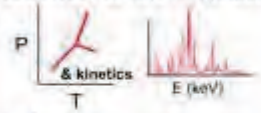
Recently, two additional techniques have been commissioned for the LVP: ultrasonic interferometry (wave velocities measurements) and acoustic emission (AE) detection. The first method features a LiNb03 piezo-sensor that transmits pulses and receives echoes at specific ultrasonic sine-wave frequencies (10-60 MHz) of both P and S waves. The two-way travel time in the sample at HPHT is measured from the echoes of the top and bottom sample interfaces. Combined with length measurements of the sample by X-ray radiography, the wave velocities are calculated and compared to seismic wave propagation in the Earth's interior. The second newly available method at HPHT and stress conditions is an acoustic emission (AE) detection system [2], which uses specialised AE sensors (0.1 – 4 MHz broadband) on 6 anvils to detect and localise events in a sample prone to brittle behavior. Examples of embrittlement include transformational faulting, dehydration reactions, or other causes of sudden phase/volume changes. AE detection can be combined with X-ray diffraction and imaging to monitor the sample stress and strain rate history in situ during controlled rock deformation. The capabilities of the LVP, detector set ups and scientific case studies will be presented, demonstrating the competitive capabilities of the P61B station (see figure attached).

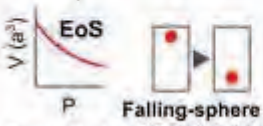
We encourage the submission of proposals for beam time or apply to try out the LVP at the station without X-rays first (see instructions on the beamline website). If unsure about the conditions of the experiment, or you are only familiar with the diamond anvil cell, do not hesitate to contact Dr. Farla or Dr. Bhat to discuss potential solutions to carry out your HPHT in situ experiments in the LVP.

[1] R. Farla et al., 'Extreme conditions research using the large-volume press at the P61B endstation, PETRA III', J Synchrotron Rad, vol. 29, no. 2, Art. no. 2, Mar. 2022, doi: 10.1107/S1600577522001047.

[2] S. Ma, J. Gasc, and R. Farla, 'Acoustic emission detection of micro-cracks under high-pressure and high temperature in a deformation large-volume apparatus at the endstation P61B, PETRA III', Review of Scientific Instruments, vol. 94, no. 2, p. 023901, Feb. 2023, doi: 10.1063/5.0107630.

Phase relations & discovery of new HP phases





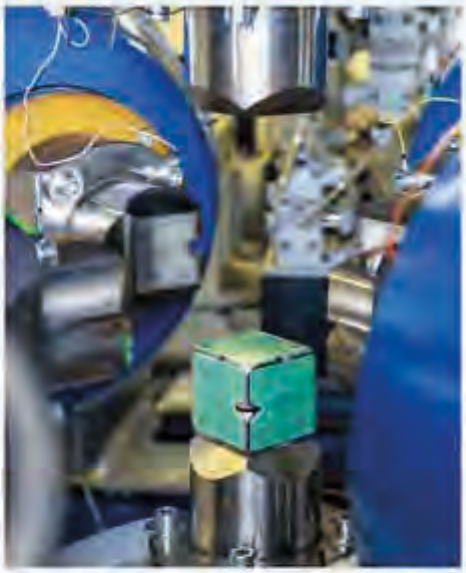
Falling-sphere viscosimetry

Controlled rock deformation

Ultrasonic Interferometry (10-60 MHz)

Acoustic Emission detection (0.1 - 4 MHz)

... and more!



http://tiny.cc/petra3p61

P61B LVP

Manuscript

P61B white-beam LVP station

(30 - 160 keV, >10^{14} ph/s/mm^2 int. flux)

Instrumentation:

- Energy-dispersive XRD
  - 2x Ge-detectors (2θ: 3 - 20°)
- Radiography
  - X-ray microscope with:
    - sCMOS Camera 5.5 MP (6.5 µm pixel size)
    - 5x & 10x magnification
    - GGG:Eu / GAGG:Ce scintillators
- AC & DC heating systems
- Waveform generator/Oscilloscopes
- AE system

The 'Aster-15' LVP

- 15 MN (5 MN per axis)
- 5-axis press stages (incl. press rotation)
- 3 Modes of Operation:
  - Kawai MA6-8 (26 & 32 mm anvils)
    General user: up to 20 GPa
    Advanced user: > 50 GPa
  - Cubic MA6-6 (incl. SD and cBN anvils)
    Controlled anisotropic compression
  - Drickamer (uniaxial) compression

BN under high pressure revisited

Dr Julio Pellicer-Porres[1], Dr Alfredo Segura[1], Dr Ramón Cusco[2], Dr Lluís Artús[2], Dr James H. Edgar[3], Dr Jiahan Li[3]
[1]MALTA-Consolider Team, ICMUV, University of Valencia, Burjassot, Spain, [2]Geo3Bcn-CSIC, Barcelona, Spain, [3]Tim Taylor Department of Chemical Engineering, Manhattan, United States

Nitrides, Borides and Carbides 1, July 24, 2023, 14:00–16:00

Hexagonal boron nitride, h-BN, is an ubiquitous layered material with unique properties as a dielectricinsulator, strong ultraviolet emitter and natural optical hyperbolic material. In the present days it has attracted attention due to its electronic and photonic applications based on graphene and related two-dimensionalmaterials. The recent availability of good quality single crystals brings the possibility to improve its characterization, both in ambient conditions and at high-pressure.

We have performed high pressure experiments with h-BN single crystals, including X-ray diffraction (XRD), Raman scattering [1] and infrared spectroscopy [2]. Raman scattering experiments have also been performed on isotopically enriched samples [3]. Single crystal XRD complements previous powder diffraction experiments, where the quality of the sample and the existence of turbostratic defects originated controversial results about the h-BN equation of state. We have characterised under high pressure the Raman active E2g high and low frequency modes, as well as the E1u(TO), E1u(LO), A2u(TO) and A2u(LO) infrared active modes[3] up to the transition to the wurtzite phase at 10.5 GPa. We interpret the high-pressure evolution of the in-plane modes in terms of the intra and interlayer interactions. The softening of the A2u(TO) mode is induced by dynamical buckling of the flat honeycomb layers. The wurtzite phase is metastable and is maintained on decompression down to ambient pressure.

The pressure evolution of the frequencies of Raman active modes does not display any systematic departures related to isotopic mass. Only a weak signature of the van der Waals interactions was observed by comparing the pressure dependence of the E2g low interlayer shear mode in isotopically pure samples. At low pressures, where van der Waals forces dominate the interlayer interactions, the mode frequencies diverge faster than at high pressures, where Pauli repulsion sets in. Finally, the linewidth of the high-frequency E2g mode changes very little with pressure, in contrast to the case of ZnO, where the effects of anharmonic decay are strongly modulated by isotopic composition and pressure effects.

[1] R. Cuscó, J. Pellicer-Porres, J. H. Edgar, J. Li, A. Segura, and L. Artús, Pressure Dependence of the Interlayer and Intralayer E2g Raman-Active Modes of Hexagonal BN up to the Wurtzite Phase Transition, Phys. Rev. B102, 1 (2020).
[2] A. Segura, R. Cuscó, T. Taniguchi, K. Watanabe, G. Cassabois, B. Gil, and L. Artús, High-Pressure Softening of the Out-of-Plane A2u (Transverse-Optic) Mode of Hexagonal Boron Nitride Induced by Dynamical Buckling, J. Phys. Chem. C 123, 17491 (2019).
[3] R. Cuscó, J. Pellicer-Porres, J. H. Edgar, J. Li, A. Segura, and L. Artús, Phonons of Hexagonal BN under Pressure: Effects of Isotopic Composition, Phys. Rev. B103, 085204 (2021).

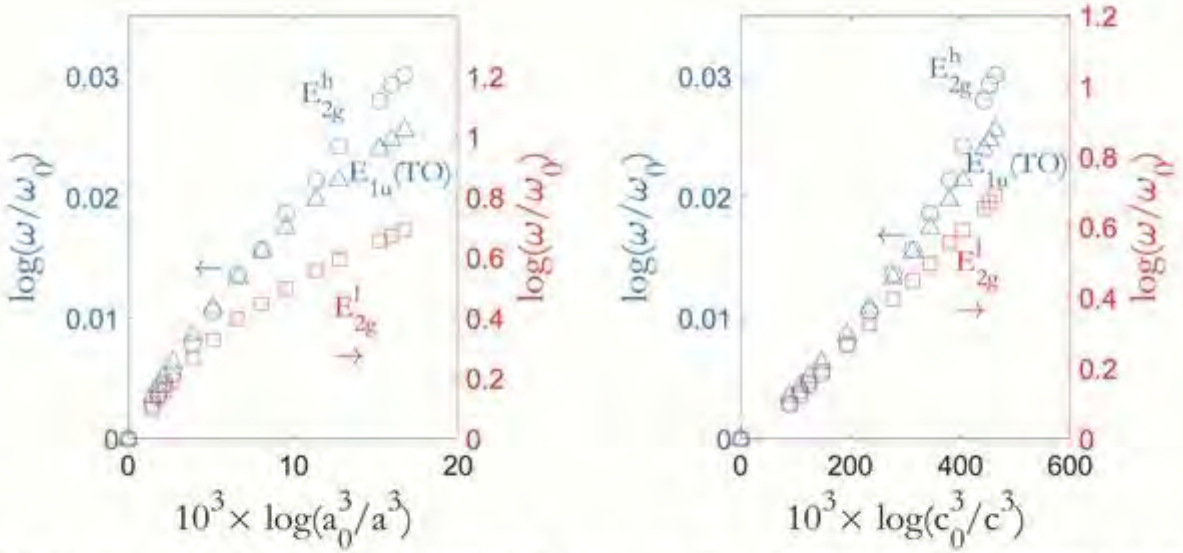


Fig.1. Evolution of the in-plane BN modes under high pressure. The independent variable corresponds to the lattice parameter measured at a given pressure. The logarithmic frequencies of the E^{h}_{2g} and E_{1u}(TO) modes, represented in blue symbols, must be read using the left axis. Those of E^{l}_{2g}, red symbols, employing the right one.

Anomalous polarization enhancement in a vdW ferroelectric material under pressure

Xiaodong Yao[1], Yinxin Bai[1], Ying Liu[1], Junling Wang[1], Jinlong Zhu[1]
[1]*Southern University of Science and Technology, Shenzhen, China*

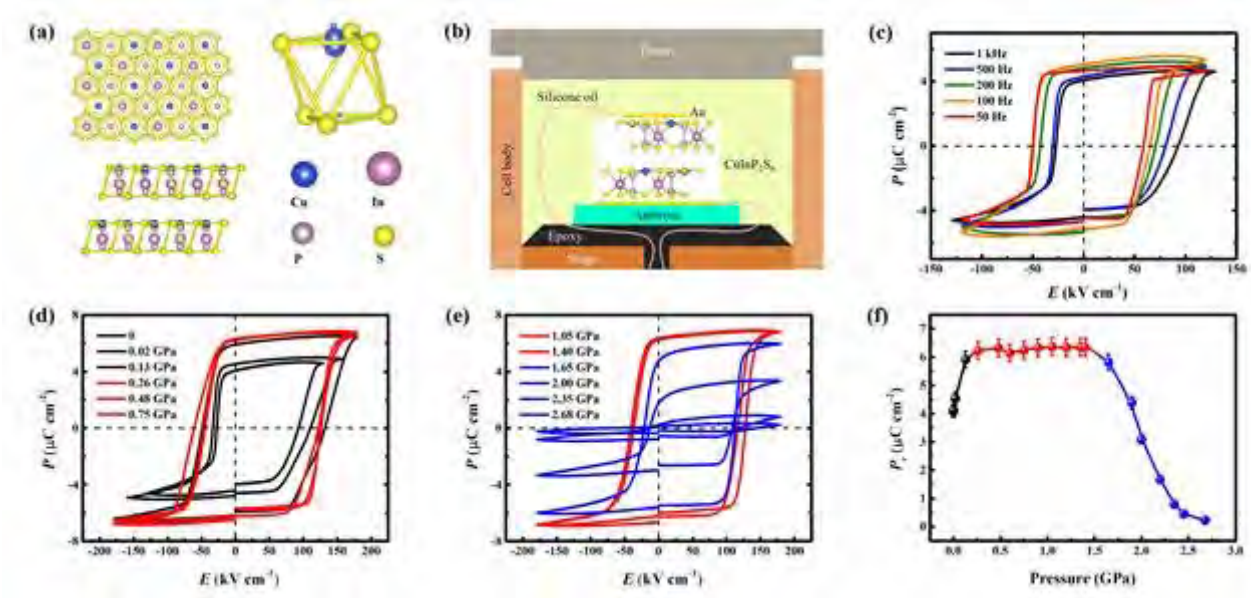
Multifunctional Materials, July 24, 2023, 10:15–12:15

Ferroelectricity is a collective behavior of electric dipoles and the orientation of dipoles can be switched by external electric field. Pressure can affect the atomic spacing and regulate the lattice symmetry, so it can greatly modify the ferroelectricity. A simple theory shows that short-range repulsions increase more rapidly than long-range attractions as pressure increases, the latter, however, favours ferroelectricity. [1]

Here we reported a vdW ferroelectric material CuInP2S6 (CIPS) that its remanent polarization (Pr) increases with pressure. The out-of-plane ferroelectricity originate from the spatial instability of Cu1+. [2] The fine single-crystal X-ray diffraction (SCXRD) experiments show that highly smeared distribution for Cu1+ and the occupancy of the interlayer site is 12% at ambient conditions. [3] Our experiment results show a hydrostatic-pressure-driven 56.5 % enhancement of the Pr at room temperature and remanent polarization increases from 4.06 to 6.36 μC cm-2 at 0.26 GPa. The large polarization state basically remains unchanged until 1.4 GPa and then the Pr gradually decreases at higher pressure, as shown in Figure 1. The high-pressure Raman spectra shows that Cu1+ migrates to interlayer site and the uniformity of CIPS framework improves with pressure up to 0.26 GPa. Simultaneously, in situ high-pressure SCXRD show that if we assume that the dipoles do not change under pressure, the volume reduction would increase the macroscopic polarization by only about 5 % (0.12 μC cm-2) at 0.26 GPa. Due to the enhanced coupling between Cu 4s and S sp orbitals in the adjacent layer as the interlayer distance reduces, it would be expected that the interlayer site is more energetically favoured [4] with the pressure increase. Above analysis suggests that even though pressure suppresses the crystal distortion, it initially forces Cu cations to largely occupy the interlayer site. These findings improve our understanding of this fascinating vdW ferroelectric material and suggest new ways to improve its properties.

Keyword: vdW ferroelectric, high pressure, polarization enhancement, spatial instability of Cu1+

[1] Physical Review Letters 35.26 (1975): 1767.
[2] Physical Review Letters 70.11 (1993): 1639.
[3] Science Advances 5.4 (2019): eaav3780.
[4] Nature Materials 19.1 (2020): 43-48.



High-pressure behaviour of Mg(IO3)2

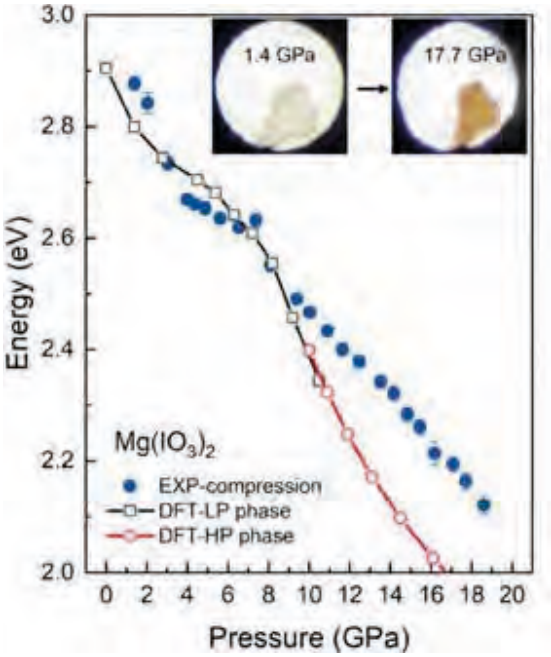
Dr. Akun Llang[1,2], Dr. Robin Turnbull[1], Dr. Catalin Popescu[3], Prof. Francisco Javier Manjon[4], Dr. Enrico Bandiello[1,4], Prof. Placida Rodriguez-Hernandez[5], Prof. Alfonso Muñoz[5], Dr. M. Jasmin[6], Dr. Ybraheem Yousef[3], Prof. Zoulikha Hebboul[7], Dr. Lan-ting Shi[8], **Prof. Daniel Errandonea**[1]

[1]Departamento de Física Aplicada — ICMUV, Univ. de València, MALTA Consolider Team, Burjassot, Spain, [2]Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom, [3]CELLS-ALBA Synchrotron Light Facility, Cerdanyola, Spain, [4]Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Univ. Polit. de València, Valencia, Spain, [5]Departamento de Física and Instituto de Materiales y Nanotecnología, MALTA Consolider Team, Univ. de La Laguna, La Laguna, Spain, [6]TKM College of Arts and Science, Kerala, India, [7]Laboratoire Physico-Chimie des Matériaux (LPCM), University Amar Telidji of Laghouat, Laghouat, Algeria, [8]Institute of High Energy Physics, Chinese Academy of Sciences (CAS), Beijing, China

Electronic Transitions 1, July 26, 2023, 16:30–18:30

Metal iodates are extremely compressible materials with a pseudo-layered crystal structure caused by the lone pair of electrons associated to the iodine atoms. Consequently, they undergo phase transitions at relative low-pressure and have a non-linear pressure dependence of many physical properties. Our group has been dedicated to the study of the behaviour of metal iodates during the last years. In this contribution we will present results on $Mg(IO_3)_2$. We have investigated the structural and vibrational behaviour of $Mg(IO_3)_2$ under compression via a combination of high-pressure synchrotron powder X-ray diffraction, Raman scattering, and infrared spectroscopy experiments [1]. Experiments have been performed under quasi-hydrostatic conditions up to 20 GPa using diamond-avil cells. We have also studied the influence of pressure on the bandgap energy by means of optical absorption measurements [2]. Experiments have been combined with state-of-the-art density-functional theory calculations. Our studies revealed that $Mg(IO_3)_2$ undergoes a pressure-induced phase transition between 7.5 and 9.7 GPa at ambient temperature from a monoclinic (space group $P2_1$) to a trigonal (space group P_3) structure. $Mg(IO_3)_2$ also exhibits the gradual formation of three secondary bonds between iodine and oxygen atoms in neighbouring $[IO3]^{-1}$ units with increasing pressure, thereby increasing the oxygen-iodine coordination from 3 to 6. The bond formation under compression is a consequence of the existence of lone electron pairs on the iodine cation. To accommodate the additional bonds, the covalent I–O bonds within the original $[IO3]^{-1}$ trigonal pyramids increase in length under increasing compression what causes a softening of several high-frequency Raman modes under compression. These results are consequences of bond transformations [3]. The appearance of additional Raman modes at 7.7 GPa and infrared modes at 9.6 GPa supports the phase transition observed in XRD experiments. Changes induced by pressure in the crystal structure and iodine coordination lead to a non-linear behavior of the bandgap energy (see the attached figure). We will report the crystal structure of the HP phase, the pressure-volume equations of state for both phases, the pressure dependence of the Raman- and infrared-active modes of both phases, and the pressure dependence of the bandgap energy. Results will be discussed under the light of DFT calculations and compared with results from other iodates. General conclusions for the behaviour of iodates under compression will be presented.

[1] Liang, A. et al. Phys. Rev. Materials 6, 044603 (2022)
[2] Liang, A. et al. Phys. Rev. B 105, 054105 (2022)
[3] Landrum, G. et al. Angew. Chem. Int. Ed. 37, 1887 (1998)


1.4 GPa
17.7 GPa
Energy (eV)
Pressure (GPa)
Mg(IO3)2
EXP-compression
DFT-LP phase
DFT-HP phase
3.0
2.8
2.6
2.4
2.2
2.0
0
2
4
6
8
10
12
14
16
18
20

A Refined EOS of bcc Bi in a Soft Pressure Medium up to 260 GPa

Daniel Campbell[1], Daniel Sneed[1], Earl O'Bannon III[1], Per Soderlind[1], Zsolt Jenei[1]
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Equation of State 2, July 27, 2023, 14:00–16:00

We present diamond anvil cell X-ray diffraction measurements up to 260 GPa of body-centred cubic Bi, stable above 10 GPa at ambient temperature, in a neon pressure medium. The symmetric structure and high compressibility of bcc Bi make it an appealing pressure calibrant for multimegabar experiments. Our new equation of state parameters show a notable difference from prior work, especially at highest compression. Anisotropic stress on Bi is quite low across the entire pressure range, and deviations in our P-V curve from those previously reported show the effect of using a soft pressure medium. This study highlights the importance of soft pressure media in reducing pressure anisotropy and obtaining accurate equations of state at extreme compression.

Recent in situ experimental and theoretical advances in severe plastic deformations, strain-induced phase transformations, and nanostructure evolution under high-pressure

Professor Valery I Levitas[1]
[1]*Iowa State University of Science and Technology, Ames, United States*

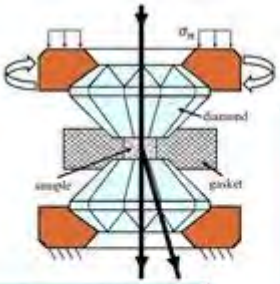
Static Studies of Elements 1, July 25, 2023, 14:00–16:00

The main problem in studying plasticity, plastic strain-induced phase transformations (PTs), and structural changes is that they depend on five components of the plastic strain tensor and its entire path[1], making huge number of independent parameters. New in situ experimental results are obtained for carbon[2], Zr[3,4], and Si[5] under compression in the diamond anvil cell (DAC) and torsion in rotational DAC (RDAC). Drastic reduction (by one to two orders of magnitude[3-5]) of the PT pressure compared with hydrostatic loading and appearance of new phases are demonstrated. The rough diamond anvils (rough-DA) are introduced[4,5] to reach maximum friction equal to the yield strength in shear, which allows the determination of pressure-dependent yield strength and intensification of plastic flow and PTs. It is found in situ that after severe plastic deformations, crystallite size and dislocation density of α and ω-Zr are getting pressure-, strain- and strain-path-independent, reach steady values before and after PT, and depend solely on the volume fraction of ω-Zr during PT[4]. The minimum pressure for plastic strain-induced α-ω PT and the pressure-dependent yield strength of ω-Zr are also independent of plastic strain- and strain-path[3,4]. PT pressure was reduced from 1.36 GPa with smooth-DA to 0.67 GPa with rough-DA, consistent with two-time smaller crystallite size and larger dislocation density.

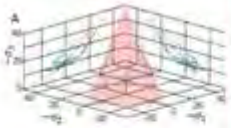
Predicted theoretical correlation between the direct and inverse Hall-Petch effect of the grain size on yield strength and the minimum pressure for strain-induced PT is confirmed for Si-I-II PT[5]. Results are interpreted using developed four-scale theories for plastic strain-induced PTs[1], which fundamentally differ from traditional pressure-induced PTs. Molecular dynamic[6] and first-principle[7] simulations were used to determine lattice PT conditions of perfect crystals under six stress components. At the nanoscale and microscale, nucleation at various evolving dislocation configurations was studied utilizing developed nanoscale[8] and scale-free[9] phase-field approaches. Possibility of reducing PT pressure by more than an order of magnitude due to stress concentration at the dislocation pileup is proven. At the microscale, strain-controlled kinetic equation was derived and utilised in the large-strain macroscopic theory for coupled PTs and plasticity. At the macroscale, the behavior of the sample in DAC/RDAC is studied using the finite element approach[10]. The obtained results create new opportunities in material design, synthesis, and processing of nanostructured materials by severe plastic deformations at achievable-in-industry pressure.

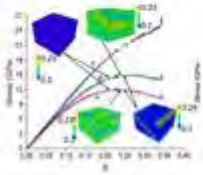
[1] V.I. Levitas, Material Transactions 60 (2019) 1294-1301, invited review.
[2] Y. Gao, Y. Ma, Q. An, V.I. Levitas, Y. Zhang, B. Feng, J. Chaudhuri, W.A. Goddard, Carbon 146 (2019) 364-368.
[3] K.K. Pandey, V.I. Levitas, Acta Materialia 196 (2020) 338-346.
[4] F. Lin, V.I. Levitas, K.K. Pandey, S. Yesudhas, C. Park (2022) https://doi.org/10.48550/arXiv.2208.08022.
[5] S. Yesudhas, V.I. Levitas, F. Lin, K.K. Pandey, J. Smith (2023) https://arxiv.org/abs/2303.04407.
[6] V.I. Levitas, H. Chen, L. Xiong, PRL 118 (2017) 025701.
[7] N.A. Zarkevich, H. Chen, V.I. Levitas, D.D. Johnson, PRL 121 (2018) 165701.
[8] M. Javanbakht, V.I. Levitas, PRB 94 (2016) 214104.
[9] S.E. Esfahani, I. Ghamarian, V.I. Levitas, Acta Materialia 196 (2020) 430-443.
[10] B. Feng, V.I. Levitas, W. Li, Int J Plasticity 113 (2019) 236-254.

Four-Scale Approach

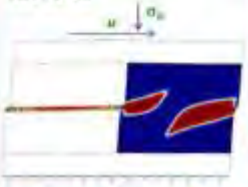


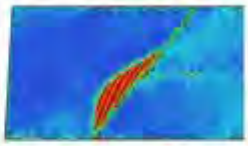
Atomistic modeling
Stress-strain curves, lattice instability criteria under complex loading: MD, DFT

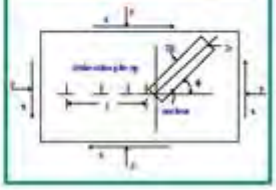




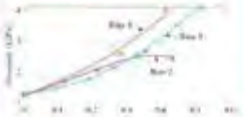
Nanoscale modeling
Interaction between PT and discrete dislocations: analytical, phase field, and MD methods

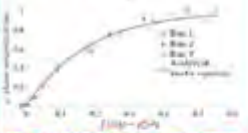


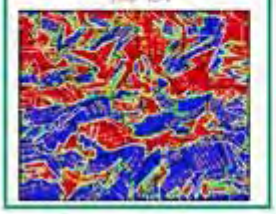




Microscale modeling
Kinetic equation for strain-induced PTs: analytical, scale-free phase field, and micromechanics methods







Macroscale modeling
Evolution of stress, strain, and concentration of phases fields in a sample in RDAC: analytical and FEM

Quantum sensing using the nitrogen vacancy (NV) centre under high-pressure

Mr. Kin On Ho[1], Prof. Swee Kuan Goh[1], Prof. Sen Yang[2]
[1]Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China, [2]Department of Physics and the IAS Centre for Quantum Technologies, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China

Instrumentation and Techniques 2, July 27, 2023, 10:15–12:15

Modern material science demands high sensitivity and resolution for discovering intriguing results. Many exotic features in electrical transport and magnetism are found at ambient pressure, yet setting up the experiments under pressure is often limited by the available tools. In view of this issue, a robust sensor is of uttermost importance for searching novel properties under pressure. A promising candidate for developing high-pressure techniques is the nitrogen vacancy (NV) centre in diamonds. It can work as an in-situ sensor for primary magnetic field or electric field sensing, while simultaneously performing as a wide-range pressure gauge. Recent works have demonstrated the robustness of implementing NV centres under pressure, such as capturing both classical and quantum phase transitions under pressure. These reveal the bright potential of NV sensing in future modern material science. In this presentation, I will briefly review the background of the NV centre under pressure. Our recent works will be introduced for paving the road to probe different material properties under pressure. At last, the proposal for future NV sensing under ultra-high pressure and probing exotic features will be discussed.

[1] Spectroscopy Study on NV Sensors in Diamond-based High-pressure Devices, K. O. Ho, M. Y. Leung, W. Wang, J. Xie, K. Y. Yip, J. Wu, S. K. Goh, A. Denisenko, J. Wrachtrup, and S. Yang, arxiv.2301.05462.
[2] Probing the Evolution of the Electron Spin Wave Function of the Nitrogen-Vacancy Centre in Diamond via Pressure Tuning, K. O. Ho, M. Y. Leung, P. Reddy, J. Xie, K. C. Wong, Y. Jiang, W. Zhang, K. Y. Yip, W. K. Leung, Y. Y. Pang, K. Y. Yu, S. K. Goh, M. W. Doherty, and S. Yang, Phys. Rev. Appl. 18, 064042 (2022).
[3] Probing Local Pressure Environment in Anvil Cells with Nitrogen-Vacancy (NV-) Centres in Diamond, K. O. Ho, M. Y. Leung, Y. Jiang, K. P. Ao, W. Zhang, K. Y. Yip, Y. Y. Pang, K. C. Wong, S. K. Goh, and S. Yang, Phys. Rev. Appl. 13, 024041 (2020).
[4] Measuring magnetic field texture in correlated electron systems under extreme conditions, K. Y. Yip, K. O. Ho, K. Y. Yu, Y. Chen, W. Zhang, S. Kasahara, Y. Mizukami, T. Shibauchi, Y. Matsuda, S. K. Goh, S. Yang, Science 366, 1355 (2019).

Lamellar amorphization in quartz and its relation to the formation of a rosiaite-structured high-pressure phase of silica

Mr. Christoph Otzen[1], Dr. Hanns-Peter Liermann[2], Prof. Dr. Falko Langenhorst[3,4]
[1]Institute of Earth and Environmental Sciences, Faculty of Environment and Natural Resources, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany, [2]German Electron Synchrotron DESY, Hamburg, Germany, [3]Institute for Geosciences, Friedrich Schiller University Jena, Jena, Germany, [4]Hawai'i Institute of Geophysics and Planetology, School of Ocean and Earth Science and Technology, University of Hawai'i at Manoa, Honolulu, United States

Minerals Under High Pressure, July 24, 2023, 16:30–18:30

The mineral quartz develops lamellae of glass when exposed to extreme pressure-temperature conditions during asteroid or meteorite impacts (Langenhorst 2002). These so-called planar deformation features (PDFs) provide the most reliable indications of past impact events on the surface of the Earth. Despite the significance of PDFs, the mechanisms leading to their formation has been unclear.

In order to simulate the pressure-time profiles of impacts on longer time scales, we rapidly compressed (0.5 GPa/s) and decompressed single crystals of quartz uniaxially along the crystallographic c axis using the double-sided membrane-driven diamond anvil cell (Sinogeikin et al. 2015). During the compression synchrotron X-ray diffraction images were collected to observe the crystallographic changes. A selection of recovered samples was investigated using the transmission electron microscope (TEM).

The time-resolved X-ray diffraction images reveal a high-pressure phase transition above 15 GPa. The single crystal-like reflections can be ascribed to a high-pressure phase with a hexagonally closest-packed arrangement of oxygen atoms, while silicon atoms are distributed over octahedral interstices similar to the structure of the mineral rosiaite ($PbSb_2O_6$). The reflections indicate additionally that the rosiaite-structured phase forms distinct crystallographic orientation relationships to quartz. Upon decompression, the rosiaite-structured phase collapses to glass. This results in the formation of amorphous lamellae as observed in the TEM. Shapes, sizes and crystallographic orientations of the amorphous lamellae resemble remarkably those of PDFs formed in naturally shocked quartz. This means that amorphization of quartz occurs over a large range of time scales during decompression from pressures above approximately 15 GPa. The observations also provide a formation mechanism and an explanation for the crystallographic orientations of the lamellae through formation and collapse of rosiaite-structured silica.

[1] Langenhorst (2002), Bulletin of Geosciences 77, 4, 265–282
Sinogeikin et al. (2015), Review of Scientific Instruments 86, 7, 072209

Finite Element Method applied to MHz X-ray diffraction in Diamond Anvil Cell

Mr Nicolas Jaisle[1], Dr. David Cébron[1], Dr. Guillaume Morard[1], Dr. Zuzana Konôpková[2], Dr. Rachel J Husband[3], Dr. Junior Professor Clemens Prescher[4], Dr. Cornelius Strohm[3], Ms Hélène Ginestet[5], Dr. Pr. Sébastien Merkel[5]

[1]Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, IRD, Univ. Gustave Eiffel, ISTerre, Grenobe, France, [2]European XFEL GmbH, Holzkoppel 4, Schenefeld, Germany, [3]DESY Deutsches Elektronen-Synchrotron, Notkestr. 85, Hamburg, Germany, [4]Institute of Earth and Environmental Sciences, Albert-Ludwigs University of Freiburg, Freiburg, Germany, [5]Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 – UMET, F-59000, Lille, France

Developments at XFELs & Lasers, July 24, 2023, 14:00–16:00

The study of magma ocean crystallization and partial melting in the deep Earth is of prime interest to understand terrestrial planets evolution from early days up to late differentiated bodies. This understanding of planets mass distribution and chemical evolutionary pathway goes along with the determination of phase diagram and partial melting properties. In that context, we describe a combined experimental and numerical approach to study pure Fe and FeSiO alloys under high pressure and temperature.

A new fiber Laser Heating Diamond Anvil Cell (LH-DAC) setup, combined with MHz X-ray Diffraction (XRD) at the European X-ray Free Electron Laser (EuXFEL) was used to overcome possible issues within LH-DAC experiments when working with alloys. These potential biases, often designated as chemical migration, are mainly related to the temperature gradients (inherent to LH) within the sample. The presented setup is based on pulsed laser heating, which aims to limit the duration of huge temperature gradients within the sample.

To enhance experimental results, we present a Finite Element Model (FEM) reproducing experimental temperatures and pressures over the experiments µs time scales. A good agreement is found between experimental and numerical values by adjusting less constrained parameters as intensity, iron thermal conductivity and liquid KCl thermal conductivity. We use model outputs (by thermal stress corrected temperature maps) to reconcile Streak Optical Pyrometry (SOP) and XRD data by exploiting model capabilities to sound for temperature and pressure gradients. Moreover, models stress and strain calculations allow for thermal pressure determination over sample and pressure transmitting medium, crucial for accurate XRD interpretation.

Novel low-Z materials for combined X-ray and large-volume-press studies

Longjian Xie[1]
[1]*Department of Earth Sciences, University College London, London, United Kingdom*

Instrumentation and Techniques 1, July 26, 2023, 10:15–12:15

Large-volume press, which can generate pressures over 100 GPa at high temperatures in a large volume, is an important device for high-pressure studies of Earth and material sciences. X-ray observation is an important tool to characterise materials. The combination of large-volume press and X-ray observation is, thus, an excellent in situ method to study the high-pressure behaviours of material. X-ray transparent materials (i.e. low-Z materials), especially heater and pressure medium, are essential for in situ high-pressure experiments. Graphite and boron-epoxy are traditional low-Z materials used as heaters and pressure media at pressures lower than 10 GPa. However, graphite cannot be used as a heater anymore due to the graphite-diamond conversion at pressures higher than 10 GPa. Boron-epoxy frequently causes blowout at pressures higher than 10 GPa. Here, I developed a boron-doped diamond as a heating element and a boron-MgO composite as a pressure medium for pressures higher than 10 GPa. The boron-doped diamond heater can generate temperatures as high as 4000 K and the boron-MgO composite pressure medium can generate pressures to 25 GPa without sacrificing its X-ray transparency. These novel low-Z materials enable various in situ X-ray measurements at pressure higher than 10 GPa such as viscosity measurements by falling sphere viscometry and density measurements by X-ray absorption method.

Measurement of Electrical Conductivity of Water and Heavy Water under Reverberating Shock Compression

Tsutomu Mashimo[1], Hideaki Isamu[1], Ryohei Inaba[1], Xun Liu[2], Williams Nellis[3]
[1]Kumamoto University, Kumamoto 860-8555, Japan, [2]Wuhan University of Technology, Wuhan, China, [3]Harvard University, Boston, United States

Outer Planets and Exoplanets 1, July 26, 2023, 10:15–12:15

Water (H2O) is predicted to exist in ice giants such as Uranus and Neptune as one of the major components between a rocky core and a gaseous atmosphere with ammonia (NH3) and some hydrocarbons. Under high-pressure extreme conditions in such ice giant, water and other components can be electrical conductors, which have been assumed to be the source of magnetic field of the planets. In this work, the electrical conductivities of water and heavy water (D2O) were measured under shock compression up to 114 GPa. We used a reverberating shock compression in order to obtain the higher pressures than those by single shock compression, supressing the temperature. We used the sapphire (Al2O3) and CVD polycrystalline diamond as anvil for the reverberating shock experiments to discuss the temperature effect on the conductive state of water. The result showed that the electrical conductivity increased exponentially with increasing pressures up to ~20 GPa and converged to a certain value. There was not large difference in electrical conductivity between using diamond and sapphire anvils, which indicated that the electrical conductivity does not depend on the temperature much. In addition, there was not large difference between water and heavy water despite the difference in weight of hydrogen and deuterium. The conductivity behaviour and the application will be discussed at the conference.

Study of liquid silicates using laser-driven shock compression

Guillaume Morard[1], Jean-Alexis Hernandez[2], Alessandra Ravasio[3], D Sokaras[4], Hae Ja Lee[4], Eric Galtier[4], S Glenzer[4], Tommaso Vinci[3], Silvia Pandolfi[4], Silvia Boccato[5], Clemens Prescher[6], Julien Chantel[7], Sebastien Merkel[7], Wendy L Mao[8], Arianna E Gleason[8], Roberto Alonso-Mori[4], S-H Shim[9]
[1]ISTerre-Université Grenoble Alpes-CNRS, Grenoble, France, [2]ESRF, Grenoble, France, [3]LULI, Palaiseau, France, [4]SLAC, Stanford, United States, [5]IMPMC, Paris, France, [6]University of Freiburg, Freiburg, Germany, [7]UMET, Lille, France, [8]Stanford University, Stanford, United States, [9]Arizona State University, Tempe, United States

Outer Planets and Exoplanets 1, July 26, 2023, 10:15–12:15

Building models of early planetary evolution is crucial to constrain the history of our planet, of the solar system, and for understanding the diversity of exoplanets. Early processes include global scale shock events, large scale melting, gravitational segregation of materials, and partitioning of elements into different layers. These early processes are critical as the chemical compositions of the different layers of a planet is set at this stage.

The temporal evolution of a magma ocean in its latter stage, i.e., after most of material has been accreted, is controlled by magma ocean convection, whose regime depends on the composition and temperature profiles. Establishing a density profile requires thermodynamic models for the relationship between density and composition. Thermal expansion and compressibility of liquid silicates are also important to estimate the temperature profiles of the magma ocean (with an adiabatic assumption). These examples demonstrate that physical properties of liquid silicates are key to establishing early planetary structures and to understanding the dynamics of an early magma ocean (e.g., full convection or stratified convection).

At the MEC instrument of LCLS, we have been able to probe shock-driven liquid silicates with in situ X-ray diffraction at combined high-pressures and -temperatures. The experimental setup allows synchronization of a laser drive (80 J focused with a 150 µm Phase Plate), inducing a shock wave in a 50 µm thick target ((Mg,Fe)SiO3 glass with variable Fe content), and an X-ray pulse produced by the Free Electron Laser (17 keV energy, duration of ~50 fs, focus spot on target of ~50 um diameter). Probing at a time just before the breakout allows homogeneous P-T conditions to be obtained in the shocked silicate, up to 350 GPa and ~15,000 K, determined by a VISAR measurement on the rear surface of the sample. The XRD patterns from 4 ePIX detectors were combined using DIOPTAS (Prescher et al, 2015) for a Q range between 17 and 90 nm-1. Then, the local structure, as well as the density, were recovered using Amorpheus software (Boccato et al, 2022).

Fast and confocal Brillouin spectroscopy for the study of molecular systems at planetary interiors conditions

Dr Alexis Forestier[1,2], Gunnar Weck[1,2], Frédéric Datchi[3], Paul Loubeyre[1,2]
[1]CEA DAM DIF, Arpajon, France, [2]Laboratoire Matière en Conditions Extrêmes (LMCE), Université Paris-Saclay, CEA, Bruyères-le-Châtel, France, [3]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), UMR CNRS 7590, Sorbonne Université, Muséum National d'Histoire Naturelle, Paris, France

Instrumentation and Techniques 3, July 26, 2023, 14:00–16:00

Brillouin spectroscopy is a powerful tool to probe the melting curve, phase transitions, as well as to measure fluid equation of state and refractive index from sound velocity data. Usually performed with a Tandem Fabry-Perot interferometer (TFP), Brillouin acquisitions last from a few minutes to a few hours in the diamond anvil cell [1]. Consequently, Brillouin studies at high pressure and high temperature are still rare. To overcome this limit, we have developed a new set-up (ref. 2) based on the spatial dispersion of the Brillouin scattered light from a Virtually Imaged Phased Array (VIPA). The Brillouin spectrum is directly recorded on a two-dimensional CMOS sensor, which allows more than 10-fold speed up in acquisition time compared to the usual TFP. Moreover, the system is coupled using single-mode fibres, which allows excellent spatial resolution and confocality at the sample. As illustrated in figure 1, our approach is particularly suited for laser heating measurements in the diamond anvil cell and has the potential to become an important platform to study warm dense molecular systems at planetary interiors conditions.

These systems, based on the elements C, H, N, O at P = 1–200 GPa and T = 300–5000 K, exhibit rich and complex phase diagrams that remain little explored [3]. Ab-initio calculations predict very interesting phenomena, e.g., liquid-liquid transitions between polymeric and molecular N2 and CO2 [4,5], as well as multiple fluid states (molecular, ionised and plasma) in water [3]. This complexity has important consequences on planetary bodies. For example, conductive shells of superionic water ice in the interiors of Neptune and Uranus are thought to be responsible for their non-symmetric, non-dipolar magnetic fields [3].

We will present detailed comparisons between the hyperfine spectrometer and the TFP in terms of implementation and performance. Brillouin data on fluid H2O will be presented and compared to previous experiments, validating our approach from a metrological point of view. Measurements of the melting curve of N2 in the laser-heated DAC will be presented. Through several examples, we will illustrate the new possibilities offered by this technique for the study of warm dense molecular systems.

[1] Kimura and Murakami, J. Chem. Phys. (in press)
[2] Forestier et al. High Press. Res 42, n°3, 259 (2022)
[3] Redmer et al. Icarus 211, n°1, 798 (2011)
[4] Boates and Bonev, Phys. Rev. Lett. 102, n°1, 015701 (2009)
[5] Boates et al. Proc. Natl. Acad. Sci. U.S.A 109 n°37, 14808 (2012)

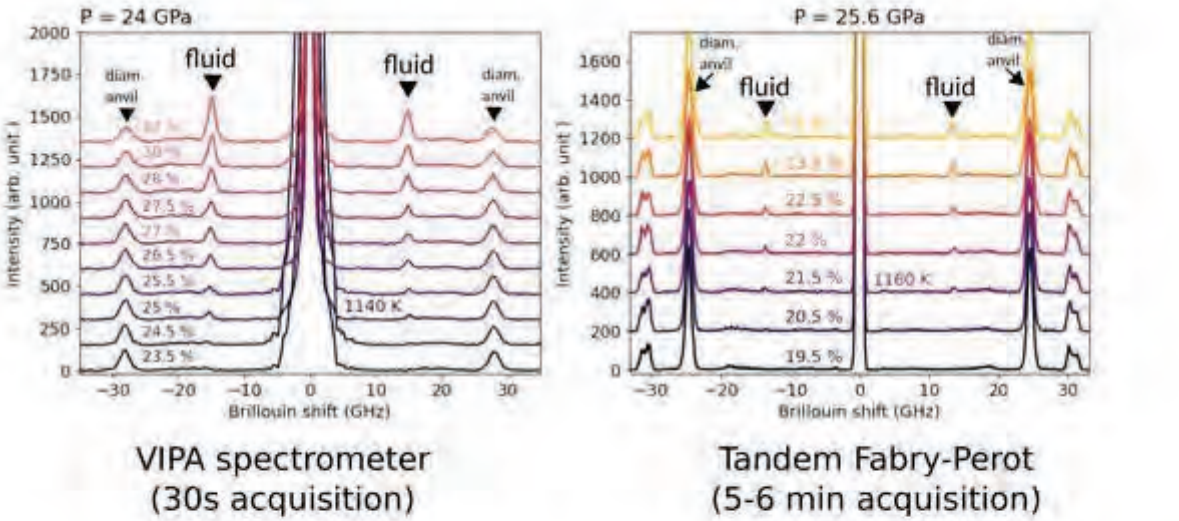


Figure 1: Brillouin spectroscopy in the DAC under CO_2 laser-heating. The sample is H_2O. Left : spectra collected with the VIPA spectrometer. Right : spectra collected using the Tandem Fabry-Perot Interferometer under similar conditions. CO_2 heating laser power values are indicated for each spectra in %. Acquisition times per spectrum are indicated.

Chemistry of Low Z Mixtures at Icy Giant Conditions

Michael Stevenson[1], Zhiyu He[1], Benjamin Heuser[1,2], Lisa Zinta[1], Divyanshu Ranjan[1,2], Mandy Bethkenhagen[3], Martin French[1], Armin Bergermann[1], Ronald Redmer[1], Thomas Cowan[2], Oliver Humphries[4], Julien Lütgert[1], Katya Voigt[2], Anja Schuster[2], Frederic Lefevre[5], Tommaso Vinci[5], Emma McBride[6], Nicholas Hartley[7], Arianna Gleason[7], Siegfried Glenzer[7], Silvia Pandolfi[8], Adrien Descamps[7], Benjamin Ofori-Okai[7], Christopher Schoenwaelder[7], Griffin Glenn[7], Luke Fletcher[7], Jean-Alexis Hernandez[9], Alessandra Ravasio[5], Dominik Kraus[1,2]

[1]University of Rostock, Rostock, Germany, [2]Helmholtz-Zentrum Dresden-Rosendorf, Dresden, Germany, [3]Institute of Science and Technology Austria, Austria, [4]European XFEL, Hamburg, Germany, [5]Laboratoire LULI, Ecole Polytechnique, Palaiseau, France, [6]Queen's University Belfast, Belfast, UK, [7]SLAC National Accelerator Laboratory, Menlo Park, United States, [8]IMPMC – Sorbonne Université, Paris, France, [9]The European Synchrotron Radiation Facility, Grenoble, France

Outer Planets and Exoplanets 2, July 26, 2023, 16:30–18:30

Extreme conditions are ubiquitous in nature. Much of the matter in the universe exists under high pressures and temperatures. Of interest, are the planetary interiors of the icy giants, Uranus and Neptune. These planets have particularly complex magnetic fields [1]. To understand these complex magnetic fields the conditions and composition of these planetary interiors need to be determined. The interiors of these planets are understood to contain mixtures of water, ammonia, and hydrocarbons [2].

To understand the behaviours observed in ice giant planets it is of the upmost importance to study their constituents. Several behaviours have been suggested for instance, as the mechanism of the complex magnetic fields observed for the icy giants. For example, the presence of either, high pressure superionic ammonia and water ices [3-5] or, metallic hydrogen formed by the de-mixing of hydrocarbons [6,7].

To study icy giants both isolated water and plastics acting as “synthetic planets” have been shock-compressed to icy giant interior conditions. The water was shock compressed into the superionic region, of the water phase diagram, with the use of reverberating shocks to determine the structures of ice under these conditions. The previously reported bcc and fcc superionic phases were observed and at higher P-T conditions a new ice phase became evident. These compression experiments also investigated hydrocarbon de-mixing under planetary interior conditions for several bioplastics. The bioplastics allowed for different planetary stoichiometries to be studied in this case simulating several different carbon:water ratios and determining the effect of the presence of oxygen in nanodiamond formation in shocked plastics [8].

Ongoing and future campaigns at XFEL, synchrotron, and laser facilities study the behaviour of the hydrogen in de-mixed shock compressed plastics and de-mixing in various plastic stoichiometries (e.g., CHNO) to simulate differing planetary interior mixtures. New plastic “slurry” targets are also being investigated [9]. These slurries may allow the investigation of chemistry in a variety of mixture stoichiometries present in planetary interiors as well as allow novel materials synthesis under extreme conditions.

[1] W.J. Nellis, J. Phys.: Conf. Ser. 950, 042046 (2017).
[2] M. D. Hofstadter et al., Ice Giants: Pre-Decadal Survey Mission Study Report, NASA-JPL report JPL- D-100520 (2017).
[3] Cavazzoni C et al., Science, 1;283(5398):44-6 (1999).
[4] M. Millot et al., Nat. Phys. 14, 3 (2018).
[5] M. Millot et al., Nat. 569, 7755 (2019).
[6] W.J. Nellis, AIP Conference Proceedings 1793, 090002 (2017).
[7] D. Kraus et al., Nat Astron 1, 606-611 (2017).
[8] Z. He et al., Sci. Adv., 8, 35 (2022).
[9] R. Smith et al., J. Appl. Phys., 131 (2022).

Theoretical investigation on the reactivity of fluorine and bromine at high pressure: emergence of novel bromine fluorides

Ms. Madhavi Dalsaniya[1,2], Mr. Deepak Upadhyay[2], Mr. Krzysztof Jan Kurzydłowski[1], Mr. Dominik Kurzydłowski[2]

[1]Faculty of Materials Science and Engineering, Warsaw University of Technology, Wołoska 141, 02-507, Warsaw, Poland, Warsaw, Poland, [2]Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University in Warsaw, 01-038, Warsaw, Poland, Poland

Chemical Bonding 1, July 24, 2023, 14:00–16:00

Investigation of the properties of halogens and halogen-rich materials under large compression is a new and largely unexplored research area in high pressure (HP) sciences [1-3]. Particular interest is the reactivity of fluorine which has unique properties at ambient conditions due to its small size, large electronegativity, and extremely high oxidizing power [4]. The few theoretical studies on the high-pressure properties of fluorine-containing systems conducted so far strongly indicate that the chemistry of this element becomes even more unique at large compression [5-7]. Here we model the reactivity of fluorine with bromine at atmospheric pressure up to 100 GPa by using the r2-SCAN DFT approach [8] with the Vienna Ab Inition Simulation Package (VASP). We explore the stability and phase transition sequence of BrFn (n = 1 – 7) compounds. The obtained convex hull diagram shows that pressure does not lead to stabilization of BrF which is an unstable fluoride at ambient conditions.

Surprisingly bromine trifluoride (BrF3) is predicted to decompose above 21 GPa into BrF5 and BrF2. The latter compound is a novel bromine fluoride with a formally open shell (21 valence electrons). Analysis of the electronic structure of this compound points to an interesting interplay between ionic and covalent bonding. These theoretical calculations provide important insights into the properties and behavior of BrFn compounds and can help guide experimental investigations into these systems.

Key words: High pressure, phase transitions, halogens, density functional theory.

[1] C. Wang, Y. Liu, X. Chen, P. Lv, H. Sun, and X. Liu, Phys. Chem. Chem. Phys., 22, 5, 3066–3072 (2020).
[2] M.H. Dalsaniya, K.J. Kurzydłowski, and D. Kurzydłowski, Phys. Rev. B, 106, 11, 115128 (2022).
[3] E. Bykova, I.G. Batyrev, M. Bykov, E. Edmund, S. Chariton, V.B. Prakapenka, and A. F. Goncharov, arXiv preprint arXiv:2301.05657 (2023).
[4] M. Rahm, T. Zeng, and R. Hoffmann, J. Am. Chem. Soc., 141, 1, 342–351 (2018).
[5] J. Lin, S. Zhang, W. Guan, G. Yang, & Y. Ma, J. Am. Chem. Soc., 140, 30, 9545–9550 (2018).
[6] D. Luo, J. Lv, F. Peng, Y. Wang, G. Yang, M. Rahm, and Y. Ma., Chem. Sci., 10, 8, 2543-2550 (2019).
[7] D. Kurzydłowski, M. Derzsi, E. Zurek, and W. Grochala, Chem. Eur. J., 27, 17, 5536–5545 (2021).
[8] J. W. Furness, A. D. Kaplan, J. Ning, J. P. Perdew, and J. Sun, J. Phys. Chem. Lett. 11, 8208 (2020).

Phase diagram of tin under extreme conditions

Robin Fréville[1,2], Dr Agnès Dewaele[1,2], Dr Philippe Faure[3], Dr Nicolas Guignot[4], Dr Mohamed Mezouar[5]

[1]CEA, DAM, DIF, F-91297 Arpajon, France, [2]Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, 91680 Bruyères-le-Châtel, France, [3]CEA, DAM, VALDUC, Is-sur-Tille, F-21120, France, [4]Synchrotron SOLEIL, BP48, 91192 Gif-sur-Yvette Cedex, France, [5]European Synchrotron Radiation Facility, BP220, 34043 Grenoble Cedex, France

Static Studies of Elements 2, July 26, 2023, 16:30–18:30

Tin lands an intermediate position between semi-conducting (Si, Ge) and metallic (Pb) elements of the group 14. It presents then unusual bonding changes as a function of pressure and temperature. At ambient conditions, Sn is stable in its metallic phase β-Sn (space group: I41/amd). At room temperature, and around 10.8 GPa, Sn undergoes a phase transition to a body-centred tetragonal bct-Sn (space group: I4/mmm) structure. The transition line ends with a β-bct-liquid triple point at 2.8 GPa and 577 K [1].

Upon further compression at room temperature, two Sn polymorphs are observed: a distortion to obtain a body-centred orthorhombic bco-Sn (space group: Immm) structure at 32.5 GPa; and then a sluggish evolution to a fully cubic bcc-Sn (space group: Im-3 m) structure. One current challenge on Tin is to determine solid phase stability domains under high temperature and the precise melting curve at high pressure (around the Mbar range) [2].

X-Ray Diffraction (XRD) in Diamond Anvil Cells (DAC) coupled with in situ laser heating experiments were conducted up to ~100 GPa. The stability domain of the bcc phase has been measured and is wider than previously thought. In particular, while its melting line agrees with ref [3] up to 70 GPa, it is higher above that pressure. A discussion between the two different diagnostics is presented which involve chemical reaction. The stability of hcp high pressure phase is confirmed. [4]

[1] G. Deffrennes, P. Faure, F. Bottin, J.-M. Joubert et B. Oudot, «Tin (Sn) at high-pressure: Reviex, X-ray diffraction, DFT calculations, and Gibbs energy modeling,» Journal of Alloys and Compounds, vol. 919, n° %1165675, 2022.

[2] A. Lazicki, J. R. Rygg, F. Coppari, R. Smith, D. Fratanduono, R. G. Kraus, G. W. Collins, R. Briggs, D. G. Braun, D. C. Swift et J. H. Eggert, «X-ray diffraction of Solid Tin to 1.2 TPa,» Physical Review Letters, vol. 115, n° %1075502, 2015.

[3] R. Briggs, D. Daisenberger, O. Lord, A. Salamat, E. Bailey, M. J. Walter et P. F. McMillan, «High-pressure melting behaviour of tin up to 105 GPa,» Physical Review B, vol. 95, n° %1054102, 2017.

[4] A. Salamat, G. Garbarino, A. Dewaele, P. Bouvier, S. Petitgirard, C. J. Pickard, P. F. McMillan et M. Mezouar, «Dense close-packed phase of tin above 157 GPa observed experimentally via angle-dispersive X-ray diffraction,» Physical Review B, vol. 84, n° %1140104, 2011.

Kinetic behaviour of Molecular Nitrogen

Jinwei Yan[1], Prof. Philip Dalladay-Simpson, Dr. Xiaodi Liu, Prof. Federico Gorelli, Prof. Chris Pickard, Pro. Eugene Gregoryanz
[1]University of Edinburgh, Edinburgh, United Kingdom, [2]University of Science and Technology of China, Hefei, China, [3]Institute of Solid-State Physics, HFIPS, Chinese Academic of Science, Hefei, China

Other Molecular Systems, July 27, 2023, 10:15–12:15

Nitrogen is the 7th most abundant element in the Universe and a major constituent of air on Earth. Its triple bonding is responsible for one of the most complicated phase diagrams known today. In fact, the phenomena observed in compressed nitrogen could provide many textbook examples for condensed matter physics. At low pressure, nitrogen solidifies into the orientationally disordered states (β). Furthermore, N2 goes through several solid molecular phases, with each subsequent one having lower symmetry with increasing pressure. At pressures above 4.9 GPa, nitrogen phases exhibit Davydov splitting caused by 2 types of molecules present in the lattice. When nitrogen is heated between 40-100 GPa (ε(ζ)-N2), it transforms into ι(θ)-N2 [1]. These two phases can be quenched to 300 K and occupy the phase space normally associated with ε(ζ). Above 130 GPa, nitrogen intermolecular bonding could be broken, resulting in an amorphous semiconductor (η). By heating η-N, single bonded nitrogen polymers (cg-N, lp-N, bp-N…) could be crystallised.

Recently, a novel molecular phase λ-N2 was discovered at low temperatures [2]. There are several interesting questions arising about the nature and properties of λ-N2. Considering the vast amount of experimental work done on nitrogen, it is intriguing why this prominent phase was not seen and described in the previous studies [3,4]. The Raman spectra of λ-N2 appear to be almost identical to those of θ-N2, but these phases are separated in the P-T space by almost 100 GPa and 1000 K at the points of their formation [2]. The (meta)stability of the ι, θ, and λ modifications is also striking even though λ-N2 forms at low temperatures, it can be recovered at 300 K; once recovered, it occupies the entire phase space of ε, ζ, and κ--the same way ι and θ do when quenched from high temperatures.

By combining newly developed fast compression techniques based on dynamic Diamond Anvil Cells (d-DACs) with Raman spectroscopy [5], we study the behaviour of N2 under dynamic rate compression between 10 and 300 K. Our research shows that kinetics play a fundamental role in the formation of a novel low-temperature phase named λ-N2. Its formation is controlled by fast compression overcoming a “pressure band gap,” where the compression rate increases rapidly with temperature. Based on DFT calculation results, we speculate on the formation mechanism of λ-N2 behind our experimental observations.

[1] R. Turnbull, et. al, Nature Communications 9, 4717 (2018)
[2] M. Frost, et. al, Physical Review B 93, 024113(2016)
[3] B. Steven, et. al, Journal of Physical Chemistry 88, 2522 (1984)
[4] R. Bini, et. al, Journal of Physical Chemistry 112, 8522(2000)
[5] J. Yan, et. al, Review of Scientific Instruments 93, 063901 (2022)

Mechanical properties of high-pressure synthesised hexagonal silicon

Dr. Tao Liang[1]
[1]*Center for High Pressure Science and Technology Advanced Research (HPSTAR), Pudong, China*

Ceramics and Composites, July 24, 2023, 14:00–16:00

Hexagonal silicon (Si-IV, also known as lonsdaleite or wurtzite Si) has recently attracted considerable research interest due to its extraordinary optical properties and possibility to convert into a direct semiconductor under strain with great potential for applications. Although Si-IV has been obtained by chemical vapor deposition or epitaxial growth on gallium phosphide nanowires, synthesizing pure Si-IV through chemical reactions is quite challenging. Fortunately, Si-IV can also be synthesised through solid-state phase transitions under high pressure. In this talk, I will first introduce the synthetic method of Si-IV by application of high pressure. And the mechanical properties investigation results of Si-IV will also be presented by combining nanoindentation and in situ high-pressure synchrotron X-ray diffraction study. The investigation results indicate that the elastic moduli and hardness of Si-IV are close to those of the common diamond cubic silicon, which are beneficial for integrating Si-IV into conventional Si-based devices and its photovoltaic and optoelectronic applications.

High-Pressure Synthesis of Ultraincompressible and Recoverable Carbon Nitrides

Dr Dominique Laniel[1], Florian Trybel[2], Andrey Aslandukov[3], Saiana Khandarkhaeva[3], Timofey Fedotenko[4], Yuqing Yin[3], Nobuyoshi Miyajima[3], Ferenc Tasnadi[2], Alena Ponomareva[5], Nityasagar Jena[2], Gunnar Weck[6], Fariia Iasmin[3], Bjoern Winkler[7], Adrien Néri[3], Stella Chariton[8], Carlotta Giacobbe[9], Jonathan Wright[9], Gaston Garbarino[9], Björn Wehinger[9], Anna Pakhomova[9], Mohamed Mezouar[9], Vitali Prakapenka[8], Victor Milman[10], Wolfgang Schnick[11], Igor Abrikosov[2], Leonid Dubrovinsky[3], Natalia Dubrovinskaia[3]

[1]University Of Edinburgh, Edinburgh, United Kingdom, [2]University of Linköping, Linköping, Sweden, [3]University of Bayreuth, Bayreuth, Germany, [4]DESY, Hamburg, Germany, [5]NUST "MISIS", Moscow, Russia, [6]CEA, Arpajon, France, [7]University of Frankfürt, Frankfürt, Germany, [8]APS, Lemont, United States, [9]ESRF, Grenoble, France, [10]Dassault Systèmes BIOVIA, Cambridge, United Kingdom, [11]University of Munich, Munich, Germany

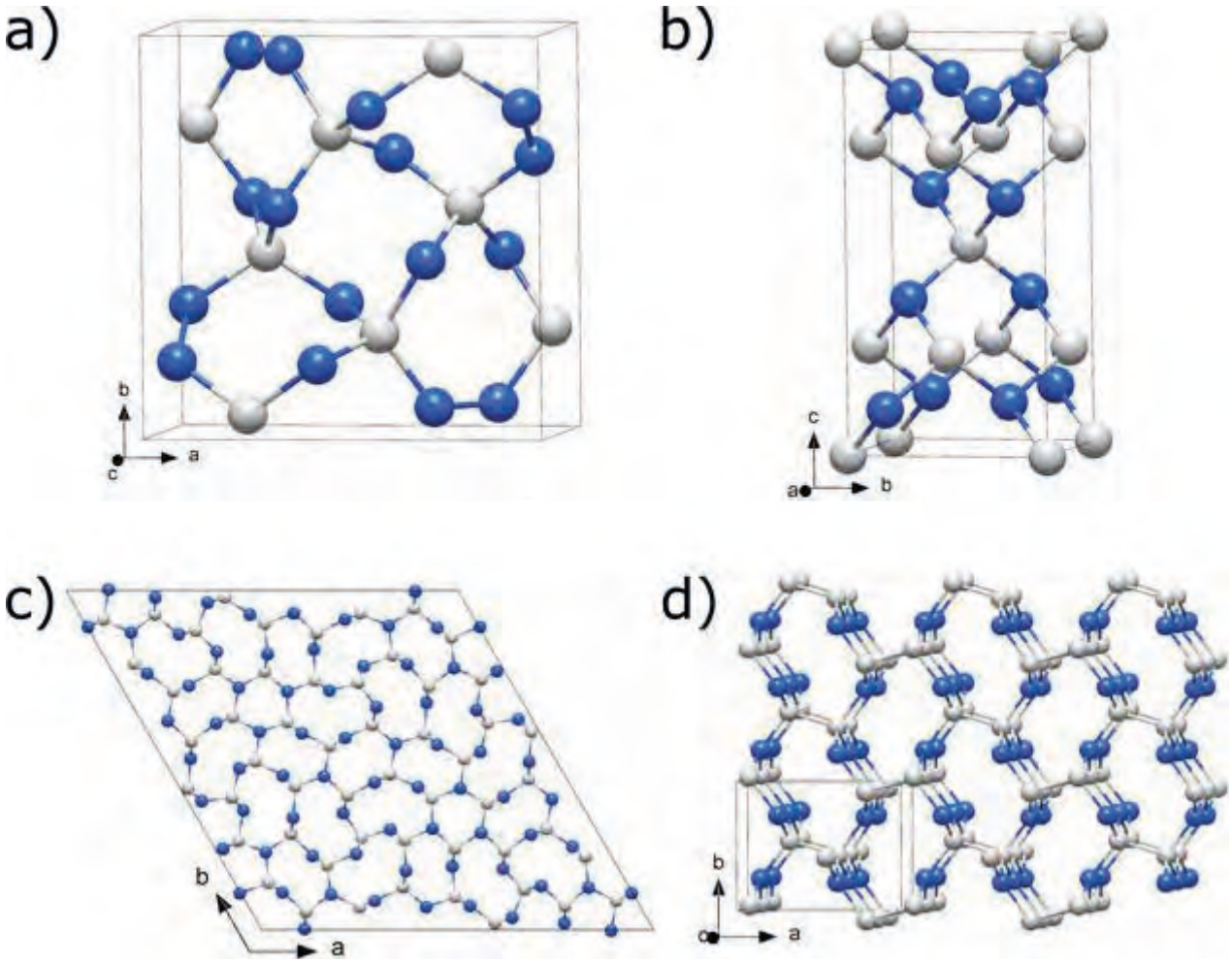
Nitrides, Borides and Carbides 2, July 25, 2023, 14:00–16:00

Carbon nitrides are one of the holy grails of materials science ever since the seminal paper of Liu and Cohen [1]. They predicted that a fully saturated polymeric C3N4 solid comprised of corner-sharing CN4 units could be formed and would have exceptional mechanical properties; likely to have a hardness greater than diamonds. In the last three decades, momentous efforts were devoted to the synthesis of such materials through a multitude of experimental approaches [2]. Yet, no credible and reproducible claim of such compounds was reported.

Here, we will present results that bring this quest to an end. Laser-heated diamond anvil cell experiments on carbon-nitrogen precursors were performed up to 137 GPa. Four carbon nitrides were synthesised, oP8-CN [3], tI14-C3N4, hP126-C3N4 and tI24-CN2, and their crystal structure was solved (Figure 1) employing single-crystal X-ray diffraction. These solids form remarkable polymeric structures with fully saturated C and N atoms, producing either corner-sharing C(CN3) or CN4 tetrahedra.

Upon the samples' decompression, all four compounds were found to be recoverable at ambient conditions – a feat never before accomplished for megabar-synthesised materials – and stable in air. As expected from their crystal chemistry, these C-N compounds are ultra-incompressible, with an experimental bulk modulus ranging between 351 and 429 GPa. Ab-initio calculations revealed the solids' superhardness, computed to be between 78.0 and 86.8 GPa based on a microscope hardness model – exceeding even that of c-BN (62.3 GPa) and closely approaching diamond's (89.2 GPa). This is qualitatively supported by diamond anvil indentation experiments using the recoverable materials. Further experiments and calculations suggest the multifunctional properties of these solids, featuring piezoelectricity, wide band gap, tunable photoluminescence and high energy density, underlining their attractivity.

[1] Liu, A. (1989). Science 245, 841-842.
[2] Kessler, F. K. (2017). Nat. Rev. Mater. 2, 17030.
[3] Stavrou, E. (2016). Chem. Mater. 28, 6925-6933.


a)
b
a
c
b)
c
a
b
c)
b
a
d)
b
a

Does similar folds mean similar folding pathways? A comparative high-pressure NMR study of the unfolding of two Ig-fold modules.

Dr Isaline Herrada[1], Mr Saotome Tomoki[2], Ms Mounia Lahfa[1], Dr Yin-Shan Yang[3], Dr Philippe Barthe[1], Dr Karine De Guillen[4], Prof Yutaka Kuroda[2], **Prof. Christian Roumestand**[1]
[1]Centre de Biochimie Structurale, University of Montpellier, Montpellier, France, [2]Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, Tokyo, Japan, [3]Centre de Biochimie Structurale, CNRS UMR5048, Montpellier, France, [4]Centre de Biochimie Structurale, INSERM U1054, Montpellier, France

Bio/Life Sciences and Soft Matter, July 26, 2023, 10:15–12:15

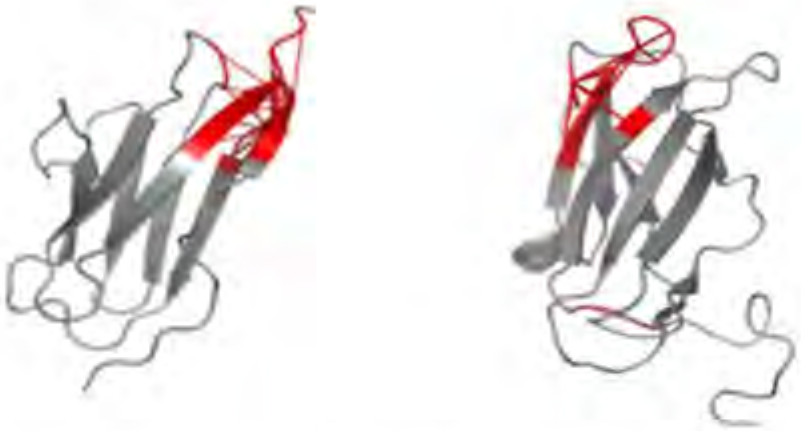
Titin is a giant multi-modular protein found in vertebrate striated muscle. In the light band of the sarcomere, its structure consists in a repetition of Ig-fold modules, which partial unfolding has been invoked in muscle elasticity.

Dengue fever is caused by an enveloped RNA flavivirus. The virus envelope consists in the association of 180 E-protein units, composed of three domains (ED1, ED2 and ED3). The ED3 domain contains two putative dominant epitopes, which are recognised by antibodies.

ED3 and Titin module adopts a characteristic Ig-like fold. In this study, we present a comparative High Pressure NMR denaturation study [1,2] of Titin I27 module [3] and ED3 domain [4]. We found that, despite a different global stability, the unfolding of these two modules started with the disruption of connections between the N- and C-termini, yielding a similar folding intermediate. On the other hand, kinetics studies show that the transition state ensemble (TSE) of ED3 is markedly more hydrated than that of I27.

It is rather striking that two proteins with unrelated function, with extremely low sequence similarity, but with a common 3D fold share similar folding pathways. Of course, the comparison of two modules is not enough to draw a general conclusion and this study should be completed by the analysis of unfolding properties of other proteins presenting this ubiquitous Ig-fold.

[1] J. Roche, C.A. Royer, and C. Roumestand. Monitoring protein folding through high pressure NMR Spectroscopy. Prog. Nucl. Magn. Reson. Spectrosc. 102-103, 15-31 (2017).
[2] J. Roche, C.A. Royer, and C. Roumestand. Exploring Protein Conformational Landscapes Using High-Pressure NMR. Methods Enzymol. 614, 293-320 (2019).
[3] I. Herrada, P. Barthe, M. Vanheusden, K. DeGuillen, L. Mammri, S. Delbecq, F. Rico, and C. Roumestand. Monitoring Unfolding of Titin I27 Single and Bi Domain with High-Pressure NMR Spectroscopy. Biophys. J. 11 (52), 341-352 (2018).
[4] T. Saotome, M. Doret, M. Kulkarni, Y.-S. Yang, P. Barthe, Y. Kuroda, C. Roumestand. Folding of the Ig-Like Domain of the Dengue Virus Envelope Protein Analyzed by High-Hydrostatic-Pressure NMR at a Residue-Level Resolution. Biomolecules, 9 (8). pii: E309. doi: 10.3390/biom9080309 (2019).



Ribbon 3D structures of Titin I27 (left) and ED3 from dengue envelope (right). The red color indicates the partial unfolding of these two domains when submitted to high hydrostatic pressure (600 bar), as seen by HP-NMR.

Multiple-axis diamond anvil cell: MDAC

Guoyin Shen[1], Richard Ferry[1], Curtis Kenney-Benson[1], Eric Rod[1]
[1]*Argonne National Laboratory, Lemont, United States*

Instrumentation and Techniques 3, July 26, 2023, 14:00–16:00

While significant progresses have been made in the development of diamond anvil cell (DAC) technology in the last five decades, there remains intrinsic limitations in the conventional approaches. Large pressure and temperature gradients in the DAC inevitably exist in the extremely small and thin, disk-like sample, making precise experiments and their characterization difficult. We have designed and fabricated a multiple-axis diamond anvil cell (MDAC). The MDAC adopts the concepts of multi-anvil compression but uses single crystal diamonds as the anvil material. Preliminary data show that the MDAC can generate extreme pressure conditions with larger sample volume under more hydrostatic stress conditions. The use of single crystal diamond anvils provides multiple accessible windows for optical and X-ray probes, as well as for heating the sample using laser. We will present the performance of the MDAC, together with various gasket designs and associated sample configurations.

The Concept of Generalised Pressure

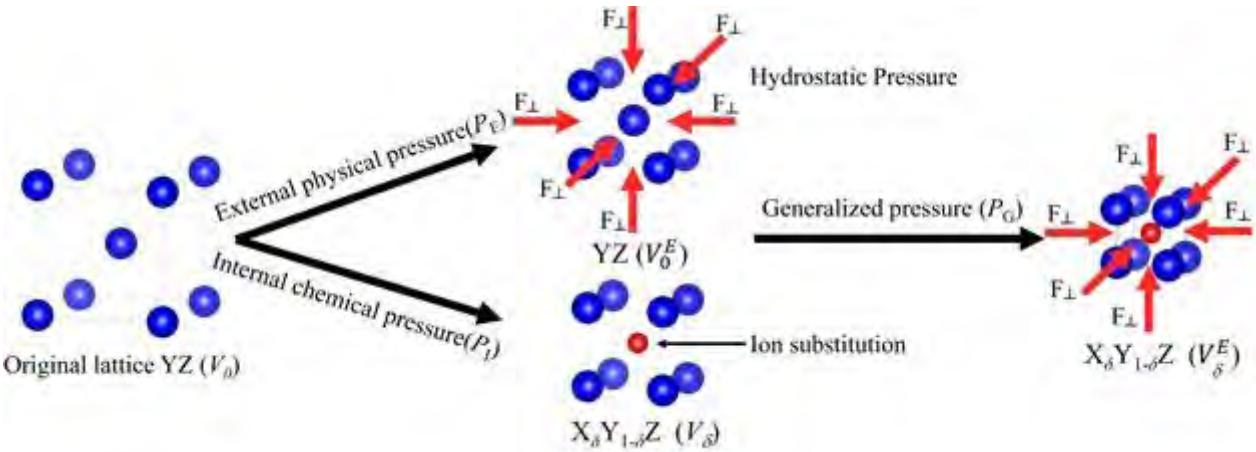
Li Lei[1], Yu Tao[1], LeiLei Zhang[1]
[1]*Sichuan University, Chengdu, China*

Equation of State 2, July 27, 2023, 14:00–16:00

The concept of chemical pressure can be traced as early as in 1991 in the research of the superconductor alloy system. In 2004, Ashcroft proposed that the “chemical precompression” of hydrogen could be realised by IVa hydrides which have higher average valence electron density than that of pure hydrogen. Such a lower metallization pressure in hydrogen dominant-rich metallic alloys is partially attributed to the chemical pressure induced by inclusion of other elements.

Chemical pressure (or “chemical precompression”) has a similar effect on changing the properties of matter as physical pressure does and has been wildly accepted to describe precompression phenomena induced by ion substitution, including positive pressure and negative pressure. However, it is still unclear to what extent the chemical pressure is equivalent to physical pressure in scale. Is there a generalised scale to quantify all kinds of pressure factors, including the chemical pressure and physical pressure?

Here, we propose a concept of generalised pressure to achieve the unification of all similar pressure factors, including internal chemical pressure and external physical pressure. The generalised pressure is the ensemble of all kinds of pressure factors based on the equivalence principle in the pressure-driven volume strain of crystal lattice or any other measurable physical quantity dominated by pressure. The equation of state for generalised pressure can elucidate the equivalent relationship between the chemical and physical pressure. We have also employed a high-pressure experiment to verify the proposed concept.



Pressure dependence of alloy solution phase diagrams: Experiments and thermodynamic modelling

Professor Guy Makov[1], Ms Shir Ben-Shalom[1], Mr Iuri Kirshon[1], Dr Yaron Greenberg[2], Dr Moran Emuna[2], Dr Eyal Yahel[2], Professor Joonho Lee[3]
[1]Ben-Gurion University, Israel, [2]NRCN, Israel, [3]Korea University, South Korea

Phase Diagrams – Metals, July 27, 2023, 10:15–12:15

The experimental construction of phase diagrams requires accurate and well equilibrated thermo-physical measurements, in addition to structural studies, to obtain the equilibrium thermodynamic conditions. Hence, it took the community many decades to map the phase space of thousands of binary systems at ambient conditions. Pressure affects phase diagrams both by altering the interactions, which control the nature of the diagram, and through the emergence of new elemental and alloy phases. Determining structures under pressure is well-developed. However, measuring thermophysical properties and their transitions under pressure is technically challenging and consequently rarer. Therefore, it is useful to combine experimental measurements and thermodynamic modelling to explore the pressure evolution of alloy systems.

In the present contribution we study the pressure evolution of several alloy systems through a combination of experimental techniques and thermodynamic modelling. Specifically, we studied several types of alloy systems, including isomorphous Bi-Sb, eutectic Ga-In, monotectic Bi-Ga with a liquid miscibility gap and the ternary Bi-Sb-Pb system. Through a thermodynamic model, supported by physical measurements of sound velocity and density, we were able to construct phase diagrams up to several GPa of these alloys. To validate our predictions, we undertook high-pressure measurements including X-ray diffraction in a diamond anvil cell (DAC), resistivity and differential thermal analysis (DTA) in a Paris-Edinburgh (PE) large volume press. These studies validate our thermodynamic model predictions of the pressure dependence of the alloy systems; including changes in the nature of the diagram from isomorphous to eutectic, disappearance of the miscibility gap, shifts of eutectic points and the evolution of interaction parameters with pressure.

A novel differential thermal analysis measurements of phase transitions at high pressure and temperatures

Eyal Yahel[1], Mr. Yuri Kirshon[2], Mrs. Shir Ben-Shalom[2], Dr. Yaron Greenberg[1], Prof. Guy Makov[2]
[1]Physics Department, Nuclear Research Center – Negev, Beer Sheva, Israel, [2]Materials Engineering Department, Beer Sheva, Israel

Instrumentation and Techniques 4, July 26, 2023, 16:30–18:30

Thermal measurements of high-pressure transitions in metals provide thermodynamic insight into the properties of phases and phase transitions.

An innovative pressure cell, designed for sensitive differential thermal analysis (DTA) measurements at elevated temperatures (ambient to ca. 1000 K) and high pressures (up to 6 GPa), implemented in the 'Paris-Edinburgh' (PE) tabletop press, is presented.

The new cell's design enables measurements of thermal properties across the phase transitions. This capability is demonstrated on the phase transitions in indium, tin, and antimony. These thermal measurements were able to capture small changes such as in solid-solid transitions. The melting curves of the selected metals, based on the DTA measurements, were mapped onto the phase diagrams, together with the subtler transitions in the solid phase. Based on these unique measurements, the enthalpy of transitions between solid phases was evaluated and found to be significantly smaller than upon melting.

By consolidating the transitions obtained from the DTA curves during isobaric measurements, the high-pressure phase diagram of the elements was reconstructed and compared with previous experimental results obtained by other methods.

Hence, we demonstrated a new experimental capability to explore with relatively high sensitivity phase diagrams of materials.

In situ Pressure Control System for Neutron Scattering Cells: Applications for Low Temperature Physics

Antonio M. dos Santos[1], Jamie J. Molaison[1], Stas V. Sinogeikin[2]
[1]Oak Ridge National Laboratory, Oak Ridge, United States, [2]DAC Tools, LLC, Naperville, United States

Instrumentation and Techniques 1, July 26, 2023, 10:15–12:15

Measurements at high pressure play a key role in condensed matter research as pressure allows the tuning of the electron-lattice coupling, drive the appearance (or suppression) of new phases or phenomena and provide experimental validation or improved parametrization of computational models [1]. The combination of these with very low temperature is often required, especially in the context of condensed matter research, as it allows the observation of systems as close to their ground state as possible. [2]

Neutron scattering techniques are notorious for simultaneously probing the lattice and spin degrees of freedom and are uniquely sensitive to the magnetic ordering. In addition, the weak interaction of neutron beams with samples does not result in temperature increase or sample damage. Consequently, the coupling of neutron techniques with high pressure has always been an invaluable research strategy in condensed matter physics.
However, the relatively low neutron flux available and weak scattering length implies the need for relatively large samples and long measurement times – when compared with other techniques – and poses strong constraints on cooling due to the necessary large mass of the high-pressure devices, limiting the lowest accessible temperature and the number of pressure points sampled.
One of the most ubiquitous pressure devices for condensed matter research is the clamp cell: it is compatible with both powdered and single crystal samples and the relatively large sample space allowed the development of a variety of measurements at pressure, well beyond neutron diffraction (e.g. transport, magnetization) [3]. However, in conventional designs, clamp cell requires pressure changes to be “clamped” at ambient temperature. This is problematic as it leads to significant down time during temperature excursions and the frequent cell manipulation can reduce reliability and result in sample misalignment during the experiment.

We addressed these issues by developing of a bellows-driven clamp cell. This device allows access to the full range of pressure of most designs and relies on the gas output from a commercial cylinder fitted with a computer-controlled regulator. In parallel we developed a sister device designed for a large-culet Diamond Anvil Cell (DAC), that reaches significantly higher loads on the piston by means of a lever-based force multiplier, albeit at the expense of piston travel. [4]
We will present neutron data from these devices, along with a strain gauge-based testing station that allows assessing the performance of these devices at all temperatures and even in the absence of neutron beam.
A portion of this research used resources at the SNS, a DOE Office of Science User Facility operated by the ORNL. This development was based in part on work supported by the U.S. DoE, Office of Science, SBIR Phase I program under Award Number DE SC 0019678 to DAC Tools LLC.

[1] R.J. Hemley and N.W. Ashcroft, Physics Today 51(8) pg. 26 Aug. 1998
[2] Y. Feng , R. Jaramillo et. al., Rev. Sci. Inst. 81(4) pg. 041301 Apr. 2010;
[3] Uwatoko Y, Todo S, et al. J Phys: Cond. Matter. 14(44) pg. 11291. 2002
[4] https://www.osti.gov/biblio/1600093.

Speciation and effects of water on hydrous peridotitic glasses: insights into the early evolution of rocky planets

Dr. Dmitry Bondar[1], Anthony C. Withers[1], Danilo Di Genova[1,2], Alessio Zandonà[3,4], Hongzhan Fei[1], Pedro Valdivia[1], Tomoo Katsura[1]

[1]Bayerisches Geoinstitut, University of Bayreuth, Universitätsstraße 30, 95440, Bayreuth, Germany, [2]Institute of Environmental Geology and Geoengineering, National Research Council of Italy, Rome, Italy, [3]CNRS, CEMHTI UPR3079, Univ. Orléans, F-45071, Orléans, France, [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science (Glass and Ceramics), 11 Martensstr. 5, 91058, Erlangen, Germany

Mantles of Terrestrial Planets, July 27, 2023, 14:00–16:00

Magma oceans composed of peridotitic melt are expected to be nearly ubiquitous features in the formation of rocky planets. The molten mantles allow for the segregation of metal, thus facilitating core formation, and transport of volatile components to the surface, thus forming the atmosphere through degassing. Finally, the crystallization of the magma ocean forms the initial mantle. These processes are controlled by the properties of the ultramafic liquid, which are in turn largely dependent on speciation and concentration of volatile components, with water being the most abundant one. Therefore, it is crucial to study the speciation and effects of water on peridotitic melts to gain insights into the early evolution of rocky planets. Unfortunately, such studies are scarce due to poor glass-forming ability of extremely depolymerised hydrous peridotitic melts.
In the framework of this project, we developed a novel rapid-quench multi-anvil technique, which enabled us for the first time to quench peridotitic (KLB-1) glasses with H_2O contents from 0 to 5 wt.%, at pressures up to 4 GPa. The synthesised glasses are transparent, optically isotropic, and chemically homogeneous. Raman spectroscopy confirmed the amorphous nature of the peridotitic glasses. The subsequent research focused on determining the speciation of water, estimating melt viscosity as a function of water content, and understanding the effect of water on the structure of such highly depolymerised melts.

The speciation of water in peridotitic glasses was studied by infrared spectroscopy, which provided two important observations. First, the fraction of molecular H_2O to the bulk H_2O decreases dramatically with increasing depolymerization (Fig. 1a), and second, an (Mg,Ca)OH peak appears at 4320-4180 cm^{-1}, next to the SiOH peak, at high CaO and MgO contents (Fig. 1b). Thus, the dissolution mechanisms of water in peridotitic glasses differ dramatically from those in more polymerised glasses, e.g., from rhyolitic to basaltic. As a result, the H_2O speciation and speciation-dependent melt properties obtained using less depolymerised melts cannot be reliably extrapolated to strongly depolymerised melts.

The viscosity of peridotitic melts was investigated by a combination of methods, namely micropenetration viscometry, conventional DSC, flash DSC and Brillouin spectroscopy. Based on measurements covering thirteen orders of magnitude (from Tg to $\eta \approx 10^{-1}$ Pa s), a new temperature- and H_2O-dependent viscosity model of peridotitic melts was developed. These data are necessary when modelling solidification and differentiation processes in a hydrous magma ocean.

Finally, our data shed some light on the effect of water on the polymerization degree of the melt structure. On the one hand, Raman data indicate a shift of the high-wavenumber envelope to higher wavenumbers with increasing water content, suggesting polymerization. On the other hand, FTIR data demonstrate that the proportions of (Mg,Ca)OH and (Si,Al)OH species remain constant over a wide range of water contents, suggesting a negligible effect of water on polymerization. Finally, we observed clear decreases in viscosity and glass transition temperature with increasing water contents, which favor the latter hypothesis.

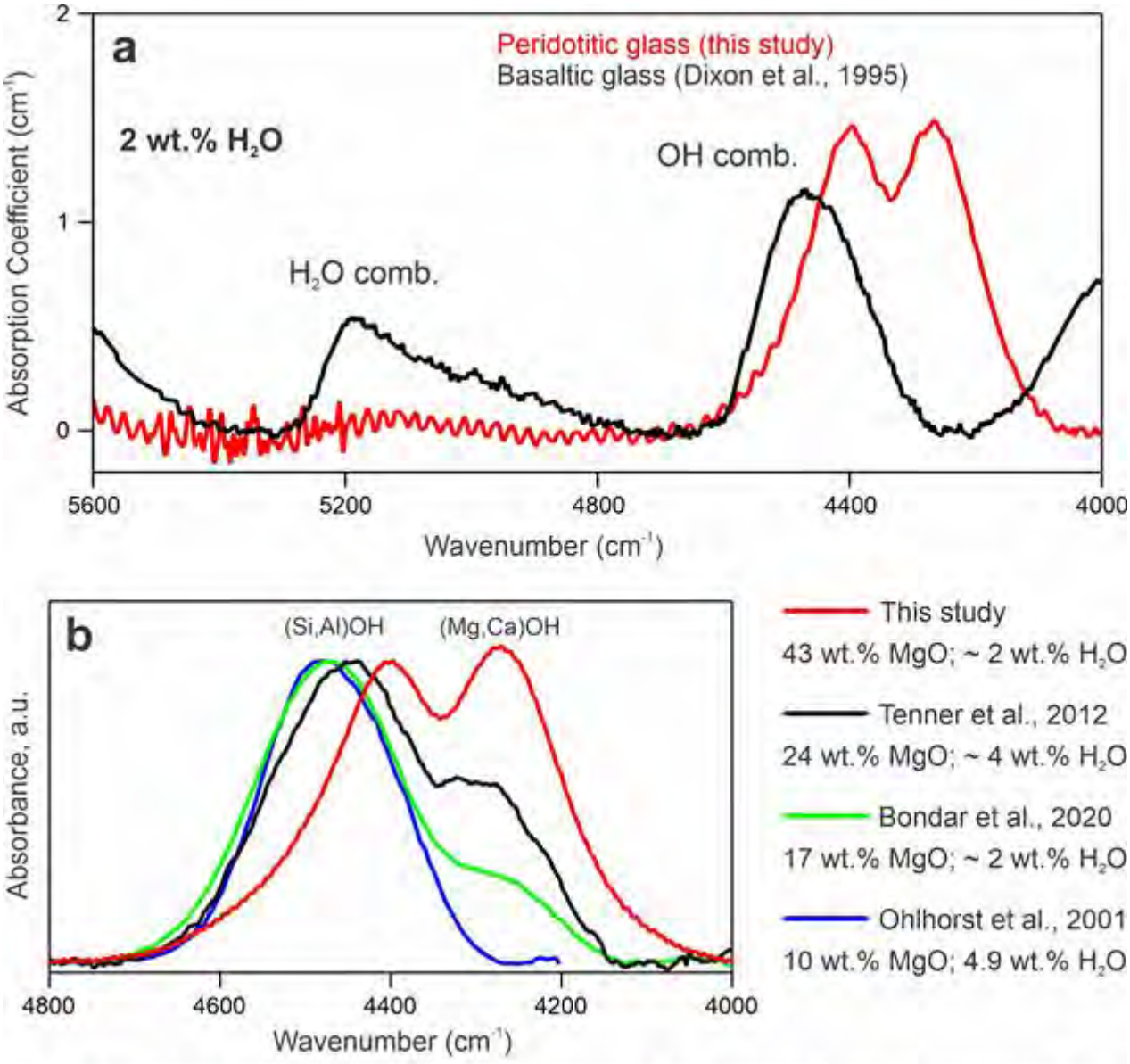


Fig. 1. a – comparison between near-infrared spectra of basaltic and peridotitic glasses; b – occurrence and growth of a lower-frequency combination band related to OH with increasing MgO concentration.

Dense ammonia-containing composite systems in ice giants at high pressures

Wan Xu[1]
[1]*Chinese Academy of Sciences, Hefei, China*

Outer Planets and Exoplanets 2, July 26, 2023, 16:30–18:30

Hydrogen, ammonia and water have plenty cosmic abundance and play prominent roles in constituting the interior structure of ice planets e.g. Uranus. During the early formation of planets, the primitive atmosphere is under high compression, which makes the investigations of the properties of these materials under high pressure cover the fields of materials science, earth science and planetary science. Using Diamond anvil cells to generate static high pressures, we carried out Raman and synchrotron radiation XRD around the composite ammonia-water and ammonia-hydrogen systems to above megabar pressure respectively. We observed the spontaneous ionization of Ammonia-hemihydrate and the formation of Ammonia-hydrogen compounds under compression. These studies would be significant for the exploration of the formation, evolution and internal structure of ice giants.

New Frontiers in nuclear magnetic resonance for high-pressure research and Geo-science

Dr. Thomas Meier[1]
[1]*Center for High Pressure Science and Technology Advanced Research, Beijing, China*

Instrumentation and Techniques 4, July 26, 2023, 16:30–18:30

Nuclear Magnetic Resonance (NMR) is one of the most widespread and versatile spectroscopic probe of contemporary natural sciences. An application in high-pressure or experimental geo-sciences was however regarded unfeasible until recently. In this talk, I will summarise recent developments in both experiment and method of high-pressure small-scale NMR methods. These developments include the implementation of NMR-crystallographic methods using a combination of high- and low-resolution techniques as well as the opportunity for hydrogen or water quantification in in situ DAC based experiments or nominally anhydrous minerals under ex-situ investigation.

[1] Meier, T., et al., (2020). Nuclear spin coupling crossover in dense molecular hydrogen. Nature Communications, 11(1), 1–7
[2] Meier, T., et al., (2020). Proton mobility in metallic copper hydride from high-pressure nuclear magnetic resonance. Physical Review B, 102(16), 1–8.
[3] Meier, T., et al., (2021). In situ high-pressure nuclear magnetic resonance crystallography in one and two dimensions. Matter and Radiation at Extremes, 6(6), 068402.
[4] Meier, T., et al., (2022). Structural independence of hydrogen-bond symmetrisation dynamics at extreme pressure conditions. Nature Communications, 13(1), 1–8.
[5] Meier, T., Laniel, D., & Trybel, F. (2022). Direct Hydrogen Quantification in High-pressure Metal Hydrides, Matter and Radiation at Extremes, 8, 1-10

Experimental evidence for the high-PT body-centred cubic Fe

Professor Anatoly Belonoshko[1], Grigory Smirnov[2]
[1]KTH, Stockholm, Sweden, [2]HSE University, Moscow, Russia

Cores of Terrestrial Planets, July 24, 2023, 14:00–16:00

Experiments at extreme conditions become increasingly complex. The interpretation of the observations is at times not straightforward, especially considering that the experiments as such are aimed at observing the materials that have no precedents among known ones. In such a situation it is tempting to assign the observations to the materials that have familiar properties. To avoid such mistakes, interpretations have to rely on the solid theoretical basis rather than on the past experience of a researcher. We present interpretation of two multi-shock experiments 1,2 on iron where the pressures as high as 10 Mbar and temperatures up to 10,000 have been reached. The collected spectroscopy data are unique. However, the interpretation demonstrated certain flaws. We provide new interpretation on the basis of large-scale ab initio molecular dynamics and obtain excellent match between the experimental data and properties of the long debated high-pressure-temperature body-centred cubic phase of iron. The phase possesses unique properties3,4,5 that made its manifestation being interpreted incorrectly.

[1] Ping, Y.et al. (2013). Phys. Rev. Lett.,. 111, 065501.
[2] Kraus et al. (2022). Science, 375, 2021.
[3] Belonoshko A. B. et al., (2017). Nature Geoscience, 10, 312.
[4] Belonoshko A. B. et al. (2019). Nature Communications, 10, 2483.
[5] Belonoshko, A. B. & Smirnov, G. (2023). J. Phys: Cond. Matter (in review).

Nuclear magnetic resonance in lanthanum polyhydrides up to 1.5 Mbar

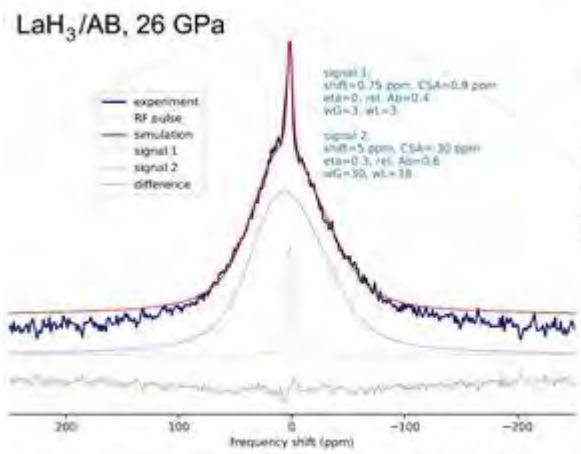
Dr. Di Zhou[1], Dr. Dmitrii Semenok[1], Dr. Thomas Meier[1]
[1]*Center for High Pressure Science and Technology Advanced Research, Beijing, China*

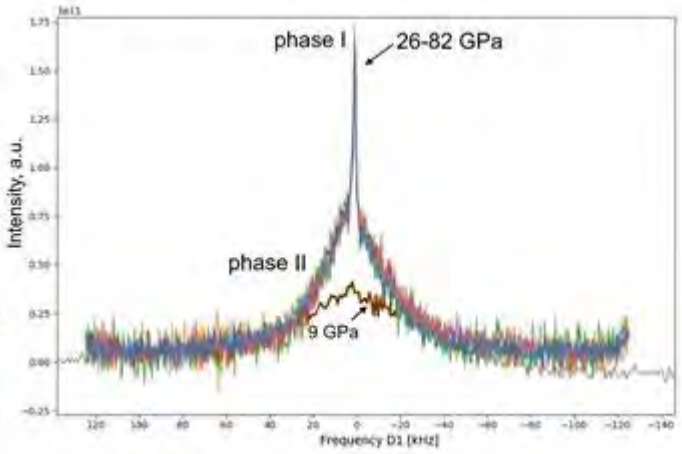
Hydrides 3, July 25, 2023, 14:00–16:00

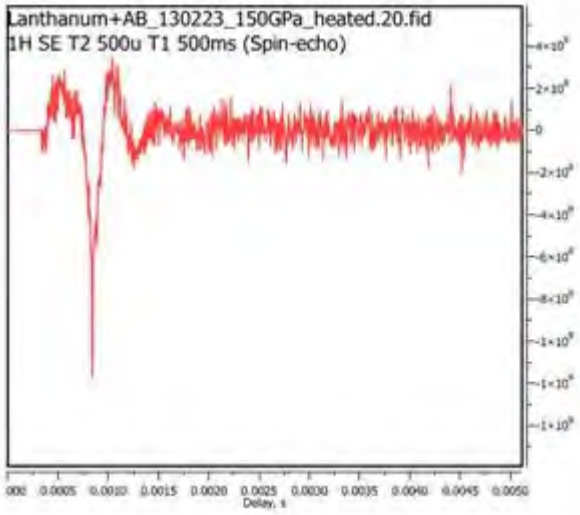
Lanthanum decahydride LaH10 is a superhydride with the highest critical temperature (TC ≈ 250 K) among known polyhydrides whose parameters are well reproducible. For this reason, the La-H system is one of the most attractive objects for research. In this work, the formation of lanthanum polyhydrides was studied by nuclear magnetic resonance (NMR) in diamond cells at pressures up to 150 GPa at room temperature. To detect nuclear induction signals, from the hydrogen spin system in our microscopic samples (d ≈ 30 μm, t = 5 μm), we used a system of Lenz lenses sputtered on the diamond anvils. LaH3 was used as a starting material with ammonia borane (NH3BH3, AB) as the hydrogen source.

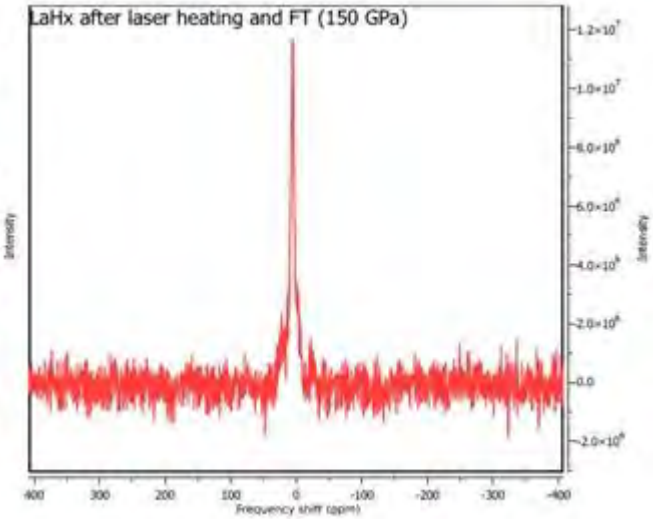
We found that the 1H-NMR spectra of LaH3 recorded at pressures from 5 to 150 GPa, contain two signals of different widths, the NMR shift of which practically does not change with increasing pressure (Figure 1). A wide signal (FWHM ≈75 ppm) corresponds to hydrogen atoms rigidly localised in the LaH3 crystal structure, and a much narrower signal possibly corresponds to a sub-system of hydrogen atoms with enhanced mobility.

Laser heating of our LaH3/NH3BH3 sample was carried out at 150 GPa. As a result, a new narrow Spin-echo signal appeared, which was not previously observed. This new signal exhibits surprisingly sharp spectral features as well as spin-spin relaxation times (T2) approaching spin-lattice relaxation times (T1), a tell-tale indication that this new spin system lies in the “extreme narrowing limit” of NMR, characteristic for liquids and high mobility ionic conductors. This indicates that in the structure of lanthanum hydrides exists a fraction of diffusion-active hydrogen atoms even at room temperature. This observation of a high mobility hydrogen sub-species in lanthanum hydrides underlines previous similar findings in iron- and copper hydrides using NMR.


LaH3/AB, 26 GPa
experiment
RF pulse
simulation
signal 1
signal 2
difference
signal 1:
shift=0.75 ppm, CSA=0.9 ppm
eta=0, rel. Ab=0.4
wG=3, wL=3
signal 2:
shift=5 ppm, CSA=-30 ppm
eta=0.3, rel. Ab=0.6
wG=30, wL=18
frequency shift (ppm)


phase I
26-82 GPa
phase II
9 GPa
Intensity, a.u.
Frequency D1 [kHz]


Lanthanum+AB_130223_150GPa_heated.20.fid
1H SE T2 500u T1 500ms (Spin-echo)
Delay, s


LaHx after laser heating and FT (150 GPa)
Intensity
Frequency shift (ppm)

High-pressure ilmenite-type MnVO3: crystal and spin structures in the itinerant-localised-covalent regimes

Angel M. Arevalo-lopez[1], Elena Solana-Madruga, Olivier Mentre
[1]*Cnrs, Uccs, University Of Lille, Lille, France*

Magnetic Materials 1, July 24, 2023, 10:15–12:15

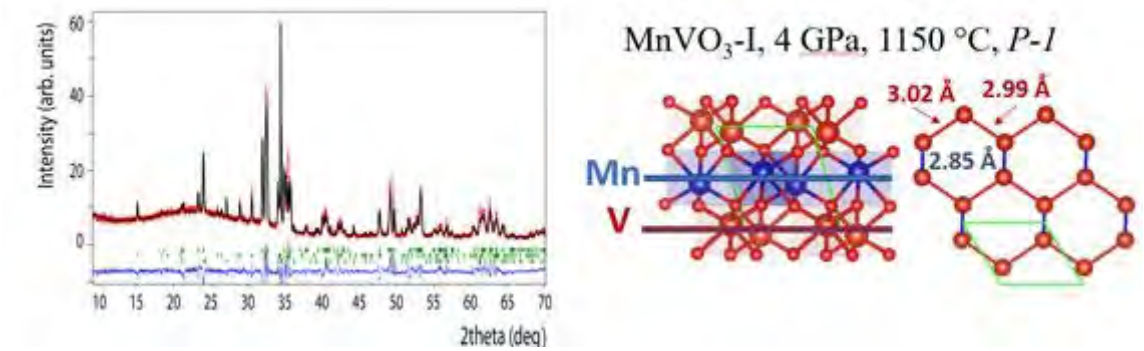
Systems with partially filled valence electrons may suffer electronic and structural changes due to instabilities, for instance the Peierls transition (cation dimerization) in VO_2 accompanied by a metal-insulator transition (MIT). In here, $MnVO_3$-I in its ilmenite polyform will be presented with such instabilities.

$MnVO_3$-I was reported long time ago by Syono et al.[1] However, the triclinic symmetry (P-1) precluded the authors for a proper structural determination. We have prepared $MnVO_3$-I via high-pressure high-temperature synthesis at 4 GPa and 1100 °C with a Walker-type multi anvil apparatus. The crystal structure was solved from an isolated small single crystal. At 300 K, $MnVO_3$-I possess P-1 symmetry with a = 5.0177(7) Å, b = 5.0513(7) Å, c = 5.5210(8) Å, α = 116.679(6) °, β = 90.044(6) ° and γ = 118.924(5) ° unit cell parameters. The polymorph represents a distorted version of the ilmenite-type structure with alternating Mn-V honeycomb-layers, Fig. 1a, similar to the recently reported $MgVO_3$ and $CoVO_3$.[2,3]

The triclinic distortion in $MnVO_3$-I arises from V-V dimerization with a short bond of ≃2.85 Å as shown in Figure 1. It also shows an AFM transition at TN = 77 K with a Curie-Weiss behaviour above 250 K and presents a |θ| = 233(1) K and a μeff = 5.7(1) μB. The latter is close to the theoretical value of 5.92 μB for Mn^{2}+.

I will also present our results on the structural evolution at high-temperature along with the MIT transition and the low-temperature magnetic structure with respective refined moments of 3.7(1) μB and 0.45(1) μB for Mn and V at 1.5 K.[4]

[1] Y. Syono, S. Akimoto, Y. Endoh, J. Phys. Chem. Solids, 32, 243 (1971)
[2] H. Yamamoto, S. Kamiyama, I. Yamada, H. Kimura, J. Am. Chem. Soc., 144, 1082 (2021)
[3] S. Kamiyama, I. Yamada, M. Fukuda, Y. Okazaki, T. Nakamura, T. Nishikubo, M. Azuma, H. Kimura, H. Yamamoto. Inorg. Chem., 61, 7841 (2022)
[4] E. Solana-Madruga, O. Mentre, D. Khalyavin, F. Fauth, A. Missiul, A. M. Arevalo-Lopez. J. Mater. Chem. C, submitted.



Structural and Electronic Insights into the Role of Anagostic Bonds in Metal Dithiocarbamate Complexes

Dr. Szymon Sobczak[1], Dr. KInga Roszak[1], Prof. Andrzej Katrusiak[1]
[1]*Adam Mickiewicz University, Poznań, Poland*

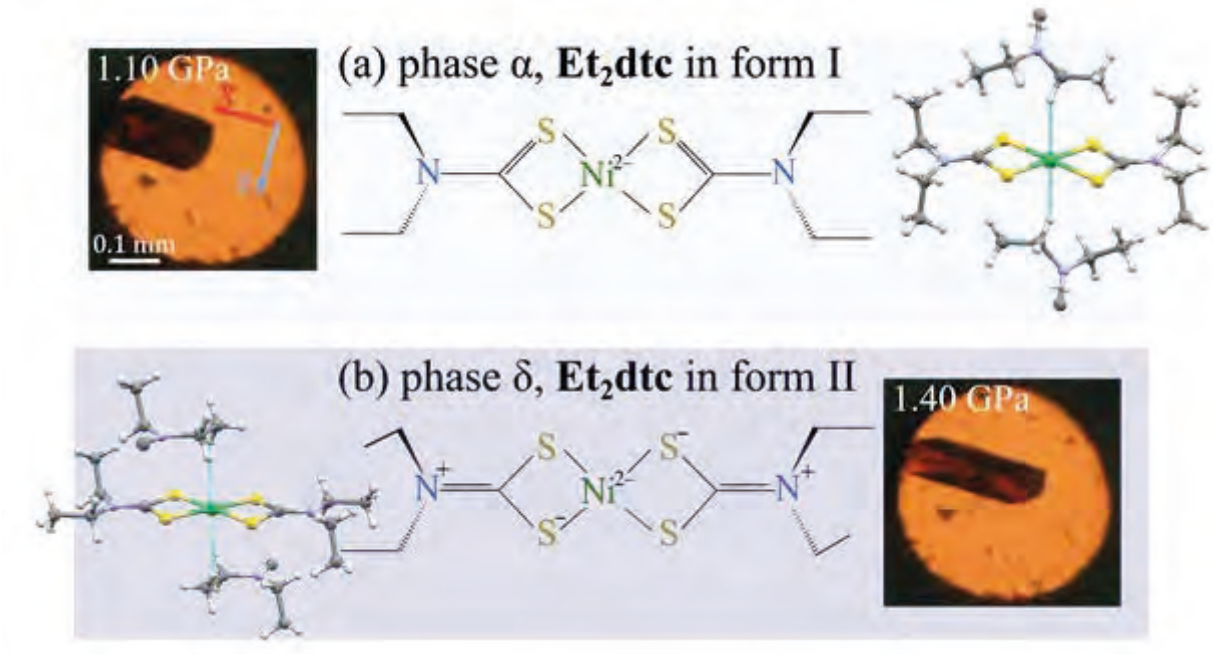
Chemical Bonding 2, July 24, 2023, 16:30–18:30

Metal dithiocarbamate complexes have garnered significant interest due to their facile synthetic routes, remarkable conducting, magnetic, and optical properties, as well as their broad spectrum of biological applications. [1] These properties can be easily tuned by functionalizing through the formation of various non-covalent interactions, such as C–H···π, S···S, S···H, O···H, and less often by the C–H···M agostic or anagostic bonds. [2]

To investigate such weak interactions, we selected a phase α of a square-planar nickel(II) bis(N,N-diethyldithiocarbamate) complex. When compressed above 1.23 GPa, a visible giant strain changes the shape of the single crystal revealing a phase transformation. This pressure-induced transformation between phases α and δ changes the H-donor of the anagostic interaction between methylene and methyl group and influences the dithiocarbamate ligand conformation. The X-ray diffraction data combined with Raman spectroscopy and quantum-mechanical calculations show that these structural changes are accompanied by increased contribution of thioureide mesomer in the resonance structure of dithiocarbamate ligand in phase δ, which is supported by the charge-assisted C–H···S- bonds. [3]

Our findings highlight the critical role of anagostic bonds in crystal cohesion forces and provide new insights into the complex relationship between conformational and electronic features in a compressed environment. These factors drastically affect the chemical properties of compounds leading to giant changes in the physicochemical properties of solid-state.

[1] Tiekink, E. R. T. Tin Dithiocarbamates: Applications and Structures. Appl. Organomet. Chem. 2008, 22 (9), 533–550.
[2] Hogarth, G. Transition Metal Dithiocarbamates: 1978-2003. In Progress in Inorganic Chemistry; 2005; Vol. 53, pp 71–561.
[3] Sobczak, S.; Roszak, K.; Katrusiak, A. Exchanged Metal-Hydrogen Anagostic Bonds and Resonance of Dithiocarbamate and Thioureide Mesomers**. Chem. – A Eur. J. 2022, 28 (45), e202201235.



High-pressure high-temperature study of plagioclase feldspar: implications for shock metamorphism

Tianqi Xie[1], Sean Shieh[1], Stella Chariton[2], Vitali Prakapenka[2]
[1]University of Western Ontario, London, Canada, [2]University of Chicago, Lemont, United States

Mantles of Terrestrial Planets, July 27, 2023, 14:00–16:00

Plagioclase feldspar is the most abundant components of igneous rocks found in the crust of Earth and lunar highland rocks. They can also be seen in lunar and Martian meteorites, and detected on the surfaces of Mars, Venus and Mercury. Knowledge of how plagioclases response to the variations of pressure and temperature is important for revealing the pressure-temperature history of natural impact events on planetary bodies as well as highly shock meteorites.

Among all the features observed in shocked plagioclase, diaplectic glass is the most diagnostic evidence of strongly shock stage. Shock-recovery experiments were used to study the formation of diaplectic glass since 1960s [1]. However, temperature from these shock experiments were not openly calculated and their timescales were much shorter than those in natural events. Furthermore, while there have been some recent static studies to demonstrate the amorphization of plagioclase [2], high-pressure and high-temperature behavior of intermediate plagioclase at pressure above 25 GPa is still poorly understood, and phase diagram reminds unclear.

In this study, we conducted high-pressure high-temperature experiments on natural intermediate plagioclase--labradorite, using in situ synchrotron X-ray diffraction and laser heating diamond anvil cell at GSECARS sector of the Advanced Photon Source, Chicago. The crystals were grounded into powder (1-3 μm), mixed with 10% platinum powder as a laser absorber and internal pressure standard. Neon was loaded as a pressure medium to maintain the samples in a quasi-hydrostatic environment and thermal insulator. 1-2 ruby spheres were used as the second pressure standard for gas-loading, operated at GSECARS. Ruby pressures are determined by the ruby fluorescence method and platinum pressure is determined by the equation of state of platinum [3].

During the experiments, amorphization and phase changes was observed, and we were able to construct the phase diagram of intermediate plagioclase with pressure ranging up to 65 GPa and temperature up to 3000K. Together with the boundary of amorphization drawn by Kubo et al. and Hugoniot curve data reported by Ahrens et al. [2, 4], we were able to constrain the pressure-temperature range for the formation of diaplectic glass. Our results suggest that diaplectic glass can form in a much wider pressure-temperature range than the ones proposed previously [1]. Furthermore, we recently measured the melting point of plagioclase feldspar under pressure up to 65GPa. We were thus able to add the melting curve to the phase diagram and further understand the formation conditions of more shock metamorphic features observed in natural impacted rocks, such as the high-pressure phases and the impact melt.

[1] Stöffler, D., Hamann, C., and Metzler, K. (2018) Meteoritics & Planetary Science 53:5- 9. 64.
[2] Kubo, T., Kimura, M., Kato, T., Nishi, M., Tominaga, A., Kikegawa, T., and Funakoshi, K. 2010. Nature Geoscience 3:41-45.
[3] Fei, Y., Ricolleau, A., Frank, M., Mibe, K., Shen G., and Prakapenka, V. 2007. Proceedings of the National Academy of Sciences of the United States of America 104:9182-6.
[4] Ahrens, T. J., Petersen, C. F., and Rosenberg, J. T. (1969) Journal of Geophysical Research 74(10):2727-2746.

Assessment of changes in enzyme activity, bioactive compound, sugar, and sensory attribute during the storage of high-pressure treated pre-packaged squash cubes

zhe chen[1], Krystian Marszałek[1], Yasin Ozdemirb[2], Zineb Benmechernene[3], Simona Fabroni[4], Sara Spilimbergo[5]

[1]Professor Waclaw Dabrowski Institute of Agriculture and Food Biotechnology, warszawa, Poland, [2]Ataturk Central Horticultural Research Institute, Turkey, [3]University of Oran, Algeria, [4]Council for Agricultural Research and Economics (CREA), Italy, [5]University of Padova, Italy

Bio/Life Sciences and Soft Matter, July 26, 2023, 10:15–12:15

The food industry has introduced a range of fresh-cut food to meet people's convenience demands. However, fresh-cut food products are susceptible to microbial and oxidative enzymes, resulting in food spoilage and nutrition degradation. To extend the shelf life and improve the quality of fresh-cut food products, an innovative process that combined high-pressure carbon dioxide with a modified atmosphere package (HPCD+MAP) was developed. In this work, 1.5 cm butternut squash cubes (8 cubes) were packaged with plastic film in a carbon dioxide environment. Then the packed squash cubes were put into the chamber equipped with a high-pressure pump. The packed squash cubes were processed at 6 MPa and 45℃ for 40 min (HPMAP-CO2) and then stored at 4 ℃ for 21 days. The control samples were packed in an air (MAP-air) or a CO2 (MAP-CO2) environment conditions as two controls. The influence of HPCD+MAP processing on the quality of fresh-cut squash: polyphenol oxidase (PPO), peroxidase (POD), total phenolic contents (TPC), antioxidant capacity, carotenoids, sugar profile, and sensory quality were investigated. The PPO and POD activities of fresh-cut squash cubes treated with HPCD+MAP showed a slight increase, while the PPO and POD activities of fresh-cut squash cubes treated with MAP-air and MAP-CO2 first increased and then gradually reduced with increasing the storage time. Furthermore, the changes in the total phenolic content and antioxidant capacity (ABTS and DPPH) of the treated squash cubes during the storage had a similar trend to the change in the PPO and POD activities of the treated squash cubes. The carotenoids and total sugar contents of squash cubes treated with HPMAP-CO2 did not change with the increased storage time. In contrast, the total carotenoids and total sugar contents of squash cubes treated with MAP-CO2 gradually decreased after 13 days of storage. Regarding sensory evaluation, the colour and smell of HPMAP-CO2-treated squash cubes had the highest score compared to MAP-air and MAP-CO2.

Keywords: Fresh-cut squash, High-pressure carbon dioxide, Modified atmosphere package, Polyphenol oxidase and peroxidase, Sensory evaluation.

Probing off-Hugoniot states in laser-driven, high-pressure experiments

Amy Coleman[1], Tom Lockard[1], Federica Coppari[1], Hong Sio[1], Andrew Krygier[1], D Alex Chin[2], Matthew Signor[2], J Ryan Rygg[2], Gilbert W Collins[2], Yuan Ping[1], James M McNaney[1]
[1]Lawrence Livermore National Laboratory, Livermore, United States, [2]Laboratory for Laser Energetics, Rochester, United States

Dynamic Studies of Elements, July 25, 2023, 10:15–12:15

When seeking to understand the behaviour of materials at extreme conditions, dynamic compression provides an invaluable tool for accessing pressures and temperatures that are vastly beyond the range of atmospheric conditions. Shock-compression gives access to pressurised states on the Hugoniot, generating large increases in temperature at high pressures, while lower-temperature states can be accessed using ramp-compression on a quasi-isentrope. Both techniques have been widely used to generate high-pressure states in a large variety of elements, but as we strive to define more comprehensive phase diagrams and to better characterise materials at extremes, we must turn to alternative techniques to generate thermodynamic compression paths that lie between the principle Hugoniot and the quasi-isentrope.

Compression generated by laser drives with complex pulse shapes, such as stepped, and shock + ramp pulses, can facilitate access to pressure and temperature states outside of those generated by pure shock and ramp compression. Thanks to high-precision laser pulse-shaping at facilities such as the Omega EP laser, we can physically realise these intricate pulse shape designs in an experimental setting and, with the implementation of diagnostics tailored to the nanosecond timescales of these compression events, we are able to probe previously unexplored regions of phase space. This talk presents novel results from off-Hugoniot experiments at the Omega-EP laser, designed to better constrain phase boundaries in elements.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

Composition of the Martian Core

Dr Jac Van Driel[1]
[1]*UCL, United Kingdom*

Cores of Terrestrial Planets, July 24, 2023, 14:00–16:00

The InSight mission is beginning to reveal fundamental constraints on Mars' deep interior structure. The most striking results are associated with the Martian core. Inversions from seismic receiver functions and geodesy suggest that the core is large and has a low density when compared to Earth. This reduced density leads some to speculate that the Martian core must contain more 'light elements' than Earth. By considering geophysical data from the recent insight mission, we perform ab initio simulations to explore the range of possible chemical compositions. We seek to constrain the Fe-S-Si-O-H-C liquid system using spin-polarised calculations with geophysical and cosmo-chemical constraints. Calculating the physical properties of iron-bearing systems (particularly in the case of the liquids) is far from straightforward as it is likely that, even at the conditions in the core of Mercury (up to 40 GPa and 4000 K), magnetism in the form of local atomic moments may alter the properties of both solid and liquid iron alloys. Indeed, pure solid iron is magnetic at these conditions, and magnetism significantly influences sub-solidus density and phase stability. Our preliminary simulations of Fe-S-Si-O-H-C iron show finite local moments, which result in a reduced density compared with non-spin-polarised simulations, modify physical properties such as density, bulk-sound velocity and heat capacity. In total, we explore over fifty different iron alloys, where a machine-learning equation of state to used to interpolate across composition, pressure and temperature. Findings from this study are directly applicable to planetary cores more extensively. Furthermore, the methods developed and implemented apply more broadly to high-pressure physics and Earth science.

Host-guest framework compounds based on silicon by high-pressure high-temperature synthesis

Julia-Maria Huebner[1], Timothy A. Strobel[1]
[1]*Carnegie Institution for Science, Washington DC, United States*

Synthesis and Properties of Novel Materials 3, July 26, 2023, 16:30–18:30

Three-dimensional framework compounds based on silicon constitute a fascinating class of inorganic phases, offering a variety of beneficial features including thermoelectric properties or superconductivity, but can also act as precursors for materials with the potential to advance silicon-based optoelectronics and energy-conversion technologies [1]. Typically, a majority of framework atoms enclose a minority of guest atoms such as alkaline, or alkali-earth metals, comprising a wide structural variety. The connectivity of the host framework is related to the octet rule, although certain deviations from this rule are generally tolerated [2].

High-pressure high-temperature methods allow access to a variety of compounds that possess novel structural motifs and properties. Furthermore, the partial replacement of silicon and therefore the transition towards ternary compounds grant another degree of freedom to add to the structural variety. This talk will highlight how both silicon substitution and the nature of the guest atom impact the resulting structure. In the first example, the incorporation of boron into the silicon framework allowed for the synthesis of clathrate I type M8-xBySi46-y (M=Na, K, Rb, Cs) [3] under high-pressure high-temperature conditions. In the case of the sodium analogue, higher pressures grant access to the rarely occurring clathrate VIII modification, a structure type that is predicted to feature promising thermoelectric efficiency [4]. Furthermore, the possibility of boron incorporation into other types of Si frameworks will be explored.

The partial substitution of silicon by germanium yields the compound Na1-xGeySi4-y featuring a novel three-dimensional arrangement of three- and four-bonded germanium and four-bonded silicon incorporating Na in extended channels. Single crystal diffraction experiments showed diffuse scattering in addition to discrete main reflections, pointing towards a certain structural latitude. Physical properties, as well as chemical and thermal stability, and the possibility of Na removal from the channels will be discussed.

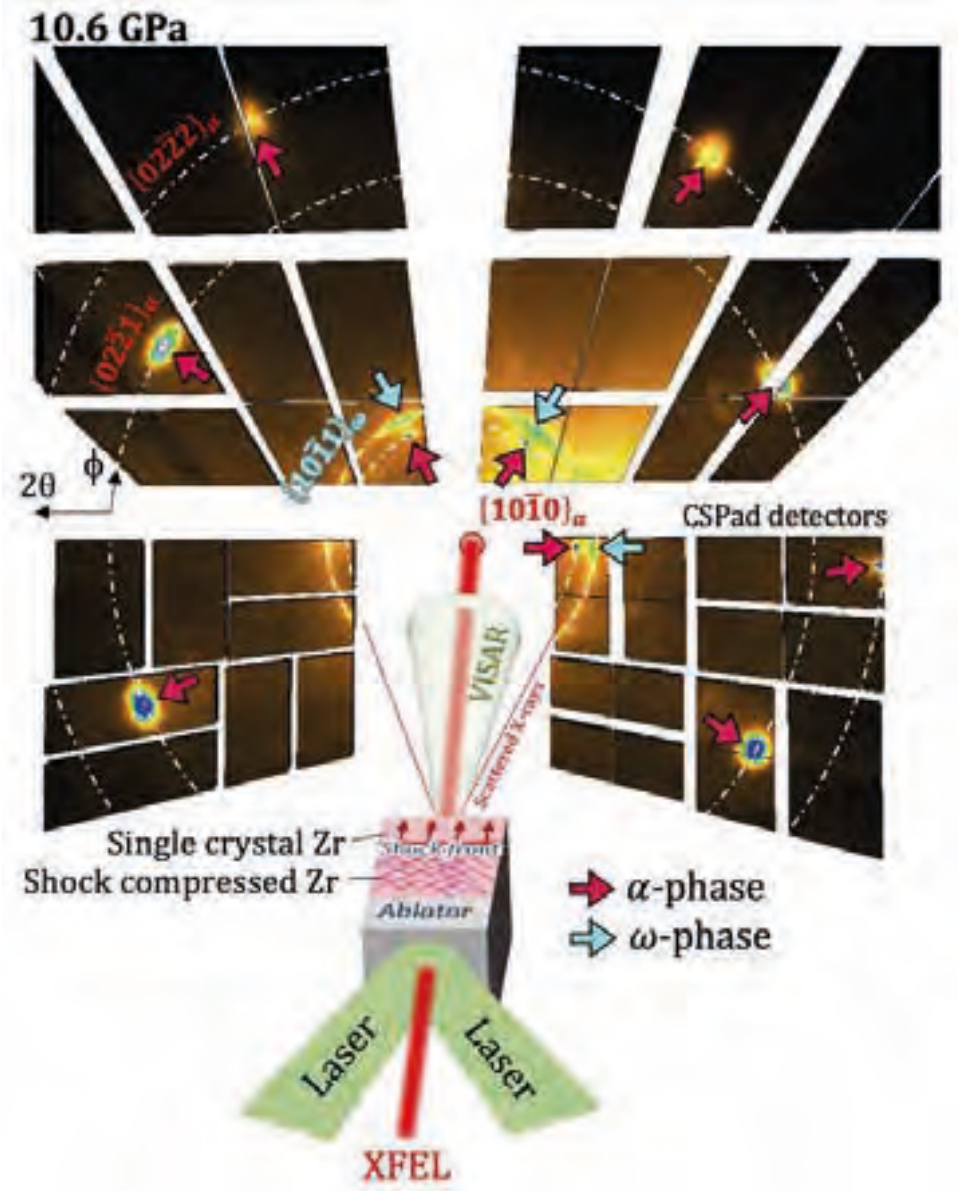
[1] Kim, D.; Stefanoski, S.; Kurakevych, O.; Strobel, T.A. Nature Mater. 2015, 14, 169–173.
[2] Bhattacharya, A.; Carbogno, C.; Böhme, B.; Baitinger, M.; Grin, Yu.; Scheffler, M. Phys. Rev. Lett. 2017, 118, 236401.
[3] Jung, W.; Lörincz, J.; Ramlau, R.; Borrmann, H.; Prots, Yu.; Haarmann, F.; Schnelle, W.; Burkhardt, U.; Baitinger, M.; Grin, Y. Angew. Chem., Int. Ed. 2007, 46, 6725– 6728.; Jung, W.; Böhme, B.; Hübner, J.-M.; Burkhardt, U.; Borrmann, H.; Bobnar, M.; Nguyen, H. D.; Pantenburg, I.; Etter, M.; Schwarz, U.; Grin, Y.; Baitinger, M. Dalton Trans. 2021, 50, 1274–1282.; Hübner, J.-M.; Jung, W.; Schmidt, M.; Bobnar, M.; Koželj, P.; Böhme, B.; Baitinger, M.; Etter, M.; Schwarz, U.; Grin, Y. Inorg. Chem. 2021, 60, 2160–2167.; Hübner, J.-M.; Jung, W.; Koželj, P.; Bobnar, M.; Cardoso-Gil, R.; Burkhardt, U.; Böhme, B.; Baitinger, M.; Schwarz, U.; Grin, Y. Z. Anorg. Allg. Chem. 2021, 647, 119–125.; Hübner, J.-M.; Carrillo-Cabrera, W.; Koželj, P.; Prots, Y.; Baitinger, M.; Schwarz, U.; Jung, W. J. Am. Chem. Soc. 2022, 144, 30, 13456–13460.
[4] Norouzzadeh, P.; Krasinski, J. S.; Myles, C. W.; Vashaee, D. Phys. Chem. Chem. Phys. 2015, 17, 8850–8859.

Complex dynamics during a shock-induced phase transition in Zr

Saranash Singh[1], Dr. Martin Gorman[1], Dr. Patrick Heighway[2], Dr. David McGonegle[3], Dr. Joel Bernier[5], Dr. Hae-Ja Lee[4], Dr. Bob Nagler[4], Dr. Jon Eggert[1], Dr. Raymond Smith[1]
[1]Lawrence Livermore National Lab, Livermore, United States, [2]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom, [3]Atomic Weapons Establishment, Reading, United Kingdom, [4]Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, United States, [5]Nuro, Mountain View, United States

Dynamic Studies of Elements, July 25, 2023, 10:15–12:15

Shock compression can cause materials to undergo structural transformations and form new phases of matter with novel material properties. The alpha-to-omega transformation in Ti, Zr, and their alloys have long been studied due to their importance to the nuclear and aerospace industries. Despite decades of investigation, the mechanisms by which this transformation occurs have remained ambiguous, with several proposals for transformation pathways and intermediate phases. This study presents femtosecond X-ray diffraction measurements on the alpha-to-omega transformation in the shock-compressed, single crystal [0001] Zr. Our in-situ X-ray diffraction measurements reveal the presence of a previously unknown intermediate disordered phase during the transition to the high-pressure omega phase. This intermediate phase is first observed at 11 GPa, at the alpha-omega transition pressure, and gradually disappears as the phase fraction of the omega phase increases. In addition to the intermediate disorder, multiple orientation relationships (ORs) corresponding to different phase transition pathways are also observed. This points to the critical role of shear stress in determining the favourability of a particular mechanism. We confirm the presence of this disordered intermediate phase using molecular dynamics simulations with a machine-learned interatomic potential. This integrated experimental and computational approach is crucial for obtaining a complete understanding of complex material transformations. The insights from this study reveal the complexity of shock-induced phase transformations and demonstrate that it is far more intricate than previously thought. Our study takes steps to reconcile the discordant results of previous experimental and theoretical investigations.


10.6 GPa
$\{02\bar{2}2\}_\alpha$
$\{02\bar{2}1\}_\omega$
$\{10\bar{1}1\}_\omega$
2θ
ϕ
$\{10\bar{1}0\}_\alpha$
CSPad detectors
VISAR
Scattered X-rays
Single crystal Zr
Shock compressed Zr
Shock front
Ablator
α-phase
ω-phase
Laser
Laser
XFEL

Observation of defects in shocked diamond below the HEL

Cara Vennari[1], Dimitri Khaghani, Eric Folsom, Kento Katagiri, Richard Briggs, Trygve Raeder, Arturas Vailionis, Chris McGuire, Trevor Hutchinson, Ray Smith, Bob Nagler, Bernard Kozioziemski, Leora Dresslehaus-Marais, Jon Eggert
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Dynamic Studies of Elements, July 25, 2023, 10:15–12:15

Diamond is well established to have strong resistance to plastic deformation and it's Hugoniot Elastic Limit (HEL) is large relative to other materials. Canonically, the propagation of shock waves through a single crystal involves an initial defect-free elastic wave followed by a plastic wave with defects. This study focuses on the defects and strain gradients generated below and at the HEL in <110> oriented single crystal diamond. This laser driven dynamic compression X- ray topography experiment was conducted at the Materials at Extreme Conditions beamline at the Linac Coherent Light Source. X-ray topography is a near field imaging technique that images defects by observing contrast in the intensity of the diffracted X-ray beam. By using a line focused X-ray beam coupled with a thick diffracting region, we generate 2D images where defect derived intracrystalline rotations generate a diffraction intensity contrast compared to the defect free regions. We shock <110> oriented diamonds that are type Ib and IIa over a range of stresses to view defects and strain gradients to visualise the physics at and below the HEL.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 through LDRD project 21- ERD-032.

In situ X-ray diffraction of iron oxides dynamically loaded to multi-megabar pressures

Ian Ocampo[1], Donghoon Kim[2], Raymond Smith[3], Federica Coppari[3], J. Ryan Rygg[4], Marius Millot[3], John H. Eggert[3], Thomas S. Duffy[1]

[1]Princeton University, Princeton, United States, [2]Carnegie Institute for Science, Washingon, United States, [3]Lawrence Livermore National Laboratory, Livermore, United States, [4]Laboratory for Laser Energetics, Rochester, United States

Cores of Terrestrial Planets, July 24, 2023, 14:00–16:00

Iron oxides are major planetary constituents that have significant influence on the geodynamic and geochemical evolution of Earth's deep interior. Iron oxides control the redox state of the mantle setting the conditions which regulate chemical speciation, transport properties, and volatile species outgassing [1] and may contribute to the low velocities anomalies observed in the lower mantle. Iron oxides have been studied extensively under the pressure-temperature conditions relevant to Earth (<150 GPa), but as planetary detection techniques improve, there are an increasing number of rocky and sub-Neptune sised exoplanets whose mass and radii can be observed [2]. Calculations based on density estimates for these planets suggest pressure-temperature (PT) profiles that greatly exceed those for Earth [5,6]. Under these extreme PT conditions, magnesium silicates are expected to undergo a series of phase transitions to a variety of highly coordinated and dense phases (i.e., ppv-MgSiO3, Th3P4-type Mg2SiO4, etc.) at TPa pressures. Recently, under quasi-static loading, iron oxides have been shown to form a homologous series of stoichiometries that are isostructural to Mg-silicates and undergo a similar series of phase transitions, yet at significantly reduced pressures (~100 GPa) [5–7]. To better model the interior mineralogy and dynamic structures of large, rocky exoplanets, experimentally validated equations of state (EOS) and phase diagrams of iron oxides are fundamental as primary planetary components and as analogue systems for Mg-silicates.

Here, we present in situ X-ray diffraction and velocimetry measurements on Fe2O3 and Fe3O4 to ~700 GPa. To achieve both high temperatures and pressures, we turn to laser-driven dynamic compression techniques (quasi-isentropic). When combined with nanosecond X-ray diffraction, atomic level structural analyses, and thus pressure-density relationships along different thermodynamic paths, can be measured providing constraints on the EOS of materials. On the nanosecond time scales of our experiments, we observe that hematite-type Fe2O3 transforms to the theta-Fe2O3 phase, predicted to be metastable under static loading conditions. Above ~350 GPa, no sample diffraction peaks are observed suggestive of pressure-induced amorphization. In contrast, we observe diffraction consistent with the crystalline Th3P4-type Fe3O4 above ~250 GPa and up to the highest achieved stress. The pressures achieved in this study extend the experimental pressure range covered in these materials by more than a factor of 3.

Part of this work was prepared by LLNL under Contract DE-AC52-07NA27344.

[1] D. J. Frost and C. A. McCammon, AREPS (2008).
[2] K. Rice et al., RAS (2019).
[3] D. Valencia, R. J. O'Connell, and D. Sasselov, Icarus (2006).
[4] F. W. Wagner, N. Tosi, F. Sohl, H. Rauer, and T. Spohn, A&A (2012).
[5] E. Bykova et al., Nat Comm. (2016).
[6] L. Bindi, R. Sinmyo, E. Bykova, S. V. Ovsyannikov, C. McCammon, I. Kupenko, L. Ismailova, L. Dubrovinsky, and X. Xie, ACS-ESC, (2021).
[7] C. C. Zurkowski, J. Yang, S. Chariton, V. B. Prakapenka, and Y. Fei, JGR Planets (2022).

Simultaneous measurements of ruby shift and unit cells of NaCl and Au in a diamond-anvil cell: new constraints on pressure scales to 20 GPa

Mr. Yanbin Wang[1], Dr. Guoyin Shen[2], Dr. Jesse Smith[2]
[1]Center for Advanced Radiation Sources, The University of Chicago, Argonne, United States, [2]HPCAT, X-ray Science Division, Argonne National Lab, Argonne, United States

Minerals Under High Pressure, July 24, 2023, 16:30–18:30

NaCl and Au are two commonly used pressure standards and many researchers have reported various equations of state (EoSs). Inter-consistency among these diffraction based EoSs has not been systematically investigated. Recently, a new ruby pressure scale has been proposed which is consistent with shock-wave data on metals, and elasticity and EoS data on ionic, covalent, and metallic materials up to 150 GPa [1]. Here we study compression behaviour of NaCl and Au in a membrane-driven diamond-anvil cell [2] with He as pressure medium, along with simultaneous ruby fluorescence measurements. Monochromatic radiation with wavelength of 0.4246 A was used for X-ray diffraction, with a beam size of ~10um (Jesse: is it ~5 um FWHM?), which covered both NaCl and Au in the DAC. An online ruby system, with its optical path reflected by an X-ray transparent carbon mirror, was used to measure ruby pressure simultaneously while X-ray diffraction was collected. Pressure was increased/decreased by a pair of membrane pressure controllers continuously, reaching 20 GPa in 2 hours. Data collection of ruby fluorescence and X-ray diffraction were automated and synchronised at 1 sec intervals. In one experiment, 7200 and 1000 measurements were conducted upon compression and decompression, respectively. Unit-cell volumes of NaCl and Au were extracted using Dioptas [3] and Multifit [4] and fitted based on the Ruby2020 pressure scale [1] to the Vinet equation of state [5].

The highly redundant measurements reveal subtle differences in materials' responses to compression and decompression. Solidification of the He pressure medium has a clear effect on the unit cells above ~14 GPa. Thus, only the compression data below He solidification pressure were used to fit equations of state for NaCl and Au. Fixing the ambient isothermal bulk moduli according to previous ultrasonic measurements [6, 7], we obtained EoSs for NaCl and Au that are consistent with Ruby2020 to within +/-0.05 GPa. These results demonstrate the potential of establishing mutually consistent pressure scales for both diffraction-based and fluorescence-based pressure scales.

[1] Shen et al., HPR, 2020 (10.1080/08957959.2020.1791107)
[2] Sinogeikin et al., RSI, 2015 (10.1063/1.4926892)
[3] Prescher & Prakapenka, HPR, 2015 (10.1080/08957959.2015.1059835)
[4] Merkel & Hilairet, JAC, 2015 (10.1107/S1600576715010390)
[5] Vinet et al., J. Phys. C, 1986 (10.1088/0022-3719/19/20/001)
[6] Spetzler et al., J. Phys. Chem. Sol., 1972 (10.1016/S0022-3697(72)80468-2); Anderson et al., JAP, 1989 (10.1063/1.342969)

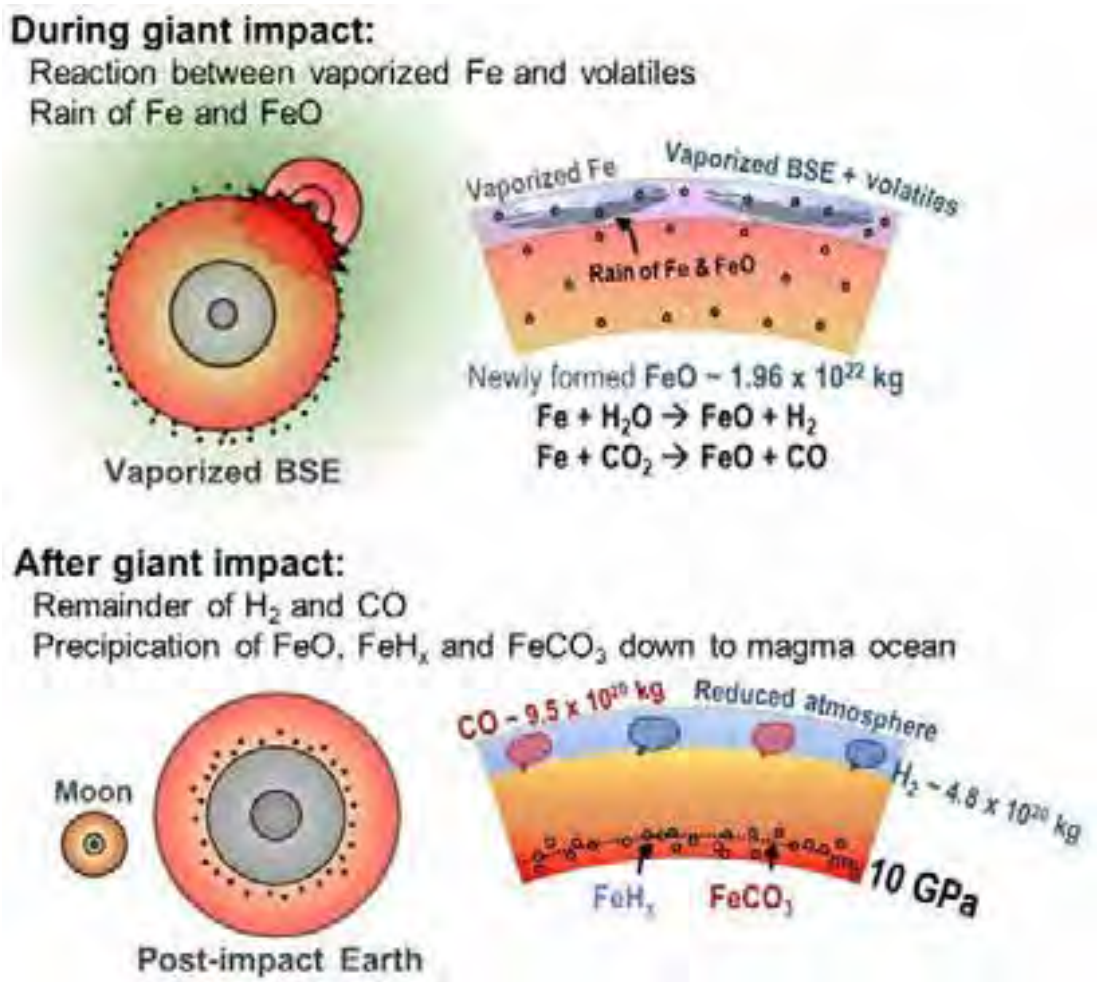
Oxidation of iron by giant impact and its implication on the formation of reduced atmosphere in the early Earth

Jinhyuk Choi[1], Rachel Husband[2], Huijeong Hwang[3], Taehyun Kim[1], Yoonah Bang[1], Seohee Yoon[1], Jeongmin Lee[1], Heehyeon Sim[1], Sangsoo Kim[4], Daewoong Nam[4], Boknam Chae[4], Hanns-Peter Liermann[2], **Prof Yongjae Lee**[1]

[1]Yonsei University, Seoul, Republic of Korea, [2]DESY, Hamburg, Germany, [3]GIST, Gwangju , Republic of Korea, [4]Pohang Accelerator Laboratory, Pohang , Republic of Korea

Secular Evolution of the Earth, July 25, 2023, 10:15–12:15

The giant impact-driven redox processes in the atmosphere and magma ocean played a crucial role in the evolution of the early Earth. However, due to the absence of rock records from that time, understanding these processes have proven challenging. Here, we present experimental results that simulate the reaction between iron and volatile components (H2O and CO2) under giant impact conditions using high-brilliance X-ray free electron laser (XFEL) as a fast heat pump and structural probe. Our results show that under XFEL pump on a compressed mixture of iron and volatiles, iron is oxidised to wüstite (FeO), while the volatiles are reduced to H2 and CO. Furthermore, iron oxidation proceeds into the formation of hydrides (γ-FeHx) and siderite (FeCO3), with an indication of a possible redox boundary near 300 km depth. Through quantitative analysis of the reaction products, we estimate theoretical constraints on the mass of the impactor and its heliocentric origin, as well as the volatile and FeO budgets in the bulk silicate Earth, supporting the Theia hypothesis. Our findings shed light on the fast and short-lived process that led to a reduced atmosphere, which is required for the emergence of prebiotic organic molecules.



Accelerating the Prediction of High-Pressure Hydrides Using Data Derived Potentials

Dr. Lewis Conway[1,2], Mr Pascal Salzbrenner[1], Professor Chris Pickard[1,2]
[1]University Of Cambridge, Cambridge, United Kingdom, [2]Advanced Institute for Materials Research, Tohoku University, Sendai, Japan

Hydrides 1, July 24, 2023, 10:15–12:15

Crystal structure prediction has been used extensively to predict a wide range of binary hydrides[1,2], which have significant implications for hydrogen storage materials and superconductivity. However, traditional DFT-based structure searching is usually limited by the number of atoms in the unit cell. I will show how Ephemeral Data-Derived Potentials (EDDPs)[3] can be used to accelerate the prediction of high-pressure hydride structures.

The potentials are trained on DFT data containing modest numbers of atoms but can be used to predict more complex structures even at stoichiometries not contained in the training data. The predicted structures are then verified using DFT calculations to reproduce known phase diagrams and predict new stable structures. The approach is easy to automate and has been applied to a wide range of binary hydride materials, predicting several previously unknown stable structure types with large unit cells, unusual stoichiometries and novel chemical motifs.

This use of machine-learned potentials for multi-species crystal structure prediction presents a new avenue to explore and revisit known phase diagrams.

[1] Zurek, Eva. ‘Hydrides of the Alkali Metals and Alkaline Earth Metals Under Pressure’. Comments on Inorganic Chemistry 37, no. 2 (4 March 2017): 78–98. https://doi.org/10.1080/02603594.2016.1196679.
[2] Song, Hao, Zihan Zhang, Tian Cui, Chris J. Pickard, Vladimir Z. Kresin, and Defang Duan. ‘High T c Superconductivity in Heavy Rare Earth Hydrides’. Chinese Physics Letters 38, no. 10 (1 October 2021): 107401. https://doi.org/10.1088/0256-307X/38/10/107401.
[3] Pickard, Chris J. ‘Ephemeral Data Derived Potentials for Random Structure Search’. Physical Review B 106, no. 1 (7 July 2022): 014102. https://doi.org/10.1103/PhysRevB.106.014102.

Dimensional crossover and re-entrant superconductivity in pressurised Kagome metals AV_3Sb_5

Ece Uykur[1], Maxim Wenzel[2], Marcos V. Faria[1], Kalliopi Mavridou[1], Andrei Luferau[1], Brenden R. Ortiz[3], Stephen D. Wilson[3], Alexander A. Tsirlin[4]
[1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany, [2]1. Physikalisches Institute, Stuttgart University, Stuttgart, Germany, [3]Materials Department, University of California Santa Barbara, Santa Barbara, United States, [4]Felix Bloch Institute for Solid-State Physics, Leipzig University, Leipzig, Germany

Electronic Transitions 2, July 25, 2023, 14:00–16:00

Non-magnetic Kagome metals, AV_3Sb_5 (A: K, Rb, Cs), offer a new promising platform for engineering topological and correlated electrons [1,2]. At ambient pressure, these compounds show a competition between an exotic charge-density wave and superconductivity that are rooted in an intricate interplay of topologically non-trivial Dirac fermions, localised flat-band electrons, and van Hove singularities in the vicinity of the Fermi level. These features can be traced back to the effectively 2D band structure of vanadium Kagome planes. We pioneered the broadband optical studies of AV_3Sb_5 and identified a significant damping of charge carriers [3,4,5], potentially related to electron-phonon coupling that has immediate implications for superconductivity.

The tunability of these properties with external means opens interesting new directions in the research of Kagome metals. For example, an unusual re-entrant superconductivity of AV_3Sb_5 was observed in transport measurements under pressure. In this presentation, I will summarise pressure evolution of AV_3Sb_5 revealed by single-crystal XRD, high-pressure infrared spectroscopy, and density-functional calculations. This combination of experimental and computational techniques allows a simultaneous probe of crystal and electronic structures under both hydrostatic and non-hydrostatic conditions. We show that, despite the initial similarity of AV_3Sb_5 with different alkaline metals (A = K, Rb, Cs) at ambient pressure, these compounds show a different sequence of pressure-induced structural phase transitions, which further depend on the extent of non-hydrostaticity of the pressure environment [6, 7].

Electronic structure calculated using experimental atomic positions and also probed directly by infrared spectroscopy reveals a dimensional crossover caused by the formation of interlayer Sb-Sb bonds [7]. The strongly 2D structures of AV_3Sb_5 become essentially 3D at elevated pressures. These changes lead to a reconstruction of the Fermi surface that clearly correlates with the re-entrant behaviour of superconductivity. We further reveal the interplay between topological and localised carriers that follow the evolution of the Fermi surface.

Our study demonstrates pressure-induced dimensional crossover as an important tool for tailoring novel electronic materials, such as Kagome metals. Concurrently, we show that their high-pressure phases intimately depend on the pressure environment and its deviation from hydrostaticity.

[1] B. R. Ortiz et al., Phys. Rev. Materials 3, 094407 (2019)
[2] H. Luo et al., Nature Communications 13, 273 (2022)
[3] E. Uykur et al., Phys. Rev. B 104, 045130 (2021)
[4] E. Uykur et al., npj Quantum Materials 7, 16 (2022)
[5] M. Wenzel et al. Phys. Rev. B 105, 245123 (2022)
[6] A. A. Tsirlin et al. SciPost Physics 12, 049 (2022)
[7] A. A. Tsirlin et al. arXiv: 2209.02794

Probing magnetism at extreme conditions at the APS-U POLAR beamline

Gilberto Fabbris[1], Daniel Haskel[1], Jörg Strempfer[1], Yongseong Choi[1]
[1]*Argonne National Laboratory, Lemont, United States*

Next Gen Synchrotrons, July 25, 2023, 14:00–16:00

Magnetic interactions play a fundamental role in quantum materials, with the high-pressure control of interatomic distances being a key parameter in tuning and understanding the emergent phenomena in these systems. Hard X-ray probes of magnetism, such as X-ray magnetic circular dichroism and magnetic diffraction, have had substantial impact due to the micron-scale beam size and the ability to penetrate the sample environment, with the Advanced Photon Source (APS) 4-ID-D beamline being amongst the leaders in this field. The APS ring is undergoing an upgrade that will largely enhance the X-ray brilliance (smaller beam) and coherence. Here, I will describe how we plan to take advantage of these enhancements at the upgraded POLAR beamline. Both X-ray scattering, and spectroscopic techniques will be available at POLAR, which will allow for cutting edge element specific magnetic measurements at high pressure, including multi-Mbar pressures, as well as real space and ptychographic magnetic imaging techniques.

Work at Argonne National Laboratory is supported by the U.S. Department of Energy, Office of Science, under contract No. DE-AC-02-06CH11357.

Modelling the Density of Earth's Magma Ocean Using Machine Learning

Isaac Taschimowitz[1], Dr Jac van Driel[1], Dr Andrew Thomson[1], Dr Paul Schofield[2], Prof John Brodholt[1]

[1]University College London, London, United Kingdom, [2]Natural History Museum, London, United Kingdom

Secular Evolution of the Earth, July 25, 2023, 10:15–12:15

Our knowledge of the high-pressure and high-temperature properties of silicate melts is very limited. This is due both to the lack of available experimental data and an accurate EoS, capable of describing the melts over a wide compositional space. This is particularly critical to understanding the magma ocean to solid transition of our planet Earth, and other terrestrial planets. As minerals crystallise the composition of the melt changes continuously and extreme composition of melt can be expected at high degrees of crystallisation. While there is a wealth of information on the densities of solids, and their response to pressure and temperature, much less is known about the density of the liquid phase in this setting, especially towards the end of the magma ocean stage.

Here, we present work modelling the density and other melt properties across a very wide compositional space. A training dataset was built from DFT simulations using the PBEsol exchange correlation functional. Simulations were performed for various compositions across a wide range of pressures (0 to 300 GPa) and temperatures (3000 to 8000 K). To define the compositional space, we have taken the 6 major oxide components of a pyrolite melt and run simulations within and including the end-member compositions. From this training dataset, a Gaussian process regression (GPR) model was trained, which can predict the density of a given composition, pressure and temperature condition. We report good cross validation scores, predicting density of a composition unseen by the model (in training and testing) for a range of pressure and temperatures. From these scores, we show that the GPR model handles fitting well even when the compositional space is relatively sparse. This method appears to overcome the two main issues outlined above: (i) lack of available data and (ii) poor description of liquid behaviour from present EoS.

Whilst the complete crystallisation sequence of the magma ocean is still unknown, we have provided a model which, once this sequence is determined, might be used to predict melt densities etc. over any compositional range, and that is of use in future geodynamical simulations of Earth. This negates the need to perform individual calculations for specific compositions to obtain density information and can be implemented in these simulations regardless to any future refinement of the crystallisation sequence.

Time resolved observations of a phase transformation in dynamically compressed Pb

Martin Gorman[1], Sabrina Nagel[1], Nathan Palmer[1], Peter Nyholm, Robert Petre[1], Camelia Stan[1], Jon Eggert[1], David Bradley[1], Neal Bhandakar[1], Arthur Carpenter[1], Laura Robin Benedetti[1]
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Dynamic Studies of Elements, July 25, 2023, 10:15–12:15

Dynamic compression of matter using lasers has been a well-established method for studying pressure-driven solid-solid phase transformations. However, the investigation of the underlying mechanisms behind these transformations has been challenging due to the difficulty of performing time-resolved, nanosecond-duration diffraction measurements of the compressed sample. Fortunately, recent advances in X-ray detector technology have made it possible to perform such ultra-fast measurements.

In this study, we have utilised nanosecond-duration in situ X-ray diffraction in combination with multi-acquisition X-ray detectors to report lattice-level observations of the hexagonal close-packed (hcp) to body-centred cubic (bcc) phase transformation in Pb. We have made up to eight diffraction measurements over a duration of 10 ns on the Pb sample, which was ramp compressed to a peak pressure of 150 GPa over 15 ns. Our results provide a time-resolved view of the structural phenomena occurring on nanosecond timescales, paving the way for a better understanding of the kinetics of phase transitions under rapid pressure loading.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

High-Tc superconductivity in clathrate calcium hydride CaH6

Mr. Hongbo Wang[1]
[1]*Jilin University, Changchun, China*

Hydrides 2, July 24, 2023, 16:30–18:30

Achieving room-temperature superconductivity is one of the ultimate goals in physics since the discovery of superconductivity in 1911 [1]. While conventional Bardeen-Cooper-Schrieffer (BCS) theory predicts that atomic metallic hydrogen could be the most plausible room-temperature superconductor [2], the required high pressure is extremely challenging [3-5]. The recent discovery of rare earth and actinide superhydrides with an atomic-like hydrogen clathrate structure [6-11] has ushered in a new era of superconductivity research at high pressures. This distinct type of clathrate metal hydrides was first proposed for alkaline-earth-metal hydride CaH6 [12] that, however, has long eluded experimental synthesis, impeding an understanding of pertinent physics. Here, we report the successful synthesis of CaH6 and its measured superconducting critical temperature Tc of 215 K at 172 GPa, which is evidenced by a sharp drop of resistivity to zero and a characteristic decrease of Tc under a magnetic field up to 9 T. An estimate based on the Werthamer-Helfand-Hohenberg model gives a giant zero-temperature upper critical magnetic field of 203 T. These remarkable benchmark superconducting properties place CaH6 among the most outstanding high-Tc superhydrides, marking it as the hitherto only clathrate metal hydride outside the family of rare earth and actinide hydrides. This exceptional case raises great prospects of expanding the extraordinary class of high-Tc superhydrides to a broader variety of compounds that possess more diverse material features and physics characteristics.

[1] H.K. Onnes, Commun. Phys. Lab. Univ. Leiden 120b, 261 (1911)
[2] N.W. Ashcroft, Phys. Rev. Lett. 21, 1748 (1968)
[3] M.I. Eremets et al., Nat. Phys. 15, 1246 (2019).
[4] P. Loubeyre et al., Nature 577, 631 (2020).
[5] I.F. Silvera et al., Science 355, 715 (2017).
[6] A.P. Drozdov et al., Nature 569, 528 (2019).
[7] M. Somayazulu et al., Phys. Rev. Lett. 122, 027001 (2019).
[8] P. Kong et al., Nat. Commun. 12, 5075 (2021).
[9] W. Chen et al., Phys. Rev. Lett. 127, 117001 (2021).
[10] D.V. Semenok et al., Mater. Today 33, 36 (2020).
[11] I.A. Troyan et al., Adv. Mater. 33, 2006832 (2021).
[12] H. Wang, et al., Proc. Natl. Acad. Sci. U.S.A. 109, 6463 (2012).

Enhancing thermoelectric power in skutterudites by tuning chemical interactions under pressure

Alvaro Lobato[1], Ernesto Blancas[2], Fernando Izquierdo-Ruiz[1], Antonio M. Márquez[2], Alberto Otero-de-la-Roza[3], Jose J. Plata[2], J.M. Recio[3]

[1]Departamento de Química Física and Malta-consolider Team, Universidad Complutense de Madrid, Madrid, Spain, [2]Departamento de Química Física, Facultad de Química, Universidad de Sevilla, Sevilla, Spain, [3]Departamento de Química Física y Analítica and MALTA-Consolider Team, Facultad de Química, Universidad de Oviedo, Oviedo, Spain

Chemical Bonding 2, July 24, 2023, 16:30–18:30

The well-known efficacy of pressure to tune material properties [1] is exploited in this work to study thermoelectric properties in M@CoSb3 (M=Na, K, Mg, Ca Sr, Ba) skutterudites. CoSb3 lattice displays a quasi-degeneracy between the Co-Sb and Sb-Sb electronic levels at the conduction band. [2] This band convergence enhances the Seebeck coefficient and thus the thermoelectric figure of merit. Therefore, a detailed understanding of the chemical bonding and Sb lone pair activity is crucial to advance in improving the performance of these materials.[3]

Taking advantage of the chemical pressure-physical pressure relationship, we explore how modifications of bonding interactions affect the energetic levels in the CoSb3 structure. In particular, we provide a detailed analysis of the role played by doping and compression. By means of DFT calculations, we show how the band gap, anharmonicity, lone pair activity, and antibonding interactions affect transport properties (thermal and electrical conductivity) and the Seebeck coefficient. Finally, we discuss the opportunities that chemical and physical pressure offer to identify correlations between particular bonding patterns and thermoelectric efficiency, a connection that remains relatively unexplored to this date.

[1] L. Zhang, Y. Wang, J. Lv and Y. Ma. Nat. Rev. Mater. 2017, 2, 17005.
[2] R. Hanus, X. Guo, Y. Tang, G. Li, G. Jeffrey Snyder, and W. G. Zeier, Chem. Mater. 2017, 29, 3, 1156.
[3] Z. Wang, J. Xi, J. Ning, K. Guo, B. Duan, J. Luo, G. Jeffrey Snyder, J. Yang and W. Zhang. Chem. Mater. 2021, 33, 1046.

Acknowledgements
Financial support from the Spanish PID2021-122585NB-C21-2, PGC2018-097520-A-100 AEI and MICIN/AEI/10.13039/501100011033 projects, the Principado de Asturias-FEDER under project AYUD/2021/51036 and the “European Union Next Generation EU/PRTR” (grants PID2019-106871GB-I00 and TED2021-130874B-I00) are gratefully acknowledged. A.O.-d.-l.-R. acknowledges the financial support of the Spanish MINECO RyC-2016-20301 Ramón y Cajal Grant.

Analysis of hydrogen concentration in anorthite from angrite by developed micro-NMR technique

Yunhua Fu[1,2], Dr. Thomas Meier[1], Dr. Shijie Li[3], Dr. Lifei Zhang[2], Dr. Renbiao Tao[1]
[1]Center for High Pressure Science and Technology Advanced Research (HPSTAR), Beijing, China, [2]School of Earth and Space Sciences, Peking University, Beijing, China, [3]Center for Lunar and Planetary Sciences, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, China

Minerals Under High Pressure, July 24, 2023, 16:30–18:30

Nominally anhydrous minerals (NAMs) composing the Earth and planetary rocks (e.g., crust and mantle) could incorporate measurable amounts of dopped hydrogen in their crystal structure (Keppler et al.,2006). Therefore, confining the hydrogen concentration of NAMs in terrestrial and non-terrestrial samples is a promising endeavour. Angrite is considered to be an early-stage igneous rock at solar formation, estimated to be formed about 4.56 billion years ago from proto-planetesimal sources by crystallization. Angrite meteorites are mainly composed of high calcium pyroxene, olivine, anorthite, and other minor minerals. Hydrogen in NAMs (e.g., anorthite) can greatly affect the physical and chemical properties of minerals, playing a crucial role in the geological and dynamic evolution of the angrite parent body (APB) (Schmandt et al.,2014). However, the volatile components and properties of APB's parent magma are currently controversial (Ho et al.,1998; Sherman et al.,1989; Longhi et al.,1995).

Compared with Fourier Transform infrared spectroscopy (FTIR) and Secondary Ion Mass Spectrometer (SIMS), nuclear magnetic resonance (NMR) spectroscopy could directly obtain the absolute hydrogen concentration in NAMs without any standard calibrations. In this study, we aim to analyse the hydrogen concentration of anorthite microlites in angrite meteorites using our developed micro-NMR spectroscopy (Meier et al., 2017). Solid-state NMR experiments were done at the Centre for High Pressure Science & Technology Advanced Research (HPSTAR), China. Results indicate the average absolute hydrogen content of anorthites in Oued Namous 001 is 0.42±0.05 ppm.

Compared to the previous analysis, the hydrogen concentration of anorthites in angrite is relatively low owing to the low detection limit of our micro-NMR technique. It can be predicted that the hydrogen content of APB is very poor, and APB is a highly volatile element depleted relative to chondrites, potentially as a result of evaporative loss of volatiles during heating, partial melting, melt extraction, and degassing. At the same time, the absence of magma ocean in planetesimals would also lead to a large loss of volatiles (Peterson et al.,2023). Further studies of achondrites and chondrites across petrologic types will be required to better constrain the extent of volatile loss during planetesimal heating, melting, and differentiation.

[1] Keppler H, Smyth J R. The Mineralogical Society of America, Washington DC, USA, 2006.
[2] Schmandt B, Jacobsen S D, Becker T W, et al. Science, 2014, 344(6189): 1265-1268.
[3] Ho Y S, McKay G. Chemical engineering journal, 1998, 70(2): 115-124.
[4] Sherman S B , Treiman A H . Lunar and Planetary Science Conference, 1989.
[5] Longhi J. Geochimica Et Cosmochimica Acta, 1995, 59(11):2375-2386.
[6] Meier T, Wang N , Mager D , et al. Science Advances, 2017, 3(12):eaao5242.
[7] Peterson L D, Newcombe M E, Alexander C M O D, et al. Geochimica et Cosmochimica Acta, 2023, 340: 141-157.

Superconductivity in multiple phases of compressed AuAgTe4

Mr. Yehezkel Amiel[1], Eran Greenberg[2], Stella Chariton[3], Gyanu P. Kafle[4], Evgenia V. Komleva[5], Daniel I. Khomskii[6], Igor I. Mazin[7], Sergey V. Streltsov[5], Elena R. Margine[4], Alexander Palevski[1], Gregory Kh. Rozenberg[1]

[1]School of Physics and Astronomy, Tel Aviv University, Tel Aviv 81800, Israel, [2]Applied Physics Division, Soreq NRC, Yavne 81800, Israel, [3]GSECARS, University of Chicago, Chicago, USA, [4]Department of Physics, Applied Physics, and Astronomy, Binghamton University-SUNY, Binghamton, United States, [5]M.N. Miheev Institute of Metal Physics UB RAS, Ekaterinburg 620108, Russia, [6]Universitaet zu Koeln, Zuelpicher str. 77, 50937 Koeln,, Germany, [7]Department of Physics and Astronomy, George Mason University, Fairfax, United States

Novel Superconductors 1, July 27, 2023, 10:15–12:15

Both gold and silver are known as inert metals, which do not easily react with other chemical elements. Among the gold-containing compounds, which are not very common anyway, only a few are superconducting and the situation with the silver-based systems is similar. Besides the mineral calaverite, AuTe2, which becomes superconducting under applied pressure[1], we are aware only of one more compound combining Au and non-metallic elements, SrAuSi3, recently synthesised under high-pressure[2]. Therefore, finding new superconducting compounds of gold (and silver) is a challenge.

Here we report combined single-crystal X-ray diffraction, Raman, and resistivity measurements, as well as first-principles calculations, to explore the effect of hydrostatic pressure on the properties of the sylvanite mineral, AuAgTe4. Our experimental studies up to ~30 GPa, supported by density functional theory, reveal a reversible structural phase transition at ~5 GPa from a low-pressure (LP) monoclinic P2/c to high-pressure (HP) P2/m phase[3], resulting in almost identical coordinations of Au and Ag ions, with rather uniform interatomic distances, and breaking of the Te–Te dimers. Our resistivity measurements revealed superconductivity in both phases, the LP and HP. However, the LP phase becomes superconducting only above ~1.5 GPa and shows an almost linear increase of the critical temperature with pressure up to ~6 GPa (with a maximum Tc ≈ 2.5 K) followed by a slower decrease. The HP P2/m phase, once it occurs, has a higher critical temperature of ~3.5 K and shows a trend to a sluggish Tc decrease under pressure. With further pressure increase above ~26 GPa we observe evidence of an additional structural phase transition to the HP-II phase characterised by a critical temperature of ~3.3 K. Upon decompression, the Tc(P) behaviour shows a significant hysteresis, a signature of an irreversible phase transition. Namely, Tc(P) demonstrates a nonmonotonous dome-like behaviour reaching a maximum of 3.84 K at 3.2 GPa and remaining rather high, 2.5 K, even at 0.6 GPa.

Our first-principles computations demonstrate that most probably the superconductivity here is of a conventional type, with the low-energy phonon modes dominating the electron-phonon interactions. Although breaking of the Te–Te dimers is not directly responsible for the onset of superconductivity in AuAgTe4, it results in an appreciable increase in the critical temperature following the transition into the P2/m phase. This is due to an increase in the electronic density of states at the Fermi level related to closing of the pseudogap and to the phonon softening. Thus, along with the discovery of a new superconducting compound of gold/silver, our results advance understanding of the mechanism of the superconductivity in Au-containing compounds, which may pave the way to the discovery of novel ones.

Acknowledgments: This research was supported by the Israel Science Foundation (Grant No. 1748/20) and by National Science Foundation (Award Nos. DMR-2035518 and OAC-2103991).

[1] Sh. Kitagawa, et al., J. Phys. Soc. Jpn. 2013, 82, 113704.
[2] M. Isobe, et al. Chem. Mater. 2014, 26, 2155
[3] A. V. Ushakov et al., J. Phys.: Condens. Matter 2019, 31, 235601.

Discovery of new superconductor Sn3S4 by Original Diamond Anvil Cell using boron doped diamond electrode

Dr. Yoshihiko Takano[1,2], Ryo Matsumoto[1], Kensei Terashima[1]
[1]National Institute for Materials Science, Tsukuba, Japan, [2]University of Tsukuba, Tsukuba, Japan

Novel Superconductors 1, July 27, 2023, 10:15–12:15

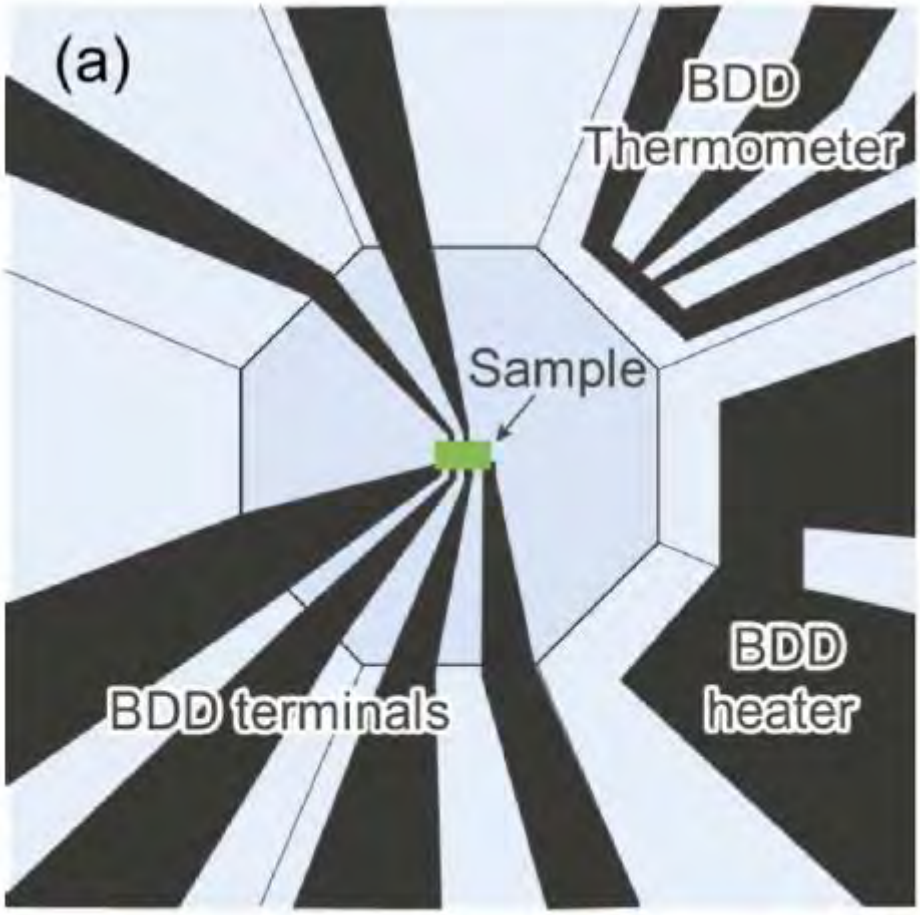
Recent reports of hydride superconductors attract much attention due to their extremely high transition temperature Tc. These materials need to be synthesised at high pressure since it was unstable at ambient condition. Laser heating is generally used for high pressure high temperature synthesis using diamond anvil cell. However, by laser heating, sample temperature is not stable and homogeneous. To overcome this problem, we have developed new high-pressure high-temperature synthesis system using originally designed diamond anvil with Joule heating circuit [1,2].

Our originally designed diamond anvil has 6 electrodes for sample, thermometer circuit, and heater circuit. The 6 electrodes are prepared for sample transport measurements of 4 terminal resistivity and Hall effect. Electrical current was applied through the heater circuit to induce Joule heat up to 1000°C. The temperature is measured by resistive thermometer and feedback to temperature controller. We can measure the sample resistivity during sample heating process.

We have synthesised Sn3S4 using SnS and SnS2 as a starting material. The pressure was applied above 30GPa and then heated up to 800K. The obtained sample was analysed by X-ray diffraction patterns which shows good matching with cubic Sn3S4. The temperature dependence of resistivity was measured by physical properties measurements system (PPMS) down to 2K. The drop of resistance due to superconductivity was observed at ~25GPa and the Tc increase with decreasing pressure. The maximum Tc was observed at 13.3K under ~5GPa. Bellow 5GPa, the superconductivity disappears due to the decomposition of Sn3S4 phase.

We have successfully discovered new superconductor Sn3S4 and related materials under high pressure using originally designed heater diamond anvil cell [2-4].

[1] R. Matsumoto et al., Rev. Sci. Instrum., 87, 076103 (2016).
[2] R. Matsumoto et al., Inorg. Chem., 61, 4476−4483 (2022).
[3] H. Yu et al., Phys. Rev. Lett. 118, 137002 (2017).
[4] J. M. Gonzalez et al., J. Chem. Phys. 148, 194701 (2018).


(a)
BDD
Thermometer
Sample
BDD terminals
BDD
heater

New opportunities at the Nuclear Resonance Beamline of ESRF with submicron spatial resolution

Ilya Kupenko[1], Georgios Aprilis[1], Sergey Yaroslavtsev[1], Jean-Philippe Celse[1], Xiang Li[1,2], Susanne Müller[1,2], Dimitrios Bessas[1], Alexander Chumakov[1]
[1]ESRF-The European Synchrotron, Grenoble, France, [2]Institute for Mineralogy, University of Münster, Münster, Germany

Next Gen Synchrotrons, July 25, 2023, 14:00–16:00

The nuclear resonant scattering based on the Mössbauer effect in iron has proven to be an important spectroscopic method to address the most advanced scientific issues in various scientific fields and is indispensable in Earth sciences. Particularly, experiments at extreme pressure and temperature conditions coupled with nuclear resonance techniques have provided many exciting results in the fields of experimental geosciences, solid-state physics, chemistry, and material sciences. Such achievements only became possible due to advances and developments in synchrotron radiation techniques as well as the evolution of tools for generating extreme conditions.

Synchrotron Mössbauer Source (SMS) spectroscopy [1] is the ultimate method to characterise the electronic states of iron atoms, enabling an accurate determination of oxidation and spin states, phase analysis, magnetic structure, and phase transitions in iron-bearing alloys and compounds. In turn, Nuclear Inelastic Scattering (NIS) is a powerful tool for studying lattice dynamics that provides access to vibrational and thermodynamic properties [2]. Moreover, the measured phonon density of states provides the Debye phonon average velocity, which together with density and bulk modulus are the necessary parameters for calculating the compressional velocity and shear velocity of the material. In fact, NIS is one of the few methods that allow sound velocity determination in the megabar pressure range.

The ESRF-EBS upgrade resulted in a significant reduction of the beam size at the nuclear resonance beamline. The beamline is now equipped with the submicron precision positioning system compatible with the beam size of 0.6 x 0.6 μm^2 provided through the short-focal distance Kirkpatrick-Baez mirrors.

In this contribution, I would like to report the recent advances in nuclear resonance methods coupled with experiments at extreme pressure-temperature conditions. In particular, I will discuss the first examples of experiments employing submicron spatial resolution and will present their applications to studies of geologically-relevant materials.

[1] Potapkin, V. et al. The ^{57}Fe synchrotron Mössbauer source at the ESRF. J. Synchrotron Radiat. 19, 559–569 (2012).
[2] Chumakov, A. I. & Sturhahn, W. Experimental aspects of inelastic nuclear resonance scattering. Hyperfine Interact. 123–124, 781–808 (1999).

Developments at PSICHE, Synchrotron SOLEIL, for science at extreme conditions

Andrew King[1], Laura Henry[1,2], Pierre Piault[1], Agnès Dewaele[2], Jean-Pierre Deslandes[1], Jean-Paul Itié[1], Nicolas Guignot[1]
[1]Synchrotron Soleil, Saint Aubin, France, [2]CEA DAM DIF, Arpajon, France

Facility Development 2, July 27, 2023, 14:00–16:00

The PSICHE beamline at Synchrotron SOLEIL proposes a range of techniques for science at extreme conditions for a wide range of communities. The beamline specialises in combining diffraction and imaging techniques and can work in both polychromatic and monochromatic modes [1]. This presentation will showcase a number of recent developments, illustrated with examples from user experiments.

Unique to PSICHE is the possibility to perform fast tomography at extreme conditions using the UToPEC press. This is performed in the white beam experimental hutch, using filtered white beam (pink beam) illumination for high flux. This station is equipped with a multi-element energy dispersive diffraction germanium detector, mounted on a two-theta rotation system. This can be used to perform combined angle and energy-dispersive structural analysis and refinement (CAESAR) acquisitions. These are particularly suited to investigations of liquid or amorphous structures. Algorithms have been developed to optimise the data acquisition and perform the renormalisation of the dataset [2]. A recent development uses the same detector system to perform X-ray absorption measurements of density using the Beer-Lambert law without the requirement of a monochromatic incident beam [3]. This suite of complementary techniques allows complete studies of a range of materials.

The monochromatic hutch of the beamline is equipped with a laser-heated diamond anvil cell station. Advanced laser beam shaping optics allow a precise control of the temperature distribution during experiments. This is combined with a 4-colour pyrometry system for imaging of the temperature radial distribution across the sample and surroundings. This resulting data are treated and displayed in real time by a program developed at the beamline. This capability allows fine control of the conditions and reactions within and around the sample.

[1] A. King et al, Rev. Sci. Instrum. (2016). 87, 093704. https://doi.org/10.1063/1. 4961365.
[2] A. King et al, J. Appl. Cryst. (2022). 55, 218–227. https://doi.org/10.1107/S1600576722000322
[3] L. Henry et al, J. Synchrotron Rad. (2022). 29, 853–861. https://doi.org/10.1107/S1600577522003411

Recovery of Nanodiamonds Produced in Laser-Driven Shock-Experiments

Mr. Ben Heuser[1,2], Mr. Michael Stevenson[1], Mr. Dominik Kraus[1,2]
[1]University of Rostock, Rostock, Germany, [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Synthesis and Properties of Novel Materials 1, July 26, 2023, 14:00–16:00

As the generation of high-pressure states via laser induced dynamic compression becomes feasible at relatively low costs and high repetition rates of several Hz, these conditions can now be reached in many laboratories across the world.

Facilities such as the Extreme Light Infrastructure (ELI) and the DiPOLE laser at European XFEL can deliver nanosecond long pulses of several hundred Jules multiple times per second. This is a major advancement for laser drive shock physics and paves the path to the generation of micrograms of high-pressure phases via dynamic compression.

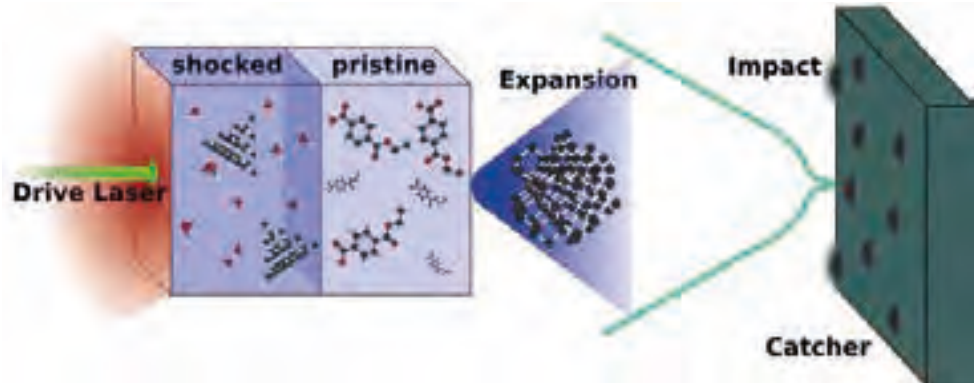
The formation of interesting forms of matter such as nanodiamonds (NDs) has been observed at the extreme shock conditions [Kraus, Nat. Astr. 2017]. Some of these materials have very interesting physical properties such as high temperature superconductivity or desirable catalytic properties in the case of NDs. The shock state persists on the nanosecond timescale and after the dynamic shock breaks out at the rear surface, the pressure drops to zero almost instantaneously and the material is ejected. The analysis of the often-metastable high-pressure phases is currently limited to in situ diagnostics (XRD, XRTS, …). To study those phases in depth they would have been recovered to ambient pressure and captured and concentrated for post analysis.

The ejection velocities can reach several tens of km/s. This makes the depressurization and deceleration of the ejected material a very challenging task. Previous experiments have been able to tailor the release path of zirconium by the application of rear side windows and recover a metastable phase to ambient pressures [Gorman, Phys. Rev. B, 2020]. However, the deceleration has not yet been solved although previous studies have done a lot of pioneering work in the field [Schuster, J. Phys. D].

In our work we study the formation and evolution of NDs from laser compressed plastic precursors [He, Sci. Adv. 2022], as well as the possibilities of intact recovery of NDs. We studied the ND release dynamics with in-situ diagnostics in an experiment at the SACLA facility and compared it to molecular dynamic simulations.

The release velocities were determined in another experiment using a high-speed camera.
To estimate the impactor size-density ratio we measured the cratering landscapes of the solid catcher materials after the experiment.

We used our results for the design of new target and catcher designs for an upcoming experiment at the ELI facility in July and will present some of the preliminary results.



Synthesis of novel rubidium superhydrides under high pressure

Mikhail Kuzovnikov[1], Busheng Wang[4], Tomas Marqueno[1], Calum Strain[1], Mengnan Wang[1], Eugene Gregoryanz[1,2,3], Eva Zurek[4], Miriam Pena-Alvarez[1], Ross T. Howie[1,2]
[1]Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom, [2]Center for High Pressure Science and Technology Advanced Research, Shanghai, China, [3]Key Laboratory of Materials Physics, Institute of Solid-State Physics, China, [4]Department of Chemistry, State University of New York at Buffalo, Buffalo, United States

Hydrides 2, July 24, 2023, 16:30–18:30

Superhydrides are a recently discovered class of materials with unusually high hydrogen content. Many superhydrides, such as bcc-CaH_6 [ma2022], bcc-YH_6 [troyan2021], hcp-YH_9 [kong2021] and fcc-LaH_{10} [drozdov2019], synthesised at pressures in excess of 150 GPa, demonstrate high temperature superconductivity. However, it remains a significant challenge to synthesise novel superhydrides at lower pressures.

Previous DFT-based ab initio calculations have predicted that rubidium should form superhydides at pressures as low as 2 GPa [hooper2012]. Here, we studied the Rb-H system in laser-heated diamond anvil cells with X-Ray diffraction and Raman spectroscopy under high hydrogen pressure up to 100 GPa.

Apart from the known monohydride RbH, we have synthesised a series of novel superhydrides via heating RbH in a hydrogen atmosphere under high pressure. These include two polymorphic modifications of a RbH_9 superhydride, two polymorphic modifications of a RbH_5 superhydride, and one superhydride with a tentative composition of RbH_{19}.

Both RbH_9 polymorphs can be synthesised via laser heating at 18-25 GPa. The highest found superhydride, RbH_{19}, can be formed via laser heating at 25-55 GPa. RbH_9 and RbH_{19} superhydrides cannot be formed via heating at 100 GPa, which suggests that their stability fields terminate at lower pressures. Instead, laser heating at 100 GPa produces one of the RbH_5 polymorphs.

All discovered rubidium superhydrides are wide-bandgap insulators containing molecular H_2 units, as manifested by their Raman spectra.

The work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement no. 948895, MetElOne).

[1] [ma2022] L. Ma et al, Phys. Rev. Lett. 128 (2022) 167001
[2] [troyan2021] I. A. Troyan et al, Adv. Mater. 33 (2021) 2006832
[3] [kong2021] P. Kong et al, Nature Commun. 12 (2021) 5075
[4] [drozdov2019] A. P. Drozdov et al, Nature 569 (2019) 528
[5] [hooper2012] J. Hooper et al, Chem. Eur. J. 18 (2012) 501

Superconductivity in YH4 Films at Very High Pressures

Dr. Jonathan Buhot[1], Dr. Owen Moulding[2], Sam Cross[1], Dr. Israel Osmond[3], Annabelle Brooks[1], Alix McCollam[4], Dr. Toni Helm[5], Dr. Nico Giordano[6], Dr. Timofey Fedotenko[6], Dr. Hanns-Peter Liermann[6], Dr. Oliver Lord[7], Dr. Sven Friedemann[1]

[1]HH Wills Physics Laboratory, University of Bristol, Bristol, United Kingdom, [2]Institut NEEL, CNRS, Univ. Grenoble Alpes, Grenoble, France, [3]The University of Edinburgh, Edinburgh, United Kingdom, [4]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, Netherlands, [5]Dresden High Magnetic Field Laboratory (HLD), Dresden, Germany, [6]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany, [7]School of Earth Sciences, University of Bristol, Bristol, United Kingdom

Hydrides 4, July 26, 2023, 14:00–16:15

The discovery of the hydride superconductor H3S in 2015 with a Tc record of 203K at 155GPa has been a cornerstone for the research on hydride at high pressures and the quest for room temperature superconductivity [1]. Since several other superhydride compounds have been synthesised, such as YH6 [2] and YH9 [3, 4], exhibiting superconductivity close to room temperature under megabar pressures. While theoretical works are paving the way to realise new hydride superconductors, their synthesis within the laboratory remains very challenging. Here we demonstrate a new approach to synthesise YH4 from an elemental yttrium film directly evaporated on the diamond anvil and ammonia borane (NH3BH3) as a hydrogen donor [5]. This method allows a more accurate control of the sample size and helps to reach high hydrogen content in the synthesis. The critical superconducting temperatures of about 70-80 K that we observe for YH4 films at 180-200 GPa are consistent with those reported by other independent groups in YH4 bulk [2, 3, 6]. The lower Tc permits us to study the upper critical field Hc2 over the full temperature range. We will present the synthesis method, the crystal structure of YH4 films obtained from X-ray diffraction, the resistivity measurements as a function of temperature and magnetic field, and Hc2(T) extracted from steady and pulsed magnetic field measurements.

[1] A. P. Drozdov, et al., Nature 525, 73 (2015).
[2] I. A. Troyan et al., Advanced Materials 33, 2006832 (2021).
[3] P. P. Kong et al., Nature Communications 12, 5075 (2021).
[4] E. Snider et al., Physical Review Letters 126, 117003 (2021).
[5] Buhot et al., Physical Review B 102, 104508 (2020).
[6] M. Shao et al., Physical Review B 104, 174509 (2021).

Phase transitions in compressed palladium trifluoride: how Pd(II)Pd(IV)F6 becomes Pd(III)F3

Dominik Kurzydłowski[1], Deepak Upadhyay[1], Kinga Zdun[1], Jakub Drapała[2], Klemen Motaln[3,4], Matic Lozinšek[3,4]

[1]Faculty of Mathematics and Natural Sciences Cardinal Stefan Wyszyński University in Warsaw, Warsaw, Poland, [2]Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland, [3]Jožef Stefan Institute, Ljubljana, Slovenia, [4]Jožef Stefan International Postgraduate School, Ljubljana, Slovenia

Magnetic Materials 2, July 26, 2023, 14:00–16:00

Fluorides are model systems for the study of pressure-induced structural transitions, as well as compression-induced reactivity. [1,2] Transition metal fluorides can exhibit high-pressure transformations involving both electronic and magnetic degrees of freedom. [3]

Palladium trifluoride adopts at ambient conditions the distorted ReO3-type structure with two inequivalent Pd sites exhibiting II and IV valency. [4] This charge ordering leads to different electron counts and spin population at both sites – Pd2+ with a d8 count has two unpaired electrons, while Pd4+ (d6) has no unpaired electrons. Recent theoretical investigation suggest that this compound should undergo two consecutive phase transitions at 19 and 57 GPa, [5] a prediction yet to be verified. Moreover, the question whether large compression will force Pd(II)Pd(IV)F6 into a metallic state, or rather a spin-1/2 semiconductor state with genuine Pd3+ cations, is still open.
Our Raman measurements indicate that palladium trifluoride retains the ambient pressure R−3 structure up to 41 GPa. Above this pressure a transformation occurs into a new phase containing Pd3+ cations. By employing hybrid DFT methods (HSE06 functional) we are able to unveil the structural and electronic changes occurring as a result of the phase transition.
In particular, we show that palladium trifluoride remains semiconducting at high pressure and exhibits a crossover from mixed valency (II and IV) to single valency (III).

[1] J. Lin, X. Du, M. Rahm, H. Yu, H. Xu and G. Yang, Angew. Chemie Int. Ed., 2020, 59, 9155–9162.
[2] D. Kurzydłowski, S. Kobyakov, Z. Mazej, S. B. Pillai, B. Chakraborty and P. K. Jha, Chem. Commun., 2020, 56, 4902–4905.
[3] S. López-Moreno, A. H. Romero, J. Mejía-López and A. Muñoz, Phys. Chem. Chem. Phys., 2016, 18, 33250–33263.
[4] A. Tressaud, N. Bartlett, J. Solid State Chem., 2001, 162, 333–340.
[5] S. Ma, L. Zhao, S. Li, T. Gao, F. Peng, Phys. Chem. Chem. Phys., 2023, 25, 6726–6732.

Molecular replacement in Clathrate Hydrates

Fernando Izquierdo-Ruiz[1,2], Alvaro Lobato[1,2], Eduardo O. Gomes[1], Alberto Otero-de-la-Roza[1,3], J. Manuel Recio[1,3]

[1]Malta Consolider Team, Spain, [2]Departamento de Química Física, Universidad Complutense de Madrid, Madrid, Spain, [3]Departamento de Química Física y Analítica, Universidad de Oviedo, Oviedo, Spain

Ice, Water and Clathrates, July 24, 2023, 10:15–12:15

Clathrate hydrates are considered very interesting materials in geology, the environmental sciences and the energy industry. Depending on the guest molecule, the use of clathrate hydrates has been proposed as a method for carbon capture (CO2) and as an energy source (methane) Below 1 GPa both CO2 and CH4 gas hydrates are stable in the cubic sI hydrate structure. The close structural relationship between the structures of the two hydrates suggests using the replacement of CO2 by methane in these systems as a carbon-neutral energy source. In order to have a successful molecular replacement, this substitution should preserve the host structure, allowing for partial substitutions without destabilizing the whole system.

By performing DFT simulations we address the thermochemistry involved in the general process x CO2(s) + (CH4)8@sI(s) --> (CO2)x(CH4)8-x@sI(s) + x CH4(s) ; x = 1—8 at pressures in the range 0–1 GPa. Electronic structure calculations for each composition are carried out taking into account the weak interactions governing the cohesion of these host-guest compounds. Energy-volume curves are fitted to analytical equations of state and enthalpy-pressure relationships are derived from them.

Our calculations allow us to determine the equilibrium compositions of the mixed gas hydrates at different hydrostatic pressures by means of the analysis of the corresponding convex hull. Employing an energy decomposition analysis, we obtain the three main components of the lattice energy, defined as: i) host deformation energy, ii) guest-guest interaction energies, and iii) guest-host interaction energies. This decomposition allows us to identify and interpret the contributions to the stability of the system. Overall, we find that mixed clathrates are thermodynamically stable under certain conditions. A way to advance in the prediction of other stable gas hydrates under pressure is also discussed.

Financial support from Spanish PID2021-122585NB-C21-2 AEI project and Principado de Asturias-FEDER under project AYUD/2021/51036 is gratefully acknowledged.

Cubic (Eu1-xYbx)2O3 nanophosphors under compression: a joint structural and spectroscopic study

Marina Teresa Candela[1,3], Fernando Aguado[2,3], Javier Ruiz-Fuertes[2], Jesús González[2,3], Rafael Valiente[1,3]

[1]Departamento de Física Aplicada, Universidad de Cantabria, Avda. Los Castros 48, 39005-Santander, Spain, [2]Departamento de Ciencias de la Tierra y Física de la Materia Condensada (CITIMAC), Universidad de Cantabria, Avda, Los Castros 48, 39005-Santander, Spain, [3]Grupo de Nanomedicina, IDIVAL-Universidad de Cantabria. Avda, Cardenal Herrera Oria, 39011-Santander, Spain

Nanoscale Systems, July 24, 2023, 16:30–18:30

Rare-earth sesquioxides (RE_2O_3) are a family of compounds that exhibit interesting physical and chemical properties, such as low phonon energies, chemical stability and a rich diversity of energy levels, which makes them interesting for optical or electronic applications, among others. These compounds crystallise in three different structural conformations at ambient conditions, denoted as A, B and C compounds, with trigonal (s.g. P-3m1), monoclinic (s.g. C2/m) and cubic (space group Ia-3) symmetries, respectively, being the stable phase mainly dependent on the RE ionic radii and on thermal treatments [1].

Introducing RE' ions in a RE_2O_3 host lattice can lead to materials with modified properties with respect to the pure compounds, as already seen in the cubic and monoclinic (Eu1-xYbx)2O3 solid solutions at ambient conditions, where a non-resonant energy transfer phenomenon between Eu3+ and Yb3+ ions has been observed, which allows to observe simultaneous visible (Eu3+) and IR (Yb3+) emission under excitation of Eu3+ ions [2].

Although the effects of pressure on the structure of RE2O3 have been widely studied [3], there is still some controversy, since some inconsistencies are found in the literature, especially with regard to the phase transitions sequence (C–B – A or C–A) or with the transition pressures depending on particle size (bulk versus nano). Moreover, the effect of pressure on rare-earth solid solutions has been scarcely investigated, although effects on the transition sequences and/or on the transition pressures have been reported for (Eu1-xHox)2O3 [4] or (Eu1-xLax)2O3 series [5], for which the pressure-concentration phase diagram has been established.

Here, we present the study of the structural evolution under high-pressure of seven nanopowder samples belonging to the cubic (Eu1-xYbx)2O3 solid solution ($0 \leq x \leq 1$), which were prepared by the sol-gel Pechini method, and all have an average size in the order of 20-60 nm. The pressure evolution of these compounds has been determined by three different techniques, including X-ray diffraction, Raman and Eu3+ photoluminescence measurements, paying special attention to possible pressure-induced phase transitions and to changes in the phase stability depending on the Yb3+ concentration. Moreover, the high-pressure behavior of these compounds has been compared to that of other RE_2O_3 solid solutions or pure compounds and the suitability of the Eu3+ luminescence as a local probe has been evaluated.

[1] M. Zinkevich. Prog. Mater. Sci. 52, 597–647 (2007).
[2] M. T. Candela et al. J. Alloys Compd. 921, 166043 (2022).
[3] F. J. Manjón et al. Crystals 9, 630 (2019).
[4] K. A. Irshad et al. J. Alloys Compd. 725, 911–915 (2017).
[5] K. A. Irshad et al. Sci. Rep. 10, 11829 (2020).

The mechanical state of the earth's crust and the force source of crustal plate movement

Duanwei He[1]
[1]*Institute of Atomic and Molecular Physics, Sichuan University, Chengdu, China*

Secular Evolution of the Earth, July 25, 2023, 10:15–12:15

The relationship between magma solidification and the force source mechanism of crustal plate movement is investigated and proposed. Crustal plate movement is the physical source of major geological activities such as earthquakes, but its driving force mechanism is still unclear. The answer to this question with a clear physical image is as follows.

First, it is found that the mechanical structure formed by the crust and lithosphere is not enough to support its self-weight. This means that any pressure fluctuation at the bottom of the lithosphere can destabilise its mechanical structure. Second, the earth as a whole dissipates heat in outer space, and its interior is in a state of liquid-solid coexistence. The solidification of molten magma since the formation of the Earth continues and leads to density change and heat release. Constrained by the rigid and brittle lithosphere of the earth's crust, the solidification of magma in the earth's interior will inevitably lead to the pressure fluctuation at the bottom of the lithosphere, which is the source of the driving force of plate movement.

Therefore, the density change accompanied by magma solidification in the earth's interior will reduce the pressure at the bottom of the crustal lithosphere and the supporting force to the rigid lithosphere. Under the action of gravity, the interaction between crustal plates will intensify, and the local stress accumulation will exceed the strength of rocks, resulting in the instability of the mechanical structure of the crustal lithosphere. The earth releases the accumulated stress through geological activities such as earthquakes and adjusts itself to achieve a new mechanical balance. The above process is repeated.

In order to verify the above point of view, the existing GPS data, day length data and the earth's net heat dissipation in outer space have been analyzed. Assuming that the earth's net heat dissipation mainly comes from the latent heat of magma solidification, the earth volume changes given by the three types of data are consistent.

High-pressure synthesis and crystal chemistry of novel Cr-Ge compounds

Takuya Sasaki[1], Kota Kanie[1], Koki Noda[1], Nico Alexander Gaida[1], Ken Niwa[1], Masashi Hasegawa[1]
[1]*Department of Materials Physics, Nagoya University, Nagoya, Japan*

Synthesis and Properties of Novel Materials 3, July 26, 2023, 16:30–18:30

Intermetallic compounds composed of transition-metal and metalloid elements have attracted attention because of their various properties, including magnetic, electronic, and superconducting properties. High-pressure conditions are a useful reaction field for synthesizing novel compounds, and many novel intermetallic compounds of transition metals and metalloids have been discovered by high-pressure synthesis. Of particular interest, intermetallic compounds, which are richer in metalloid elements than the ambient-pressure phase, tend to form under high pressure. We have focused on intermetallic compounds in the binary Cr–Ge system. In the Cr–Ge system, the most Ge-rich ambient-pressure phase is the Nowotny chimney ladder phase $Cr_{11}Ge_{19}$. We expect to synthesise novel materials in the Cr–Ge system under high pressure and present here the results of the synthesis of novel compounds using a diamond anvil cell and large-volume presses. $MoSi_2$-type $CrGe_2$, the most Ge-rich compound in the Cr–Ge system, was synthesised above 27 GPa by laser heating using a diamond anvil cell. Nowotny chimney ladder chromium germanides, $CrGe_\gamma$, with varying compositions from $\gamma = 1.737$ to $\gamma = 1.774$, were synthesised at 2~14 GPa using DIA-type and Kawai-type large-volume presses. The composition ratio γ increases with the synthesis pressure, indicating that the Nowotny chimney ladder $CrGe_\gamma$ phases became more Ge content – finally, the Cr–Ge compound changes from the Nowotny chimney ladder phase to the $MoSi_2$-type digermanide at above 27 GPa. The Nowotny chimney ladder $CrGe_\gamma$ phases are ferromagnetic regardless of their composition. The magnetic transition temperature finally increased by 270 K from the transition temperature for $Cr_{11}Ge_{19}$ as the γ became higher.
We will present and discuss the detailed crystal chemistry and magnetic properties in the Cr–Ge compound synthesised under high pressure in the presentation.

Study on Stress, Strain and Densification of Superhard Materials and Ceramics during High Pressure Sintering

Fang Peng[1]
[1]*Institute of Atomic and Molecular Physics, Sichuan University, Chengdu, China*

Ceramics and Composites, July 24, 2023, 14:00–16:00

With the development of high-pressure science and technology, the sintering quality of superhard materials and ceramic materials under high pressure and high temperature has continuously improved. Especially, the sintering of pure phase superhard materials without binder has made progress in recent years. In order to explore the sintering mechanism of pure phase superhard materials and ceramic materials, some relevant issues were discussed in this paper.
Firstly, the stress and strain of diamond and SiC particles under high pressure were studied using in situ a DAC synchrotron radiation X-ray diffraction. At different pressure, the high-pressure X-ray diffraction spectra were obtained. Based on the relationship between the stress, strain, the peak position and shape of X-ray diffraction of material samples, the stress states of diamond and SiC particles under high pressure were obtained. The study found that the stress on the sample particles is uneven, and there are different high stress regions and low stress regions. At an external load of 35.1 GPa, the stress difference on the diamond particles reaches 18.8 GPa. At an external load of 23.0GPa, the stress difference on the SiC particles reaches 11.0 GPa. With the external load increasing, the stress difference causes continuous fragmentation and densification of the material particles. This result is of great significance for understanding the mechanism of direct bonding between particles in binder free pure phase superhard materials and ceramic sintering.

Secondly, according to the above results, the pure phase sintering of cubic boron nitride (c-BN) and SiC powders was carried out using a large volume cubic press. Before reaching the sintering pressure and temperature conditions, the pressure and temperature treatment processes was introduced and allows the material particles to achieve sufficient crushing and densification. Using a large volume cubic press, the pure phase c-BN sintered bulk and SiC sintered bulk were prepared. The c-BN sintered bulk is transparent and has a hardness of 68.0 GPa, the pure phase SiC sintered bulk has a high hardness of 31.3GPa.

Nano-polycrystalline diamond anvil cells for neutron diffraction up to 100 GPa

Kazuki Komatsu[1], Keishiro Yamashita[1], Hiroyuki Kagi[1], Stefan Klotz[2], Takanori Hattori[3], Asami Sano-Furukawa[3], Shinichi Machida[4], Tetsuo Irifune[5], Shinmei Toru[5]
[1]GCRC, UTokyo, Tokyo, Japan, [2]IMPMC, Sorbonne University/CNRS, Paris, France, [3]J-PARC Center, JAEA, Tokai, Ibaraki, Japan, [4]CROSS, Tokai, Ibaraki, Japan, [5]GRC, Ehime Univ., Matsuyama, Ehime, Japan

Instrumentation and Techniques 1, July 26, 2023, 10:15–12:15

Neutron diffraction has several advantages over X-ray diffraction in accessibility to crystal structures including light elements, magnetic structures, and so on. On the other hand, the achievable pressure by neutron diffraction has long been limited up to date because neutron diffraction requires significantly larger sample volumes than the case of X-ray diffraction due to the low flux of neutron source. The current world record for the highest pressure for neutron diffraction in the published data is 94 GPa by Boehler et al. [1] taken at the SNAP beamline in SNS using diamond anvil cells (DACs) with conically supported 'Boehler-Almax' type diamond anvils. Guthrie et al. [2] managed to obtain neutron diffraction of ice VII up to 60 GPa with a quality that the structure can be refined. We have developed DACs with nano-polycrystalline diamonds (NPDs) which would be a promising material because of their hardness and toughness owing to the absence of cleavage planes [3]. We adopted a 'flat' base design of NPD anvils rather than the conical support because the supporting area of the base is large enough to support a high load.

A few years ago, we conducted neutron diffraction experiments at the PLANET beamline in J-PARC, and achieved up to 82 GPa for D20 ice VII (or X) sample with a size of 0.4 mm in diameter and 0.2 mm in thickness (sample volume is 0.025 mm3) using NPDs with a culet size of 1.0 mm [3]. We recently modified the culets into those with the size of 0.5 mm and a dip with diameter and depth of 0.3 mm and 0.05 mm, respectively (sample volume = 0.017 mm3) to obtain neutron diffraction patterns of D20 ice VII (or X) up to 100 GPa. We also used radial collimators with a diffraction gauge length of 0.5 mm [4], which preferentially reduced scattering from NPDs, although its intensities still dominate the diffraction patterns. In this presentation, we will report the recent technical achievements and the data analysis procedure using the NPDAC.

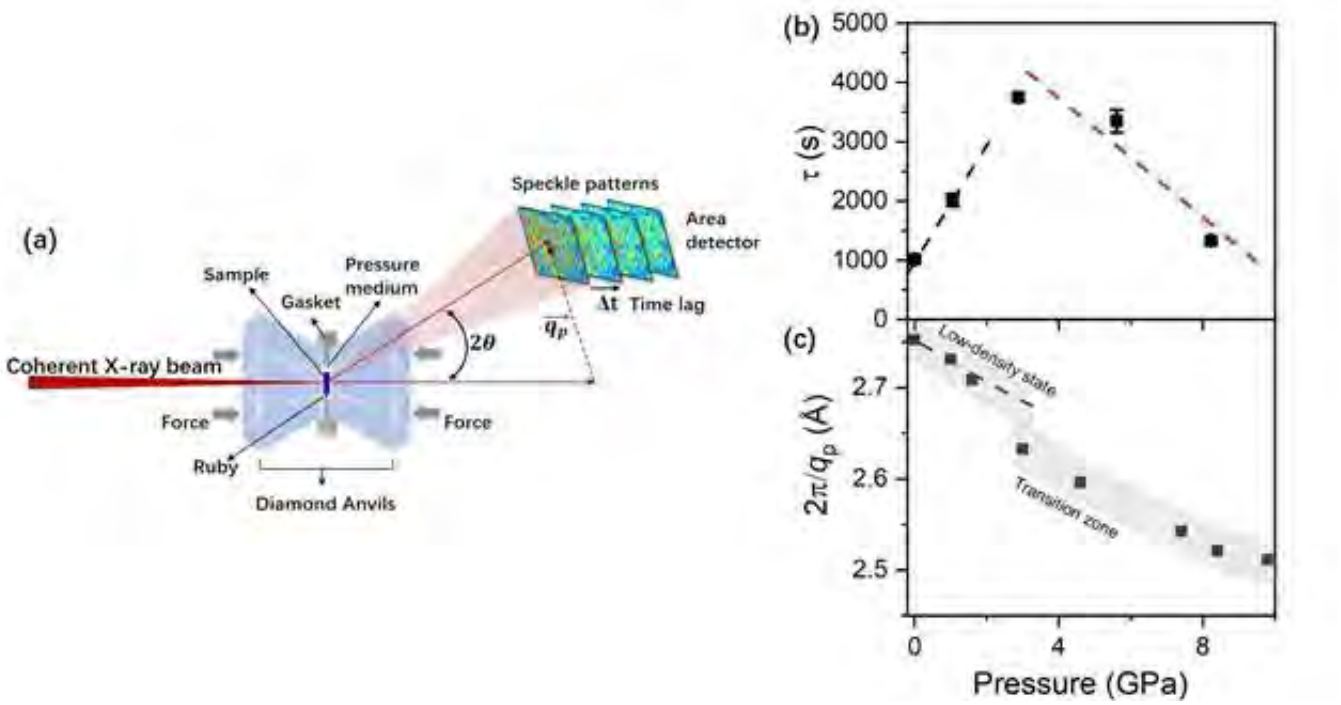
[1] Boehler, R., Guthrie, M., Molaison, J.J., dos Santos, A.M., Sinogeikin, S., Machida, S., Pradhan, N. and Tulk, C.A. (2013) High. Press. Res., 33, 546-54.
[2] Guthrie, M., Boehler, R., Molaison, J.J., Haberl, B., dos Santos, A.M. and Tulk, C. (2019) Phys. Rev. B, 99, 184112.
[3] Komatsu, K., Klotz, S., Nakano, S., Machida, S., Hattori, T., Sano-Furukawa, A., Yamashita, K. and Irifune, T. (2020) High. Press. Res., 40, 184-93.
[4] Hattori, T., in prep.

Pressure-induced non-monotonic crossover of steady relaxation dynamics in a metallic glass

Prof. Qiaoshi Zeng[1]
[1]*HPSTAR, Shanghai, China*

Synthesis and Properties of Novel Materials 1, July 26, 2023, 14:00–16:00

Relaxation dynamics, as a key to understand glass formation and glassy properties, remains an elusive and challenging issue in condensed matter physics. In this presentation, I will introduce our recent development of in situ high-pressure synchrotron high-energy X-ray photon correlation spectroscopy (Fig.1a), which enable us to probe the atomic-scale relaxation dynamics of a cerium-based metallic glass during compression. Although the sample density continuously increases, the collective atomic motion initially slows down as generally expected and then counter-intuitively accelerates with further compression (density increase), showing an unusual non-monotonic pressure-induced steady relaxation dynamics crossover at ~3 GPa. Furthermore, by combining in situ high-pressure synchrotron X-ray diffraction, the relaxation dynamics anomaly is evidenced to closely correlate with the dramatic changes in local atomic structures during compression, rather than monotonically scaling with either sample density or overall stress level (Fig.1b and c). These findings could provide new insight into relaxation dynamics and their relationship with local atomic structures of glasses. It is worth emphasizing that the technique developed and demonstrated in this work will strongly benefit from the advent of diffraction-limited synchrotron sources with largely enhanced coherent X-ray flux, allowing to dramatically extend the accessible dynamical range using high-energy X-ray.



Nonmetal-to-metal transition in dense fluid nitrogen at high pressure

Ronald Redmer[1], Armin Bergermann[1]
[1]*University of Rostock, Rostock, Germany*

Phase Diagrams – Molecular Systems, July 27, 2023, 14:00–16:00

The high-pressure phase diagram of solid nitrogen is extremely rich [1]. Recent molecular dynamics (MD) simulations on dense fluid nitrogen using density functional theory (DFT) [2-5] predict a first-order liquid-liquid phase transition (LL-PT) at about a megabar.

We have calculated the equation of state and the electrical conductivity of dense fluid nitrogen for high pressures up to several megabars by using extensive DFT-MD simulations. We have checked the convergence of the method with respect to the particle number and performed our simulations with up to 256 nitrogen atoms. We have determined the instability region of the first-order LL-PT which results from an abrupt dissociation of nitrogen molecules. This transition is accompanied by a nonmetal-to-metal transition (metallization) of the fluid and corresponding structural changes from a molecular to a polymeric phase.

The LL-PT is studied in more detail by analysing the electrical conductivity and the pair distribution function as well as the coordination number. Note that we have used the hybrid exchange-correlation functional of Heyd-Scuseria-Ernzerhof (HSE) [6] in order to determine the band gap and, thereby, the electrical conductivity in the transition region from a semi-conducting to a metallic fluid. The HSE functional yields more reliable band gaps than the Perdew-Burke-Ernzerhof (PBE) [7] functional used in the earlier studies [2-5]. Finally, we present the high-pressure phase diagram with our results for the coexistence line of the first-order LL-PT and its critical point located at T_c=3500 K, ρ_c=3.4 g/cm3, and p_c=90 GPa [8].

[1] R. Turnbull et al., Nature Commun. 9, 4717 (2018).
[2] B. Boates and S. A. Bonev, Phys. Rev. Lett. 102, 015701 (2009).
[3] K. P. Driver and B. Militzer, Phys. Rev. B 93, 064101 (2016).
[4] S. Jiang et al., Nature Commun. 9, 2624 (2018).
[5] Z. Fu et al., High Energy Dens. Phys. 31, 52 (2019).
[6] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003).
[7] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
[8] A. Bergermann and R. Redmer, submitted.

High pressure medium, solidifying at pressure beyond 5 GPa at room temperature, and related topics

Prof. Keizo Murata[1], Dr Kenji Goto[2], Dilip Bhoi[3], Stefan Klotz[4], Yoshiya Uwatoko[3], Shinji Aoki[2]
[1]Osaka Metropolitan University, Osaka, Japan, [2]Idemitsu Kosan, Japan, [3]ISSP University, Japan, [4]CNRS, IMPMC, France

Instrumentation and Techniques 4, July 26, 2023, 16:30–18:30

In the past more than years, we have developed high pressure medium, with higher solidification pressure at room temperature, P_solid@RT. We developed Daphne 7373, 7474, 7575 with P_solid@RT from 2.2 GPa to 4 GPa. We plan to show new medium candidate having P_solid@RT beyond 5 GPa and related topics with this material.

High-Pressure Behavior of δ-Phase of Formamidinium Lead Iodide by Optical Spectroscopies

Elena Stellino[1], Valentina Carpenella[2], Francesca Ripanti[1], Claudia Fasolato[3], Alessandro Nucara[4], Caterina Petrillo[1], Lorenzo Malavasi[5], Paolo Postorino[6]

[1]University of Perugia, department of physics and geology, Perugia, Italy, [2]Department of Sciences, University of Roma Tre, Roma, Italy, [3]CNR-ISC, Istituto dei Sistemi Complessi, c/o Sapienza University of Rome, Roma, Italy, [4]CNR-SPIN and Department of Physics, Sapienza University of Rome, Roma, Italy, [5]Department of Chemistry and INSTM, University of Pavia, Pavia, Italy, [6]Department of Physics, Sapienza University of Rome, Roma, Italy

Synthesis and Properties of Novel Materials 1, July 26, 2023, 14:00–16:00

The exceptional photovoltaic properties of hybrid organic-inorganic perovskites (HOIP) have attracted increasing interest in the last decades [1]. Among these materials, $FAPbI_3$ shows two structural phases: the high temperature perovskite α-phase, with direct bandgap close to the Shockley-Queisser limit, and the less photoactive non-perovskite δ-phase, stable at ambient conditions [2]. Although the presence of δ-phase has been usually regarded as a limitation for $FAPbI_3$ optoelectronic applications, recent studies have found that devices with increased stability and efficiency can be designed by mixing α- and δ-phases [3,4]. This has brought out the need for a deeper understanding of the physical properties of δ- $FAPbI_3$.

In this perspective, we present a high-pressure Raman and photoluminescence (PL) investigation on a δ-$FAPbI_3$ crystal, to study the effects of lattice compression on its vibrational and optoelectronic properties [5]. As shown in figure 1, we observe an increase in the number of Raman-active phonon peaks around 1.5 GPa, indicating a lattice transition to a lower symmetry phase. Then, above 7 GPa, the spectrum line shape turns into a nearly featureless profile suggesting the occurrence of an amorphization-like process. As for the PL spectrum, the exciton band at 2.15 eV, ascribed to the indirect gap recombination, continuously evolves in the 0-9 GPa range. Based on these results, we can draw a coherent scenario for the pressure evolution of δ-$FAPbI_3$, in which three distinct regimes can be distinguished. At ambient conditions, the crystal exhibits a dynamically disordered structure, in which the organic cation is rotationally averaged over equivalent orientations and, thus, the long-range periodicity is governed mainly by the inorganic frame. The application of pressure above 1.5 GPa inhibits the rotation of FA cations, bringing the inorganic frame to a lower-symmetry phase. Finally, above 7 GPa, a statically disordered regime takes place, in which the FA cations are locked at random orientations. Correspondingly, the octahedral chains undergo local distortions making the crystal lose its long-range periodicity. In this state, although the lack of long-range order damps the vibrational modes, the sample maintains locally an octahedral symmetry, as witnessed by the reversibility of the Raman spectrum after the compression cycle.

The absence of abrupt changes in the PL spectrum under pressure provides further support to the idea that the inorganic frame maintains the local octahedral structure.

Our results show that the pressure evolution of δ- $FAPbI_3$ shares strong similarities with that of crystals in a perovskite form [6], indicating that the driving mechanism of the amorphous-like molecular disorder in HOIP is mostly associated with octahedral compression and only to a lesser extent to the long-range lattice arrangement.

[1] Jin Y. K., et al., Chemical Reviews (2020), 120(15)7867-7918
[2] Constantinos C., et al., Inorganic Chemistry (2013), 52(15)9019–9038
[3] Jingjing Q., et al., Journal of Physical Chemistry Letters (2019), 10(9)2101-2107
[4] Zhang, J., et al., Advanced Functional Material (2022), 32, 2204642
[5] Carpenella V., ..., Stellino E., et al., Journal of Physical Chemistry C (2023), 127(5)2440–2447
[6] Capitani F., et al., Journal of Physical Chemistry C (2017), 121(50)28125-28131

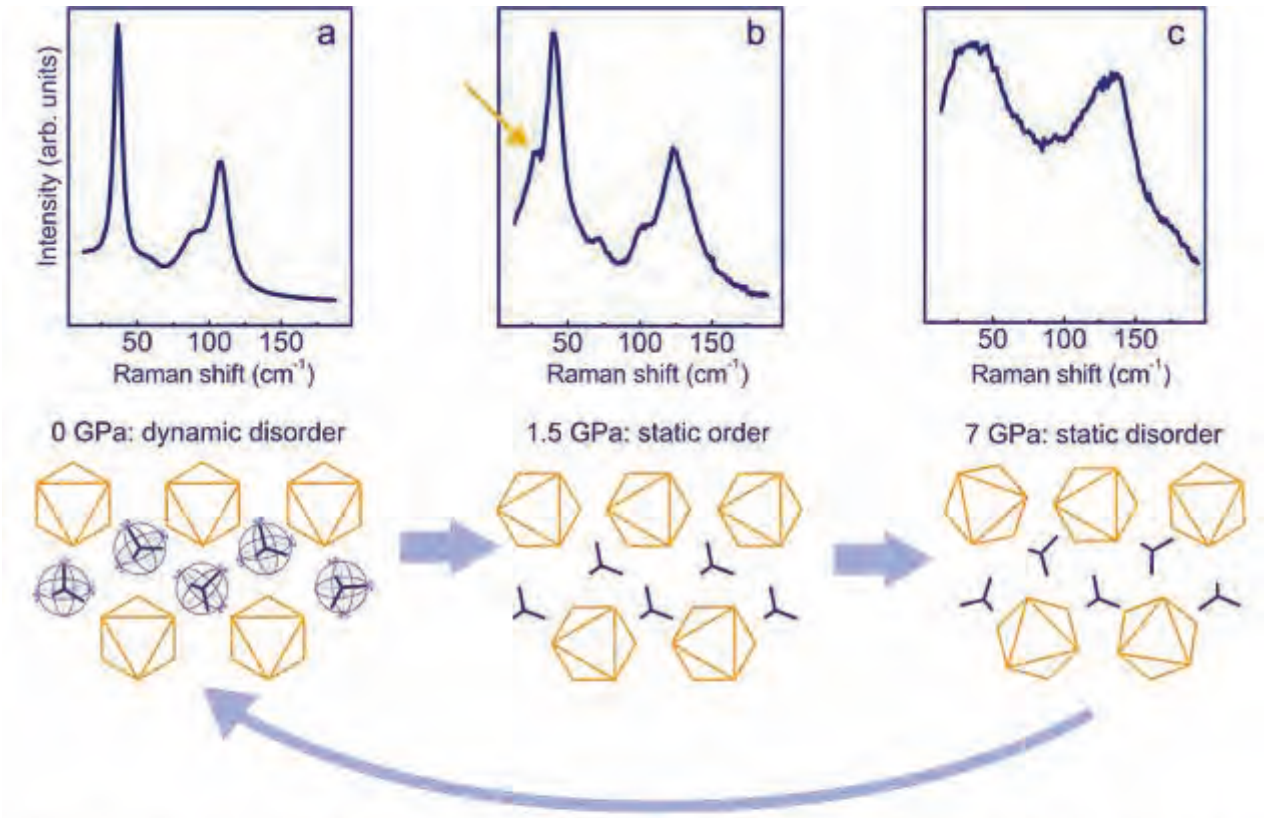


Figure 1: Evolution of the Raman spectrum of δ-FAPI under pressure. (a)showsthe Raman peaks associated with the vibrational modes of the inorganic frame at ambient pressure. (b)Raman spectrum at 1.5 GPa with the new low-frequency peak(orange arrow), which appears in correspondence with the transition to a lower-symmetry phase. (c) Amorphous-like Raman spectrum at 7 GPaassociated with the onset of a statically disordered phase, in which the long-range order of the latticeis lost.Once the pressure on the sample is released, the spectral features shown in panel (a) are recovered.At the bottom, schematic representations of the three regimes are also shown.

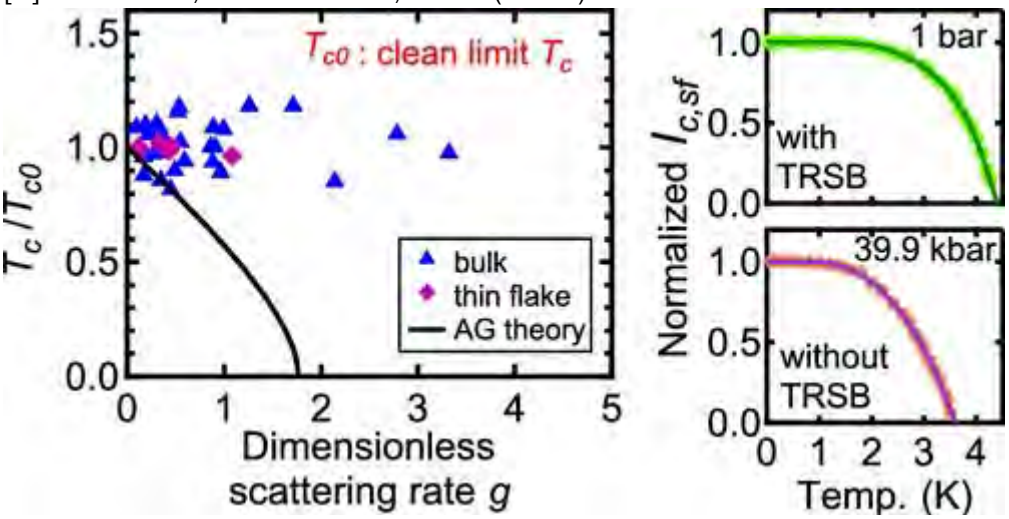
Probing the Superconducting Gap of a Kagome Metal in a Diamond Anvil Cell via Self-field Critical Current

W. Zhang[1], X.Y. Liu[1], L. Wang[1], C.W. Tsang[1], Z.Y. Wang[1], S.T. Lam[1], W.Y. Wang[1], J.Y. Xie[1], X.F. Zhou[2], Y.S. Zhao[2], S.M. Wang[2], J.L. Tallon[3], K.T. Lai[1], **Swee K. Goh**[1]
[1]The Chinese University of Hong Kong, Hong Kong, [2]Southern University of Science and Technology, China, [3]Victoria University of Wellington, New Zealand

Novel Superconductors 1, July 27, 2023, 10:15–12:15

The kagome metal CsV3Sb5 features an unusual competition between the charge-density-wave (CDW) order and superconductivity. Evidence for time-reversal symmetry breaking (TRSB) inside the CDW phase has been accumulating. Hence, the superconductivity in CsV3Sb5 emerges from a TRSB normal state, potentially resulting in an exotic superconducting state. To reveal the pairing symmetry, we first investigate the effect of nonmagnetic impurity. Our results show that the superconducting critical temperature is insensitive to disorder, pointing to conventional s-wave superconductivity [1]. Moreover, using a technique we developed to conduct transport measurements of thin flakes in a diamond anvil cell [2], we measure the self-field critical current (Ic,sf), which is related to the London penetration depth. Our Ic,sf data confirm the conventional s-wave superconductivity. Finally, we measure Ic,sf where the CDW order is removed by pressure and superconductivity emerges from the pristine normal state. Our results show that s-wave gap symmetry is retained, providing strong evidence for the presence of conventional s-wave superconductivity in CsV3Sb5 irrespective of the presence of the TRSB [1].

[1] W. Zhang et al., Nano Lett. 23, 872 (2023).
[2] J. Xie et al., Nano Lett. 21, 9310 (2021).



Neutron scattering, Raman scattering and molecular dynamics simulation study of supercritical fluid nitrogen

Dr. John Proctor[1], Dr. Ciprian Pruteanu[2], Prof. Graeme Ackland[2], Dr. John Loveday[2], Prof. Ian Morrison[1], Mr. Abdullah Al-Maiyah[1], Dr. Oliver Alderman[3]

[1]University Of Salford, United Kingdom, [2]Centre for Science at Extreme Conditions, University of Edinburgh, Edinburgh, United Kingdom, [3]ISIS Neutron and Muon Source, Didcot, United Kingdom

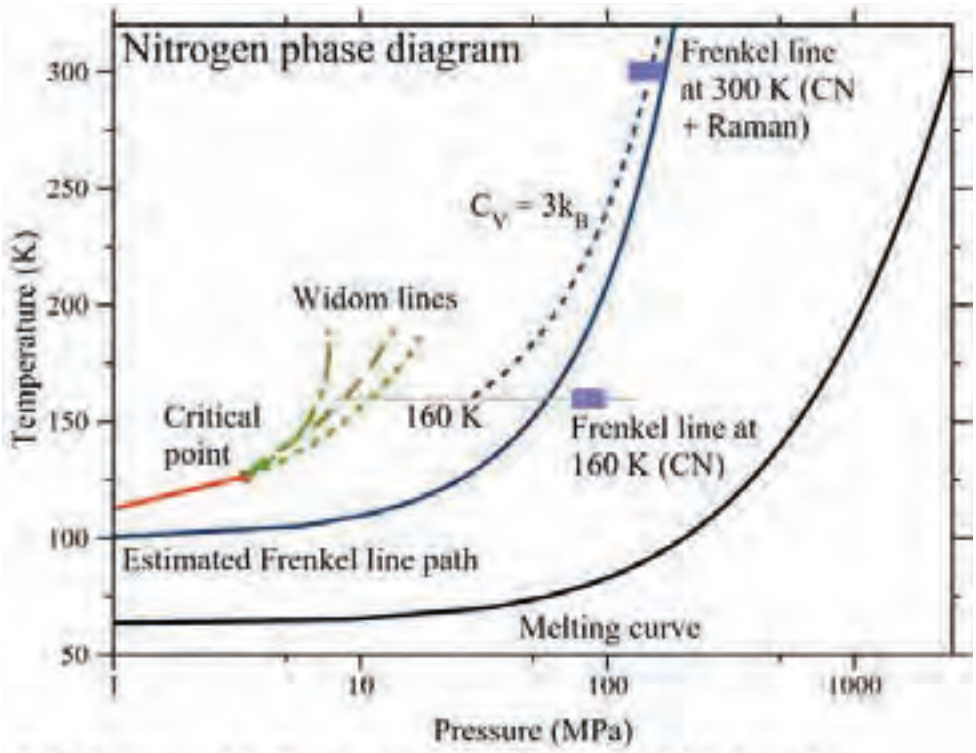
Phase Diagrams – Molecular Systems, July 27, 2023, 14:00–16:00

We have performed neutron scattering experiments on supercritical fluid Nitrogen (N2) at 300 K (2.4 T_C) and 160 K (1.3 T_C), backed up by ab initio molecular dynamics simulations at 300 K. Very recently, we have performed Raman scattering from 300 K to 400 K and are currently extending our neutron scattering investigations to 90 K (0.7 T_C) to compare with recent computational predictions that the Frenkel line extends to the triple point [1].

We have been able to reliably characterise the Frenkel line in nitrogen using both diffraction (neutron scattering) and spectroscopy methods for the same substance, backed up by simulation, and obtain a broad overview of what parameters change, and what parameters do not change, when the Frenkel line is crossed. Furthermore, we have established characterization of the Frenkel line over a far wider temperature range than previously achieved and that characterization of the Frenkel line position via diffraction and spectroscopy methods yield findings that are – at least roughly – in agreement.

Finally, our investigation includes the temperature regime in which both the Widom lines and the Frenkel line are present. We find that behaviour of nitrogen remains gas-like until the Frenkel line is crossed, and our data support the hypothesis that the Widom line transitions are driven by density increase.

[1] C.G. Pruteanu et al., J. Phys. Chem. Lett. 12, 11609 (2021).



C.G. Pruteanu, J.E. Proctor, O.L.G. Alderman and J.S. Loveday
J. Phys. Chem. B **125**, 8902 (2021).

New studies on high pressure methane and ethane up to 150 GPa

Dr Loïc Toraille[1,2], Gunnar Weck[1,2], Gaston Garbarino[3], Paul Loubeyre[1,2]
[1]CEA DAM DIF, F-91297 Arpajon, France, [2]Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, 91680 Bruyères-le-Châtel, France, [3]European Synchrotron Radiation Facility, 71, avenue des Martyrs, CS 40220 , 38043 Grenoble, France

Phase Diagrams – Molecular Systems, July 27, 2023, 14:00–16:00

The characterization of the physico-chemical properties of the C-H system under high-pressure and high-temperature is of great importance in many fields such as organic, bio and petroleum chemistry as well as in planetary science.

Surprisingly little is known about high-pressure methane (CH_4) and ethane (C_2H_6), with only a few studies mainly based on X-ray diffraction [1,2,3] (XRD) and Raman spectroscopy [2,4], often with contradictory conclusions. Depending on the compression history of CH_4, it appears that different high-pressure phases named pre-B and B can be attained. As for C_2H_6, various phase transitions reportedly witnessed with Raman spectroscopy have not been observed through XRD.

We realised numerous high-pressure experiments with varying parameters in order to successfully produce either B or pre-B CH_4, even simultaneously in one case, and were able to obtain reliable crystal structures for both phases as well as their full Raman signatures. These results give us a better understanding of the relative phase stabilities of high-pressure CH_4.

By coupling single-crystal XRD with Raman spectroscopy, Infrared absorption and ab initio calculations up to 150~GPa, we determined precisely the structure, stability regions and vibration modes of two phases of solid C_2H_6. The Raman spectroscopy in particular reveals interesting phenomena.

[1] L. Sun et al., Chemical Physics Letters 473, 72-74 (2009).
[2] E. Stavrou, et al., The Journal of Chemical Physics 155, 184503 (2021).
[3] M. Podsiadlo et al., Cryst. Growth Des. 17, 228-232 (2017).
[4] L.Q. Read et al., J Raman Spectrosc. 51, 2311– 2317 (2020).

Deuteration-enhanced Negative Thermal Expansion and Negative Area Compressibility in a 3-Dimensional Hydrogen Bonded Network

Piotr Rejnhardt[1,2], Jan Zaręba[3], Andrzej Katrusiak[4], Marek Daszkiewicz[2]
[1]Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warszawa, Poland, Warsaw, Poland, [2]Division of Structure Research, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-422 Wrocław, Poland, Wrocław, Poland, [3]Advanced Materials Engineering and Modeling Group, Faculty of Chemistry, Wroclaw University of Science and Technol-ogy, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland, Wrocław, Poland, [4]Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland, Poznań, Poland

Chemical Bonding 2, July 24, 2023, 16:30–18:30

Negative area compressibility (NAC) and negative thermal expansion (NTE) are material behaviours raising high hopes for applications such as ultrasensitive manometry and thermometry. However, the group of NAC materials is primarily limited to 2D coordination compounds whose layered structure is prone to the bidirectional compression upon pressure . Here we report an alternative strategy that does not employ formation of metal-organic systems but takes advantage of the pliability of hydrogen-bonded networks for searching materials with very rare NLC and NAC behaviours. Indeed, strong NAC property, coupled with large NTE, has been identified for the hydrogen-bonded hydrochloride salt of L-arginine homologue ((S)-2-amino-3-guanidinopropanoic acid monochloride – (HAmGP)Cl and its deuterated analogue – (DAmGP)Cl. While both structures feature isosymmetric phase transition at ca. 0.88 GPa it is discovered that the re-placement of protium with deuterium significantly boosts NAC magnitudes: phase II of (DAmGP)Cl features over two-fold higher negative area compressibility coefficient than that of nondeuterated analogue ($\beta_{2,3}$ = -17.6(27) TPa-1 for (DAmGP)Cl vs. -7.9(38) TPa-1 for (HAmGP)Cl)). What is more, deuteration enhances also NTE property (α_2 = -23.4(22) MK-1 vs. -16.1(31) MK-1 for (DAmGP)Cl and (HAmGP)Cl, respectively) of the investigated supramolecular network. Our research opens new paths to preparation of organic hydrogen-bonded materials with unique mechanical responsiveness to temperature and pressure stimuli.

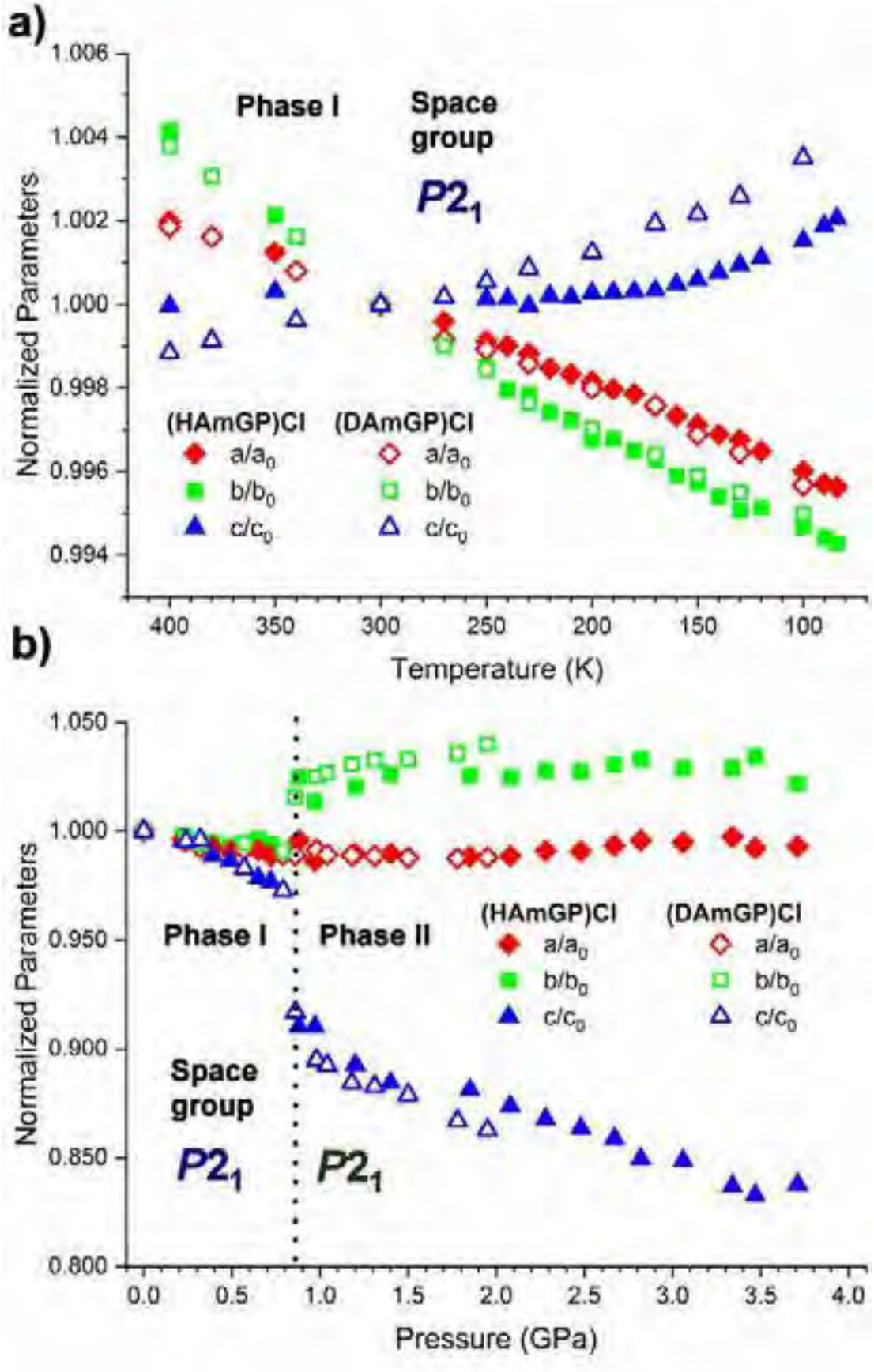


Figure caption: Relative thermal expansion (a) and compression (b) of lattice parameters a, b and c for (HAmGP)Cl (full symbols) and (DAmGP)Cl (open symbols).

Pressure tuning and Evolution of Structural, Magnetic and Electronic Properties in TMPX3 van-der-Waals Compounds

Shiyu Deng[1], Dr. Matthew J. Coak[1,2], Dr. Charles R. S. Haines[1,3], Dr. Hayrullo Hamidov[1,4], Dr. David M. Jarvis[1], Dr. Andrew Wildes[5], Cheng Liu[1], Dr. Emilio Artacho[1,6], Dr. Siddharth S. Saxena[1]

[1]University of Cambridge, Cambridge, United Kingdom, [2]University College London, London, United Kingdom, [3]University of East Anglia, Norwich, United Kingdom, [4]Navoi State University of Mining and Technologies, Navoiy, Uzbekistan, [5]Institut Laue-Langevin, Grenoble, France, [6]CIC Nanogune BRTA and DIPC, San Sebastian, Spain

Magnetic Materials 1, July 24, 2023, 10:15–12:15

Control of dimensionality in condensed matter continues to reveal novel quantum phenomena and effects. Transition metal phosphorous trichalcogenides $TMPX_3$ (TM = Mn, Fe, Ni, V, etc., X = S, Se) have proven to be ideal examples where structural, magnetic and electronic properties evolve into novel states when their dimensionality is tuned with pressure. At ambient pressure, they are two-dimensional van-der-Waals antiferromagnets with strongly correlated physics. Our recent experimental studies [1-4] have shown dimensionality crossover related pressure-induced insulator-to-metal transitions and novel magnetic phases in $FePS_3$. To elucidate the relationship between structural transitions, magnetism and electronic properties, we also performed a random structure search using first-principles calculations at high pressures and DFT+U studies [5]. We experimentally explored the coexistence of the low- and intermediate-pressure phases, and we predict a novel high-pressure phase with distinctive dimensionality and possible options for interpreting origins of metallicity.

We will also present our most recent single-crystal high-pressure X-ray study of $FePSe_3$, a similar compound to $FePS_3$ with reported high-pressure induced superconductivity occurring at 2.5 K and 9.0 GPa [6]. This new work on single crystal samples performed at the DIAMOND light source, finally provides clear crystallographic assignments related to phases which emerge with the application of pressure.

[1] C. R. S. Haines, et al., Phys. Rev. Lett., 121, 266801 (2018).
[2] M. J. Coak, et al., J. Phys. Condens. Matter, 32, 124003 (2020).
[3] M. J. Coak, et al., Phys. Rev. X, 11, 011024 (2021).
[4] D. M. Jarvis, et al., Phys. Rev. B, 107, 54106 (2023).
[5] S. Deng, et al., arXiv preprint: 2209.05353v5 (2023).
[6] Y. Wang, et al., Nat. Commun. 9, 1914 (2018).

Synchrotron spectroscopies for the study of electronic and magnetic transitions under high pressure at HPCAT

Yuming Xiao[1], Paul Chow[1], Eric Rod[1], Curtis Kenney-Benson[1], Richard Ferry[1], Arunkumar Bommannavar[1], Maddury Somayazulu[1], Nenad Velisavljevic[1,2]
[1]HPCAT, X-ray Science Division, Argonne National Laboratory, Argonne, United States, [2]Physics Division, Lawrence Livermore National Laboratory, Livermore, United States

Electronic Transitions 2, July 25, 2023, 14:00–16:00

Electronic and magnetic transitions under high pressure play a critical role in our understanding of the behaviour of materials and their properties. The 16ID-D beamline of the High-Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source (APS) is dedicated to high pressure research using spectroscopic techniques specifically for samples in diamond anvil cells. The beamline provides X-rays in the range of 4.5-37 keV with focus size ~4μ(V) x 6μ(H) FWHM. [1]

XES has been widely used to study pressure-induced spin transitions of materials by measuring satellite peaks of the Kβ1,3 line of 3d transition metals and the Lγ1 line of 4f elements. [2] The XES spectrometer at HPCAT consists of up to seven 4-inch spherically bent Si analysers and a Pilatus 100K detector. Combined with HP XRD, Wang et al. have used HP XES to study the pressure-induced spin transition and Jahn-Teller distortion in MnTe. [3] High energy resolution fluorescence detection X-ray absorption (HERFD-XAS) has been used to study valence change of Eu-based magnetic topological materials under high pressure. [4]

HPCAT has an IXS spectrometer for the study of electronic excitations at low momentum transfer and core-electron excitations (X-ray Raman scattering) at larger scattering angles with ~1.4 eV energy resolution. A full polycapillary lens is used as post-sample collimation to increase signal-to-noise ratio for HP experiments. [5] XRS experiments above Mbar have been routinely done at 16ID-D since the world's first XRS result over a Mbar was reported in 2018 from HPCAT. [6-7]

Synchronised with the APS upgrade to a new diffraction-limited storage ring, HPCAT will undergo a significant upgrade. A new revolver undulator, a HDCM and a HDMM will be installed for the 16ID-D/E beamline. Flux from the undulator will be increased by ~5-10 times depending on X-ray energy. The HDMM will provide ~2 orders of magnitude flux increase due to the wider bandpass, which makes time-resolved non-resonant XES possible with the proposed von Hamos XES spectrometer upgrade at 16ID-D. Low temperature IXS under high pressure to study dynamics of materials such as metal hydrides will become possible with a proposed cryostat compatible with polycapillary IXS setup.

This work is performed at HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA's Office of Experimental Sciences. The Advanced Photon Source is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

[1] Bommannavar et al. (2022). Phys. Chem. Minerals. 49:36.
[2] Xiao et al. (2016) High Pressure Res., 36, 315-331.
[3] Wang et al. (2022) Chem. Mater. 34, 3931.
[4] Bi et al. (2022) npj Quantum Mater, 7, 43
[5] Chow et al. (2015) Rev. Sci. Instrum. 86,072203.
[6] Lee et al. (2018) Proc. Natl. Acad. Sci. USA. 115, 5855.
[7] Kim et al. (2022) J. Am. Chem. Soc. 144, 10025.

Mesoscale mechanisms of the isostructural phase transition in Cerium.

Laura Henry[1,2,3], Nicolas Bruzy[2,3], Robin Fréville[2,3], Christophe Denoual[2,3], Eglantine Boulard[4], Andrew King[1], Nicolas Guignot[1], Bernard Amadon[2,3], Agnès Dewaele[2,3]
[1]Synchrotron Soleil, Les Ulis, France, [2]CEA DAM/DIF, Bruyères le châtel, France, [3]Laboratoire Matière en Conditions Extrêmes (LMCE), Orsay, France, [4]IMPMC, Sorbonne Université, Paris, France

Static Studies of Elements 1, July 25, 2023, 14:00–16:00

Cerium with [Xe]4f26s2 electronic structure is a light rare Earth element, the most abundant in the Earth's crust. It exhibits an unusual polymorphism with giant volume change under extreme conditions. Under ambient conditions, cerium crystallises in a cubic face centred (fcc) gamma-Ce structure. At 8 kbar and room temperature, gamma-Ce transforms into alpha-Ce, another fcc structure with a density greater by 18%. Alpha-Ce exhibits a higher thermal expansion coefficient than gamma-Ce such that their volumes converge with temperature, giving rise to a solid-solid critical point (SSCP). It is the only example of isostructural solid-solid transition and existence of a SSCP in an element. While the exact driving force of the gamma-alpha transition has been debated since 1950, it is acknowledged that 4f electrons are localised in gamma-Ce and in an itinerant metallic state in alpha-Ce. Higher bonding in the metallic state results in the large volume collapse at the transition. In situ XRD measurements have shown that gamma and alpha phases exhibit the exact same orientation [1] and ab initio modelling have emphasised the role of electronic entropy in the transformation [2]. Even though, the alpha-gamma transformation remains an enigma at the mesoscale. How does the microstructure adapt to the volume decrease at the transition, and at which cost?

We have performed fast X-ray Computed Tomography (XCT) and Energy-Dispersive X-Ray Diffraction (ED-XRD) at high pressure and temperature at the PSICHÉ beamline in SOLEIL. The combined approach has been used to unveil the mechanisms of the gamma-alpha isostructural phase transition under different loading conditions below and above the critical point, in Paris-Edinburgh Press modified for XCT measurements (UToPEc).

In situ XCT on large crystals of cerium have revealed the microstructure induced by the transition, with the apparition of large platelets, characteristic of displacive (martensitic) phase transitions. Parent and daughter crystals have identical orientations as revealed by ED-XRD and their plane of coexistence has an orientation close to (100) direction. The low strain evidenced with ED-XRD suggests a surprisingly high dislocation mobility for the scanned temperature regime. We followed the growth of the platelets: it is faster for smaller density difference between alpha and gamma phases but is also affected by the history of the sample, suggesting a multi-scale mechanism for this fascinating transformation. Based on continuum mechanics modelling and ab initio calculations, we propose a mechanism initiated by elastic instabilities in the <100> directions.

[1] F Decremps, L Belhadi, DL Farber, KT Moore, F Occelli, Melanie Gauthier, A Polian, D Antonangeli, CM Aracne-Ruddle, and B Amadon. Diffusionless γ α phase transition in polycrystalline and single- crystal cerium. Physical review letters, 106(6):065701, 2011.
[2] B Amadon, S Biermann, A Georges, and F Aryasetiawan. The α- γ transition of cerium is entropy driven. Physical review letters, 96(6):066402, 2006.

High-pressure photoluminescence study of monolayer TMDs: an extensive investigation of the role of defects induced by sample/substrate interaction

Beatrice D'Alò[1], Elena Stellino[2], Mattia Capeccia[1], Elena Blundo[1], Antonio Polimeni[1], Paolo Postorino[1]

[1]Physics Department, Sapienza University of Rome, Rome, Italy, [2]Department of Physics and Geology, Perugia University , Perugia, Italy

Nanoscale Systems, July 24, 2023, 16:30–18:30

Two-dimensional Transition Metal Dichalcogenides (TMDs) have gained considerable attention in the scientific community as potential candidates for developing 2D electronic and optoelectronic devices. Moreover, they serve as an interesting platform to investigate the effects of dimensionality on electronic properties.

TMDs bulk crystals consist of an array of covalently bonded single layers coupled through weak van der Waals (vdW) forces. These crystals can be easily exfoliated into few-layer (FL) and even single-layer (1L) flakes. Despite the weak nature of the inter-layer interaction, it plays a key role in determining the electronic properties of TMDs. Thinning TMDs down to FL-crystals reduces vdW interactions, ultimately leading to an indirect-to-direct bandgap transition in the 1L-crystal [1]. The application of high-pressure (HP) using diamond anvil cells (DACs) represents a unique tool to enhance inter-layer interactions and tune TMDs electronic properties [2]. Compressed TMDs can be then studied using photoluminescence (PL) spectroscopy: a local, non-invasive technique able to give precious insights into the main optical transitions of the samples.

However, the same inter-layer interactions which tune the electronic band structure cause a high sensitivity of the TMDs to their substrates: the latter induce defects and strain in FL-TMDs [3], further enhanced when pressure is applied. As a consequence, the PL signal dramatically decreases as pressure increases and a trion contribution due to defect states appears and dominates the high-pressure spectra. All these factors prevent a comprehensive knowledge of the high-pressure evolution of the electronic structure of FL-TMDs, giving rise to diverse interpretations in literature.

Here we report a study of defect contribution in the PL spectra of different TMDs performing HP experiments on 1L-crystals in two different conditions. In one case, we compressed 1L-TMDs exfoliated on the culet of a DAC, hence directly exposed to the formation of defects. In the other case, we applied pressure on 1L-TMDs encapsulated with hexagonal boron nitride (hBN), which proved to preserve the crystal quality of graphene and graphene-like materials in ambient conditions [3].

The encapsulation of 1L-TMDs resulted in a successful method to protect the samples from defects formation in the HP regime: thanks to this process, we were able to measure the PL signal of 1L-TMDs in uncharted pressure values. Moreover, studying the trion contributions to the PL, we could directly assess the effects of hBN-encapsulation on defects formation: the rate of pressure-induced defect creation was strongly diminished in encapsulated 1L-TMDs, in contraposition to their bare counterparts, where defects grow rapidly as pressure increases.

Our experiments provide a simple way to control defect formation in the HP regime. Compressing hBN-encapsulated 1L-TMDs, we could decouple the effects of defect creation from the evolution of the band structure of TMDs, shedding new light on the possibility to fine-tune the electronic structure of TMDs by pressure application and allowing for the PL investigation of the band structure at high pressure.

[1] L. Zhang et al., Nano Lett. 2015, 15, 2, 949–957
[2] AP. Nayak et al., Nat Commun. 2014, 5, 3731
[3] D.Rhodes et al., Nat Materials 2019, 18, 541–549

Diamond Nanothreads: Controlling Solid-State Reactivity via Reaction-Directing Heteroatoms

Dr. Samuel Dunning[1], Bo Chen[2,3], Li Zhu[4], George Cody[1], Wan Si Tang[1], Sebastiano Romi[1], Anirudh Hari[1], Dongzhou Zhang[5], Stella Chariton[6], Vitali Prakapenka[6], Maddury Somayazulu[7], Timothy Strobel[1]

[1]Carnegie Institution For Science, Washington, United States, [2]Donostia International Physics Center, Donostia San Sebastian, Spain, [3]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain, [4]Physics Department, Rutgers University-Newark, Newark, United States, [5]Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, Honolulu, United States, [6]Center for Advanced Radiation Sources, The University of Chicago, Chicago, United States, [7]X-ray Science Division, Argonne National Laboratory, Lemont, United States

Chemical Bonding 2, July 24, 2023, 16:30–18:30

High-pressure, solid-state organic synthesis can provide access to novel reaction pathways and has been shown to produce materials with bonding environments and structural motifs that are difficult or impossible to obtain through solution-phase reactions.[1] However, generalised synthetic control of these high-pressure reactions is difficult due to limitations such as geometrical/steric constraints, crystal packing, high-pressure phase changes, and multiple energetically competitive pathways. Diamond nanothreads are an emerging class of one-dimensional, crystalline carbon nanomaterials synthesised from small unsaturated ring systems (e.g., benzene[1]) that provide a unique platform to systematically study the reactivity of small molecules at pressure.

Nanothreads are typically synthesised through a series of high-pressure, solid-state [4 + 2] Diels-Alder cycloaddition reactions along the molecular stacking axis to produce polymers containing an extended sp3 carbon core. These diamond-like materials are predicted to combine the flexibility of conventional polymers with the superlative properties of diamond and several synthetic strategies have now been developed to promote nanothread formation.[2] However, as several reaction pathways are typically viable at the pressures required for nanothread synthesis reactions often result in the formation of chemically inhomogeneous products with inconsistent chemical bonding. This issue is compounded for precursors that contain pendant functional groups that can partake in additional side reactions. For nanothreads to reach their potential and find use in advanced applications, it is imperative that synthetic strategies are developed that provide improved control over C-C bond forming reactions at pressure and allow us to produce highly ordered, functionalised materials for which the structures, properties, and reactivity can be accurately determined.

Here we highlight our work on the formation of chemically homogeneous nanothread polymers from aromatic heterocyclic compounds.[3] The incorporation of less reactive “thread directing” heteroatoms limits the number of available reaction pathways to a carbon-exclusive cycloaddition reaction, allowing us to synthesise chemically homogeneous nanothreads. We will discuss the complex role that the type, extent, and relative position of heteroatom incorporation plays in the formation of nanothreads from heterocyclic compounds. We will also discuss the impact of heteroatom functionality and intermolecular forces (e.g., H-bonding) on the reactivity of precursors with pendant functionality. A particular focus will be placed on our efforts to lower reaction onset pressures, synthesise nanothreads which retain functionality, and our successes in the formation of carboxylate (-COOH) rich nanothread polymers.

[1] T. C. Fitzgibbons, M. Guthrie, E.-S. Xu, V. H. Crespi, S. K. Davidowski, G. D. Cody, N. Alem, J. V. Badding, Nature Materials 2015, 14, 43-47.

[2] a) M. D. Ward, W. S. Tang, L. Zhu, D. Popov, G. D. Cody, T. A. Strobel, Macromolecules 2019, 52, 7557-7563; b) W. S. Tang, T. A. Strobel, Journal of Physical Chemistry C 2020, 124, 25062-25070.

[3] a) S. G. Dunning, L. Zhu, B. Chen, S. Chariton, V. B. Prakapenka, M. Somayazulu, T. A. Strobel, Journal of the American Chemical Society 2022, 144, 2073-2078; b) S. G. Dunning, B. Chen, L. Zhu, G. D. Cody, S. Chariton, V. B. Prakapenka, D. Zhang, T. A. Strobel, Angewandte Chemie International Edition 2023, e202217023.

X-ray imaging of silicon under shock-compression at the LCLS: direct visualization of high-pressure phase nucleation and multi-wave kinetics

Silvia Pandolfi[1,2], Arianna Gleason[2], Thomas Hatcher[2], Daniel S Hodge[3], Hae Ja Lee[2], Dimitri Khaghani[2], Eric Cunningham[2], Hai-En Tsai[2], Gilliss Dyer[2], Richard L Sandberg[3], Eric Galtier[2], Bob Nagler[2]

[1]IMPMC – Sorbonne Université, Paris, France, [2]SLAC National Accelerator Laboratory , Menlo Park, USA, [3]Brigham Young University, Provo, United States

Instrumentation and Techniques 3, July 26, 2023, 14:00–16:00

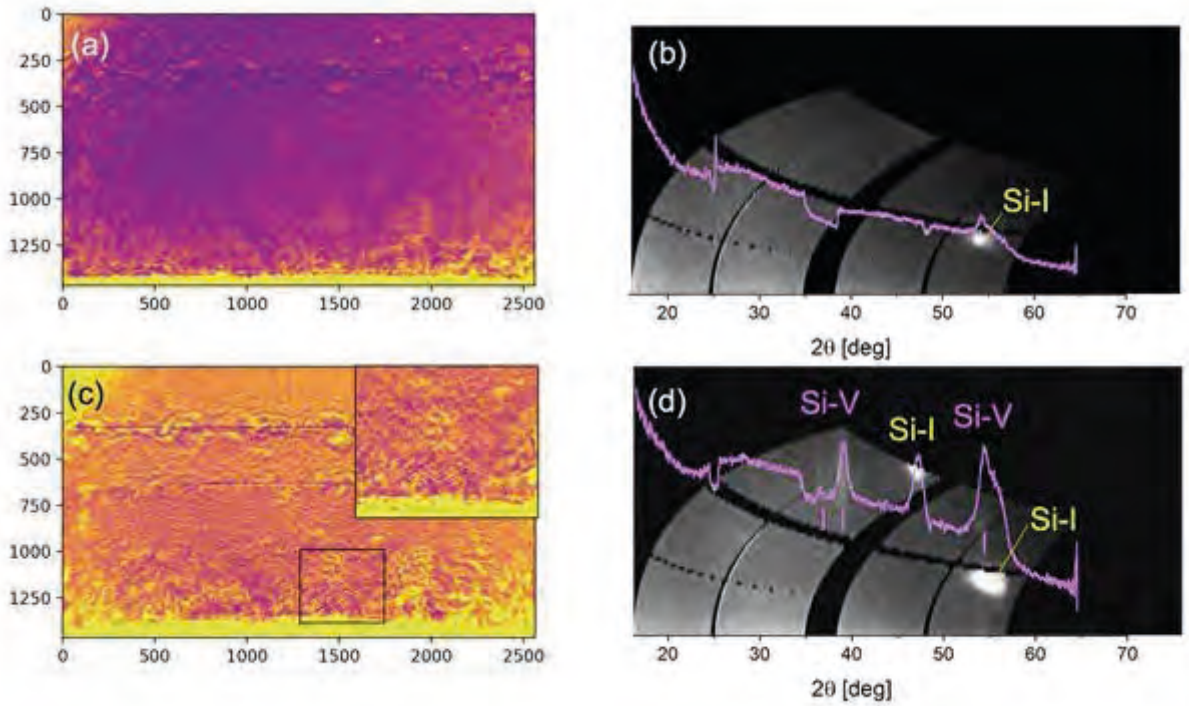
We report the first results from a new X-ray imaging diagnostic at the Matter in Extreme Conditions endstation at the Linac Cohorent Light Source and new insight on the behaviour of silicon (Si) under laser-driven shock-compression.

The multi-wave response of Si to shock loading has been debated for decades, and our recent study has demonstrated the lack of conventional plasticity using X-ray diffraction (XRD) [1]. Here, we combine XRD and X-ray imaging to visualise for the first time the growth of the high-pressure phase in situ. With the high spatial (<600nm) and temporal (<100ps) resolution of our setup, we can resolve the kinetics of Si deformation at the relevant timescales and length-scales. We show the emergence of the intermediate elastic feature previously reported and its link with the phase transitions [2], and we observe the nucleation and growth of the high-pressure phases. Interestingly, the high-pressure phase grows preferentially in a banding structure that had been predicted by MD simulations but never recorded during a shock before [3].

With these results, we demonstrate the capability of the new X-ray imaging setup at the LCLS to provide detailed information on the macroscopic and microscopic behaviour of materials under shock-compression over ultrafast (ns) timescales.

*Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515. The MEC instrument is supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences under contract No. DE-AC02-76SF00515.

[1] S. Pandolfi, et al, Nat Commun 13, 5535 (2022).
[2] S. B. Brown, et al, Sci Adv 5, eaau8044 (2019).
[3] G. Mogni, et al, Phys Rev B 89, 064104 (2014).


(a)
(b)
(c)
(d)
Si-I
Si-V
Si-I
Si-V
Si-I
2θ [deg]
2θ [deg]

Proton transfer reaction in 4,4’-bipyridine malonic acid cocrystal under pressure

Ewa Patyk-Kaźmierczak[1], Fernando Izquierdo-Ruiz[2], Alvaro Lobato[2], Michał Kaźmierczak[1], Ida Moszczyńska[1], Anna Olejniczak[1], J. Manuel Recio[3]

[1]Faculty of Chemistry, Adam Mickiewicz University In Poznań, Poznań, Poland, [2]MALTA-Consolider Team and Departamento de Química Física, University Complutense of Madrid, Madrid, Spain, [3]MALTA-Consolider Team and Departamento de Química Física y Analítica, University of Oviedo, Oviedo, Spain

Other Molecular Systems, July 27, 2023, 10:15–12:15

The solid-state chemical reactions in crystals offer noticeable advantages from the sustainability and selectivity points of view.[1] Arranging the substrates in a crystalline lattice in a predefined manner allows to steer the process in desirable direction via topochemical reactions.[2] Among stimuli known to induce such reactions, next to temperature and UV light, is high pressure. Previous reports show that compression can lead to polymerization or to proton transfer reactions.[3,4] The last type of chemical transformation is especially interesting in the context of crystals of APIs (Active Pharmaceutical Ingredients). Since cocrystals and salts can differ in terms of solubility and bioavailability,[5] the transition between the two forms can affect the performance of the final drug product. Herein, we present results of a high-pressure study of 4,4’-bipyridine and malonic acid (BIPYMA) cocrystal, aimed at inducing a proton transfer reaction in the crystal. A single crystal of BIPYMA was compressed isothermally, using Daphne 7575 oil as hydrostatic medium up to 3.10(2) GPa and measured using a 4-circle X-ray diffractometer.

Experiments were carried out using one20DAC from Almax EasyLab, with an effective opening angle of 112°, to improve the completeness of the high-pressure X-ray diffraction data. Crystal structure results are supported by high-pressure Raman spectroscopy and DFT calculations.

At pressure of ca. 3 GPa a proton transfer reaction occurs in crystals of BIPYMA. The transformation from cocrystal to salt is accompanied by the change in the symmetry of the crystal. Initially, both molecules, 4,4’-bipyridine and malonic acid, are placed in special positions, and only half of each molecule comprise the asymmetric part of the unit cell. After the transition, the symmetry is broken, which lowers the crystal symmetry from C2/c to $P2_1/c$. The proton transfer is evidenced by the shift of the Raman frequencies above 2.9 GPa, visible in the experimental and calculated Raman spectra. Analysis of the structural changes induced by the proton transfer, including alterations in the molecular geometry and aggregation, as well as the calculation of the energy barrier for the proton transfer, is presented.

Acknowledgements: This study was financed by the National Science Centre Poland, grant number 2020/39/D/ST4/00260.

Financial support from Spanish PID2021-122585NB-C21-2 AEI project and Principado de Asturias-FEDER under project AYUD/2021/51036 is gratefully acknowledged.

[1] Braga, D.; Grepioni, F. Reactions Between or Within Molecular Crystals. Angew. Chem., Int. Ed. 2004, 43, 4002– 4011, DOI: 10.1002/anie.200301721

[2] Biradha, K.; Santra, R. Crystal Engineering of Topochemical Solid State Reactions. Chem. Soc. Rev. 2013, 42, 950– 967, DOI: 10.1039/C2CS35343A

[3] Li, F.; Xu, J.; Wang, Y.; Zheng, H.; Li, K. Pressure-Induced Polymerization: Addition and Condensation Reactions. Molecules. 2021, 26(24), 7581. DOI: 10.3390/molecules26247581

[4] Casati, N.; Macchi, P.; Sironi, A. Hydrogen migration in oxalic acid di-hydrate at high pressure? Chem. Commun. 2009, 19, 2679 —2681, DOI: 10.1039/B823458B

[5] Cavanagh, K.L.; Maheshwari, C.; Rodríguez-Hornedo, N. Understanding the Differences Between Cocrystal and Salt Aqueous Solubilities. J Pharm Sci. 2018, 107, 113-120. DOI: 10.1016/j.xphs.2017.10.033.

Density driven changes in electronic properties of the binary M(IV) oxides (M=Sn, Ge, Ru)

Dr. Keith Lawler[1]
[1]*University Of Nevada, Las Vegas, Las Vegas, United States*

Electronic Transitions 1, July 26, 2023, 16:30–18:30

Density driven tailoring of a material's electronic properties is emerging as a powerful means for functional materials design. The binary metal(IV) oxides offer a rich polymorphism as function of both temperature and pressure, with many of the materials sharing similar pathways in their pressure dependent phase progression, in particular a rutile to CaCl2 phase transition. In SnO2, an anomalous increase in conductivity was observed at pressures just below that of the CaCl2 phase transition.[1] Through a combination of X-ray diffraction, Raman spectroscopy, EXAFS, and DFT it was found that the most likely mechanism for this is disordering of the oxygen sub-lattice owing to the softening of the B1g mode that drives the rutile to CaCl2 second-order phase transition. X-ray diffraction, Raman spectroscopy and EXAFS measurements confirm a similar disordering of the oxygen sublattice across the rutile to CaCl2 phase transition in GeO2.[2] DFT simulations on GeO2 indicate that the proposed disordering mechanism leads to small polaron formation which causes the change in electronic properties across the rutile to CaCl2 phase transition. Slight but measurable changes in conductance and MSRD are observed preceding the rutile to CaCl2 transition in RuO2, however a low-temperature metal-insulator transition is seen to occur above 27 GPa. This transition to an insulative state is irreversible upon warming to room temperature and is accompanied by a significant drop in pressure, suggesting the electronic transition is due to a strong structural distortion that we propose is linked to a first-order phase transition. DFT indicates this is the long sought-after fluorite-type (Fm-3m) phase of RuO2.

[1] D. Smith et al., J. Phys. Chem. Lett. 10, 5351-5356 (2019).
[2] G. A. Smith et al., Phys. Rev. B 104, 134107 (2021).

Effect of carbon on sound velocities of iron alloys and compounds at Earth's inner core conditions

Susanne Müller[1], Efim Kolesnikov[2], Xiang Li[1,2], Georgios Aprilis[1], Aleksandr Chumakov[1], Mohamed Mezouar[1], Ilya Sergeev[3], Lélia Libon[4], Wolfgang Morgenroth[4], Arno Rohrbach[2], Jasper Berndt[2], Max Wilke[4], Carmen Sanchez-Valle[2], Ilya Kupenko[1]

[1]ESRF – European Synchrotron Radiation Facility, Grenoble, France, [2]Institut für Mineralogie, Westfälische Wilhelms-Universität, Münster, Germany, [3]DESY – Deutsches Elektronen Synchrotron , Hamburg, Germany, [4]Institut für Geowissenschaften, University of Potsdam, Potsdam, Germany

Cores of Terrestrial Planets, July 24, 2023, 14:00–16:00

In order to understand the formation, evolution, and dynamics of the core of the Earth and other terrestrial planets, its composition is crucial. However, the exact constitution of the Earth's core remains enigmatic to date. It is known that the main components of the inner core are iron and nickel, but the comparison of densities and seismic velocities between pure Fe-Ni alloys and seismological models reveals a density deficit and reduced velocities in the core. These observations can be explained by the addition of 3-7 wt% light elements to Fe-Ni alloys, with the most probable candidates being H, C, O, Si, and S [1].

Metal/silicate partitioning behaviour, the high cosmochemical abundance and the isotopic signature make carbon a promising main light element in the Earth's core [2,3]. More importantly, Fe-C-alloys are able to explain the low shear wave velocity and the high Poisson ratio in the Earth's inner core [4]. Phase relation experiments showed that the solubility of carbon in solid iron decreases with pressure and temperature. Therefore, if carbon is a dominant light element in the inner core and if the outer core contains more than 3 wt% carbon, the present Fe-C-phase in the inner core is most likely Fe7C3 [5].

In order to determine sound velocities of Fe7C3 we carried out nuclear inelastic scattering and X-ray diffraction experiments in diamond anvil cells at pressures up to 175 GPa and 2300 K. We used the data to calculate sound velocities at high pressures and temperatures and extrapolated them to inner core conditions. Here, we will present the results and discuss the availability of carbon in the Earth's inner core, as well as the effect of carbon on sound velocities of carbon-bearing iron alloys.

[1] K. Hirose et al. 2021, Nat. Rev. Earth. Environ. 2, 645-658
[2] R. Dasgupta et al. 2013, Geochim. Cosmochim. Acta 201, 191-212
[3] B. J. Wood et al. 2013, Reviews in Mineralogy and Geochemistry 75, 231-250
[4] C. Prescher et al. 2015, Nat. Geoscience 8, 220-223
[5] I. Mashino, et al. 2019, Earth Planet. Sci. Lett. 515, 135

Ramp EOS measurements through phase transitions in tin up to 10 Mbar

Richard Briggs[1], Suzanne Ali[1], Dave Braun[1], Damian Swift[1], Travis Volz[1], Peter Celliers[1], Martin Gorman[1], Jon Eggert[1], Earl O'Bannon[1], Ray Smith[1], Jim McNaney[1]
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Equation of Satate 1, July 26, 2023, 14:00–16:00

An equation of state (EOS) for a material is constrained through pressure and density measurements across a wide range. Static compression experiments under 'quasi-hydrostatic' conditions are typically used in combination with in-situ X-ray diffraction to determine the pressure-volume relationship of a material (room temperature isotherms). Pressure-volumes are fit with an appropriate EOS equation, e.g. Birch-Murnaghan or Vinet, with extrapolations to very high pressure often used to compare against shockwave or ramp derived data.

Tin is a material that undergoes several solid-solid phase transitions between 0 and 200 GPa at room temperature, with large regions of coexistence observed between phases. Consequently, the experimental data used to define the EOS for each phase covers a relatively small range. Ramp compression experiments are now a well-established technique to derive a room temperature isotherm from longitudinal stress measurements via velocimetry.

In this talk, I will present ramp compression data on Sn from the National Ignition Facility. A reduced isotherm determined from low adiabat (solid tin) ramp compression shows good agreement with experimental static compression data (that are corrected using a more up-to-date ruby pressure scale). The implications of adiabatic pathways that traverse the bcc to hcp phase transition in tin will be discussed. An update to the phase diagram, based on recently published experimental data, will also be compared against existing EOS models, alongside high adiabat ramp compression experiments on NIF that begin in the liquid phase.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Modulation technique for investigation of superconductivity by magnetic susceptibility

Sasanka Munasinghe[1]
[1]*University Of Rochester, Rochester, United States*

Instrumentation and Techniques 2, July 27, 2023, 10:15–12:15

Magnetic susceptibility measurements are one of the most powerful techniques for detecting superconductivity. However, as the sample size decreases, the experimental setup for testing materials under high pressure becomes more complex. Modern measurement instruments and an improved coil system using the double-frequency modulation technique have made it possible to reduce the complexity of the setup, increase the sensitivity of the measurements, and improve the signal-to-noise ratio over a broad temperature range. The improved method uses two sets of identically wounded coils, each set consisting of a primary coil and a secondary coil. An AC magnetic field is produced by the primary coil, and the secondary coil detects the resulting induced voltage. The primary coils of two sets are connected in series with the same polarity, while the secondary coils are connected in series but with the opposite polarity to reduce the background signal. The field produced by the primary coils is the result of a superposition of a high-frequency, low-amplitude excitation signal and a low-frequency, high-amplitude modulation signal. Superposition eliminates the requirement for a separate coil to generate the modulation field. The modulation signal is used to suppress the superconductivity near the transition temperature. It suppresses superconductivity twice per cycle of the modulation signal at or slightly below the transition temperature. This results in an amplitude-modulated signal near the transition temperature. The sideband of this modulation can be used to detect the superconducting transition of materials using a single lock-in amplifier in a dual reference mode. This improved double-frequency approach was tested on previously studied MgB2 and ErBa2Cu3O7 materials, and the results displayed a distinct response during the superconducting transition with a nearly constant background.

Quantum diamond magnetometry for high-pressure sensing

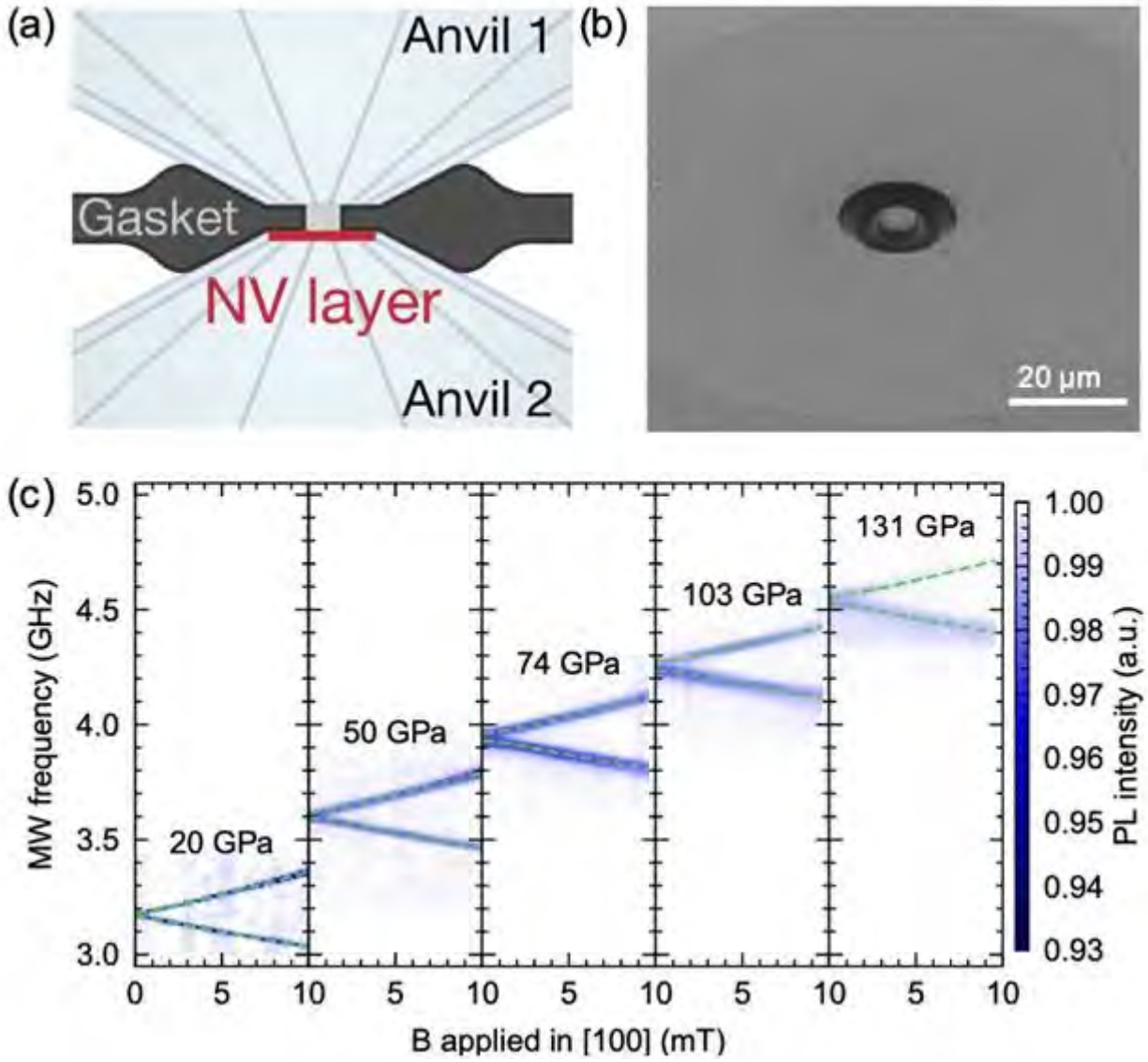
Antoine Hilberer[1], Loic Toraille[2], Cassandra Dailledouze[1], Liam Hanlon[1], MP Adam[1], Gunnar Weck[2], Martin Schmidt[1], Paul Loubeyre[2], **JF Roch**[1]
[1]Ens Paris-Saclay, Gif-sur-Yvette, France, [2]CEA, DAM, DIF, Bruyères-le-Châtel, France

Instrumentation and Techniques 2, July 27, 2023, 10:15–12:15

High-pressure magnetometry can be implemented using nitrogen-vacancy (NV) colour centres in diamond. These atomic-like quantum systems can be fabricated at the tip of diamond anvils using nitrogen ion implantation. Due to their spin properties, NV centres are highly sensitive magnetic probes, and their atomic size can allow for sub-micrometer spatial resolution. Using a customised optical microscope, we observe the spin dependent luminescence of NV centres, to perform a mapping of the magnetic field at the diamond anvil tip. Expulsion of magnetic field lines due to the Meissner effect in a superconductor leads to a decrease of the magnetic field amplitude in the close vicinity of the sample, where the NV sensors are located (1). This detection provides a direct and reproducible diagnosis of superconductivity that can be easily combined with synchrotron X-ray diffraction for structural characterization (2).

The challenge is to deploy this method at pressures above 100 GPa, in order for instance to probe the superconductivity of super-hydrides. All previous experiments reported a decrease of pressure of the NV sensitivity to the magnetic field, setting a practical limit at about 50 GPa. We found that this limit is due to the cupping of the diamond tip induced by the huge forces exerted on the anvils. The stress anisotropy then breaks the NV symmetry, and its magnetic sensitivity is blurred out. The sensitivity can be restored by ensuring hydrostatic compression. This regime can be obtained by milling a micropillar on the anvil tip. For the NV centers on the surface of the micropillar the Zeeman splitting created by an applied magnetic field is then the same at 130 GPa than at 20 GPa (3). This result significantly extends the pressure range where NV magnetic sensing and derived quantum sensing techniques can be efficiently implemented.

(1) M. Lesik, T. Plisson, L. Toraille, J. Renaud, F. Occelli, M. Schmidt, O. Salord, A. Delobbe, T. Debuisschert, L. Rondin, P. Loubeyre, and J.-F. Roch, Magnetic measurements on micrometer-sised samples under high pressure using designed nv centers. Science 366, 1359–1362 (2019).
(2) L. Toraille, A. Hilberer, T. Plisson, M. Lesik, M. Chipaux, B. Vindolet, C. Pépin, F. Occelli, M. Schmidt, T. Debuisschert, N. Guignot, J.-P. Itie, P. Loubeyre, and J.-F. Roch, Combined synchrotron X-ray diffraction and NV diamond magnetic microscopy measurements at high pressure, New J. Phys. 22, 103063 (2020).
(3) A. Hilberer, L. Toraille, C. Dailledouze, L. Hanlon, M.-P. Adam, G. Weck, M. Schmidt, P. Loubeyre, and J.-F. Roch, NV center magnetometry up to 130 GPa as if at ambient pressure, arXiv:2301.05094 (2023).


(a)
Anvil 1
Gasket
NV layer
Anvil 2
(b)
20 μm
(c)
MW frequency (GHz)
5.0
4.5
4.0
3.5
3.0
20 GPa
50 GPa
74 GPa
103 GPa
131 GPa
0
5
10
B applied in [100] (mT)
PL intensity (a.u.)
1.00
0.99
0.98
0.97
0.96
0.95
0.94
0.93

Effects of impurities and stacking fault energy on shock-induced phase changes in copper alloys

Travis Volz[1], Chris McGuire[1], Cara Vennari[1], Raymond Smith[1], Melissa Sims[2], June Wicks[2], Sally Tracy[3], Samantha Clarke[1], Richard Briggs[1], Jon Eggert[1], Andy Krygier[1]
[1]Lawrence Livermore National Laboratory, Livermore, United States, [2]Johns Hopkins University, Baltimore, United States, [3]Carnegie Institution for Science, Washington, United States

Phase Diagrams – Metals, July 27, 2023, 10:15–12:15

Recent publications suggest a relationship between stacking fault (SF) generation and the face-centred cubic (FCC) to body-centred cubic (BCC) phase transformation in shock-compressed noble metals. Metal alloying is well known to affect many material properties including stacking fault energy (SFE) and phase stability regions. To examine the effect of impurities on stacking fault generation and high-pressure phase boundaries, we performed laser-shock in situ X-ray diffraction (XRD) experiments on three copper alloys with SFEs between 10 and 90 mJ/m2. For the different Cu alloys (≥70% Cu), we found FCC to BCC transition stresses between ~130 and ~280 GPa, highlighting the large effect impurities can have on transition stress. Due to the observed linear relationship between SFE and FCC to BCC transition stress, for small impurity contents, we expect minimal phase boundary changes.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. (LLNL-ABS-846453)

Chemical thermodynamics of Earth's core materials under high pressure

Tetsuya Komabayashi[1,2], Samuel Thompson[1,2]
[1]School Of GeoSciences, University Of Edinburgh, Edinburgh, United Kingdom, [2]Centre for Science at Extreme Conditions, University Of Edinburgh, Edinburgh, United Kingdom

Cores of Terrestrial Planets, July 24, 2023, 14:00–16:00

Seismological, cosmochemical, and mineral physics studies indicate that the Earth's core is mainly composed of iron with some amounts of impurities to account for a 4–7% density deficit compared to pure iron at the relevant pressure (P) and temperature (T) conditions. Over 70 years since the first proposition by Birch (1952), the light impurities (light elements) in the core is yet to be determined even among a small number of candidate elements: Si, S, O, C, and H. Dissolution of light elements into an iron-rich core melt largely depends on how the core was formed 4.6 billion years ago and therefore, the identification of their kinds and amounts in the core will place constraints on the origin, formation, and evolution of the Earth.

One of the big hurdles towards constraining core composition is how one can examine the mixing properties of Fe-X liquids (X: Si, S, O, C, or H), while a conventional practice is assuming ideal mixing. The chemical thermodynamics for a core melt was poorly studied under core pressure. We have developed thermodynamic models which can be applicable to Earth's core P-T conditions in the systems, Fe, Fe-FeO, Fe-Si, and Fe-S. We first made high-P experiments in diamond anvil cells to determine key phase relations. Then, we assessed the equation of state of end-member liquids based on their melting P-T curves. We also evaluated their mixing properties by calculating eutectic points. From the Gibbs free energy, the crystallising point, density, seismic velocity, and isentrope of the outer core and the crystallising inner core phase will be uniquely determined by thermodynamics for a given outer core composition. The geophysically observable parameters (density and seismic velocity) can now be compared with those inferred from seismology and I will discuss the relevance of each system to the core.

Synthesis of Light-Element-Doped Lanthanum Superhydrides

Katsuya Shimizu[1], Seiji Matsumot[1], Natsumi Osaki[1], Misaki Sasaki[1], Mari Einaga[1], Yuki Nakamoto[1], Saori Kawaguchi[2], Naohisa Hirao[2], Yasuo Ohishi[2]
[1]KYOKUGEN, Osaka University, Toyonaka, Japan, [2]JASRI, Sayo, Japan

Hydrides 3, July 25, 2023, 14:00–16:00

Since the first report of high-temperature superconductivity in H3S [1], various hydrides have been investigated. Binary hydrides consisting of an element and hydrogen have been studied by exhaustive theoretical predictions and experimental verification. Among them, high-temperature superconducting transition temperatures (Tc) have been found in many rare-earth hydrides such as lanthanum hydride LaH10 was found to exhibit a transition temperature above 250 K at around 150 GPa [2,3]. However, superconductivity in these hydrides requires very high pressure exceeding 100 GPa, then high-Tc superconductivity at lower pressures is desired for future practical use. We have been studying light-element doping or substitution to rare-earth hydrides as a candidate material for such low-P and high-Tc superconductors. Here we focused on theoretical calculations[4] that LaBH8 is a superconductor at 138 K at about 70 GPa.

Lanthanum (La) and amorphous boron (B) were mixed and sealed in a diamond anvil cell together with ammonia borane (NH3BH3) as a hydrogen source. To prevent oxidation of La, mixing with B and sealing were performed in an Ar glove box. After sealing, the cell was pressurised to 100 GPa. The generated pressure was determined by the Raman edge of the diamond, and the electrical resistance of the sample was measured through a platinum electrode. The laser heating was performed simultaneously with powder XRD using focused X-rays at BL10XU in SPring-8. The electrical resistance was recorded during the heating process. There was a change in the XRD pattern at a certain laser power, but it did not match the theoretically predicted pattern of LaBH8 [4]. The diamond anvil cell was cooled down and a drop of the resistance was observed around 90 K, which is considered to be a superconducting transition. The transition temperature was found to increase to 100 K when the pressure was reduced to 93 GPa. This may indicate the additional boron element may act some effect on the transition temperature and pressure.

[1] A. P. Drozdov et al., Nature, 525, 73 (2015).
[2] M. Somayazulu et al., Phys. Rev. Lett., 122, 027001 (2018).
[3] A. P. Drozdov et al., Nature, 569, 528 (2019).
[4] Z. Zhang et al., Phys. Rev. Lett., 128, 047001 (2022).

Cobaltates as prospective Kitaev quantum spin liquids: atomic, electronic and magnetic responses of Na3Co2SbO6 under pressure

Mr. Eduardo Poldi[1,2], Dr. Gilberto Fabbris[2], Dr. Ravhi Kumar[1], Mr. Rodolfo Tartaglia[3], Dr. Dmitry Popov[2], Dr. Yan Wu[4], Mr. Nam Nguyen[1], Dr. Hyowon Park[1], Dr. H. Zheng[2], Dr. John Mitchell[2], Dr. Jiaqiang Yan[4], Dr. Russell Hemley[1], Dr. Daniel Haskel[2]

[1]University Of Illinois Chicago, Chicago, United States, [2]Argonne National Laboratory, Lemont, United States, [3]University of Campinas, Campinas, Brazil, [4]Oak Ridge National Laboratory, Oak Ridge, United States

Magnetic Materials 2, July 26, 2023, 14:00–16:00

The layered Na3Co2SbO6 compound features Co2+ ions in a trigonally distorted edge-shared O6-octahedra environment. The pseudospin-1/2 state of these ions in a honeycomb structure together with edge-shared octahedra introduces Kitaev interactions, that are predicted to be dominant in Na3Co2SbO6 if the trigonal splitting energy value Δ is reduced from about 40 meV to near zero. In this work we attempted to tune Δ by the means of isotropic compression in order to drive a transition from antiferromagnetically ordered to a disordered, quantum spin liquid phase. We conducted temperature-dependent X-ray diffraction, X-ray magnetic circular dichroism (XMCD), and X-ray Emission Spectroscopy (XES) experiments as a function of quasi-hydrostatic pressure in diamond anvil cells to explore the evolution of the atomic, electronic and magnetic structures of this cobaltate. Powder X-ray diffraction results indicate no phase transitions up to 100 GPa, and Co K-edge XMCD measurements show a decrease in the magnetic response, reaching the noise level at those pressures. Co Kβ XES data show a linear suppression of the Kβ' satellite peak from 50 to 90 GPa, in good agreement with our XMCD results. This suppression, although frequently associated with a high-spin to low-spin state transition, extends over a 40 GPa pressure interval. This observation suggests the existence of other phenomena such as changes in covalent bonding that could interfere with the spin 1/2 picture for Co atoms and cause a breakdown of the Kitaev description. We suggest that hydrostatic compression may be insufficient to drive frustration of the magnetic lattice of Na3Co2SbO6, and that the application of uniaxial strain in single crystalline samples might be needed to reach the postulated spin liquid phase.

Effects of light elements on the water partitioning between liquid metal and molten silicate under high pressure and temperature

Taku Tsuchiya[1]
[1]*Geodynamics Research Center, Japan*

Minerals Under High Pressure, July 24, 2023, 16:30–18:30

Metal/silicate water partitioning under high pressure is important to understand the water circulation in Earth's deep interior. Several studies have therefore been conducted both experimentally and theoretically. However, primarily due to the technical difficulty in quantitative analyses of hydrogen, the reported results scatter largely, such as some experiments showing siderophile behaviours of hydrogen under high pressure but some others lithophile behaviours. Recent theoretical studies suggest its siderophile behaviour, but an earlier one the opposite. Also, the theoretical studies assumed a simple molecular exchange reaction only and the stability of an experimentally suggested redox reaction has not been investigated. For this confused situation, we have started the ab initio free energy calculations of high-P,T hydrogen partition between liquid iron and molten silicate and reported some preliminary results in my previous talk of the last JpGU meeting that unlike the preconception, the exchange and redox reactions both could occur at high-P,T though hydrogen is basically siderophile. This means that oxygen is also partitioned into iron along with hydrogen. In this preliminary study, we have also examined the effects of oxidation state on the reactions and realised that the stability of exchange reaction strongly depends on the redox condition, indicating that the exchange reaction is more suppressed (hydrogen becomes lithophile under some particular conditions) and the redox reaction becomes more prominent when iron contains more oxygen atoms. These preliminary findings strongly suggest the hydrogen partition nature between liquid iron and molten silicate could be sensitive to the light element incorporation into iron, and therefore we have started to investigate the effects of other important light elements (Si and S) comprehensively. In this talk, we will present the currently obtained results and shed light on the nature of complicated hydrogen partition mechanisms between liquid iron and molten silicate under high P,T condition.

Field angle dependent magnetotransport properties of CrAs

Kai Ham Yu[1], Wei Zhang[1], King Yau Yip[1], Qun Niu[2], H. Sugawara[3], H. Kotegawa[3], Swee K. Goh[1]
[1]Department of Physics, The Chinese University of Hong Kong, Shatin, Hong Kong SAR, China, [2]High Magnetic Field Laboratory, HFIPS, Chinese Academy of Sciences (CAS), Hefei 230031, Anhui, China, [3]Department of Physics, Kobe University, Japan

Novel Superconductors 1, July 27, 2023, 10:15–12:15

CrAs is the first chromium-based superconductor with a helimagnetic transition at T_N ≃ 265 K at ambient pressure and pressure-induced superconductivity with a maximum Tc of 2.17 K at 10 kbar. The low-temperature magnetoresistance under pressure was reported to be quasilinear up to 14 T, which was attributed to a tiny Fermi pocket near the Y point of the Brillouin zone. To further explore the role of this Fermi pocket, we measure the magnetoresistance as a function of field angle in a diamond anvil cell down to 100 mK. We discuss the implication of our new data on the electronic structure of CrAs.

Continuous peak fit: a new algorithm for fitting spotty, noisy or incomplete X-ray diffraction data

Simon Hunt[1], Danielle Fenech
[1]*University Of Manchester, United Kingdom*

Instrumentation and Techniques 4, July 26, 2023, 16:30–18:30

X-ray diffraction patterns collected from samples under extreme conditions are often less ideal than those collected at ambient conditions: for example, they have higher backgrounds, lower and broader peak intensities. The relative quality of the diffraction patterns from high pressure means that much of the detailed information about the atomic and crystallographic level behaviour of materials contained in the diffraction patterns is discarded during data processing. This remains a factor despite significant improvements in detector technology which have expanded the potential resolution of diffraction measurements as well as the speed of data collection.

However, diffraction processing software has not kept pace with the advances in detector technologies, resulting in the interpretation of diffraction data being limited by the post-collection processing. This is especially true of measurements that are contingent on azimuthally dependent properties of the diffraction rings (e.g. differential strain, LPO, etc.). Processing of these properties is still undertaken by segmenting the diffraction data into segments (or cakes), down sampling the (x, y) detector space into an orthogonal (2θ, χ) and processing each segment separately. This approach has been encoded in many different software packages including Fit2D, MultiFit/Polydefix, [1,2]). However, further processing frequently assumes continuum properties (e.g. $\cos^2(2\theta)$ for differential strain [3]).

These data processing methods work well for ideal, well counted, clean data. However, for many studies at extreme conditions the data are formed of either very weak peaks, spotty peaks or highly overlapped peaks, for which the standard data processing methods are limited.

Here we present a new diffraction processing package: continuous peak fit. This package dispenses with the caking and resampling of the diffraction data. Instead, we use Fourier series or splines to describe the peak properties (d-spacing, intensity, width etc.) as a function of azimuth. This model is fit to the collected pixel intensity data, (2θ, χ, intensity) by least squares minimisation.

Testing on a sample data set shows the new approach returns significantly more precise differential strain values that enables the extraction of previously unresolvable time-dependent properties. Other samples show that consistent differential strains and LPOs can be extracted from significantly overlapping, very weak and spotty peaks.

[1] Hammersley, A. Fit2D, https://www.esrf.fr/computing/scientific/FIT2D/
[2] Merkel and Hilaret (2015) J. Appl. Cryst., 48, 1307–1313
[3] Singh et al (1998) J. Appl. Phys. 83, 7567

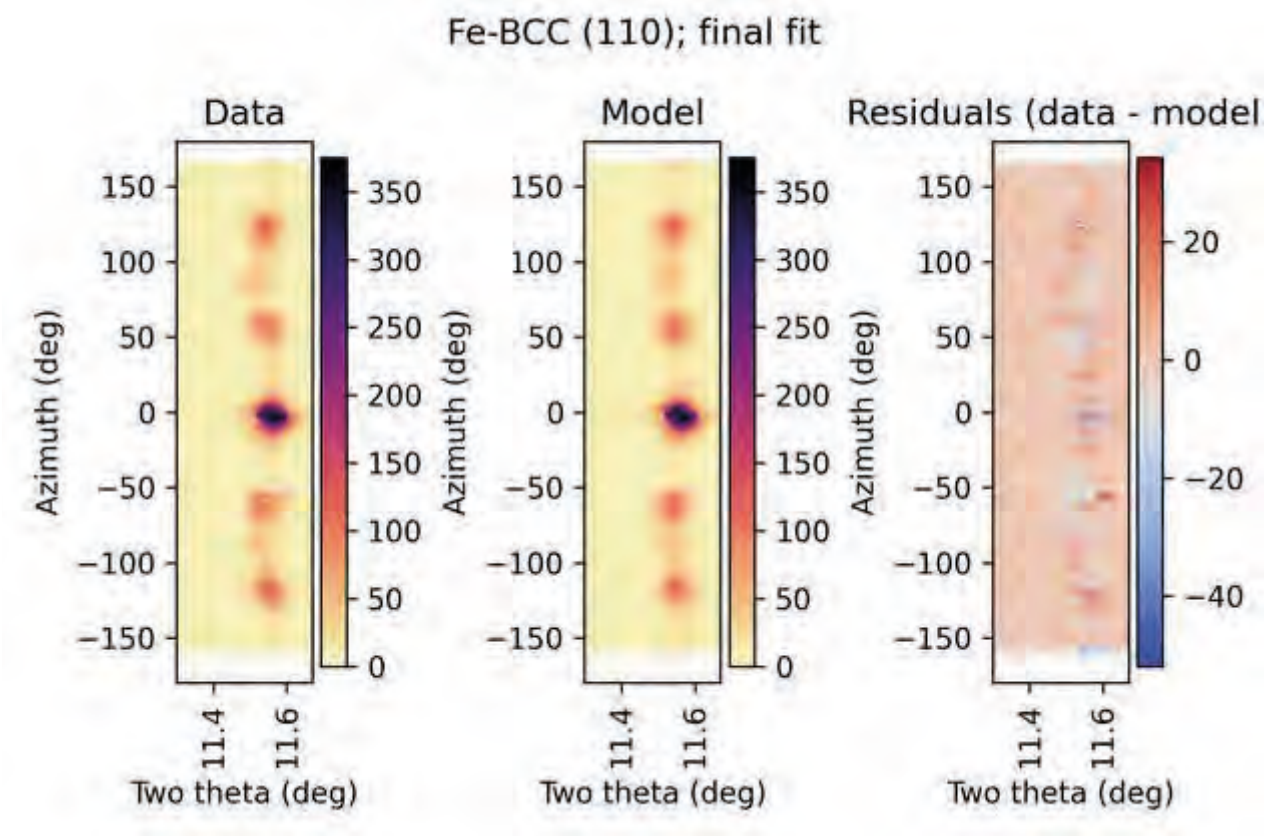


Figure: Example fit for the iron (110) peak at 2 GPa. On the left is the intensity data extracted from the (x,y) pixel observations and plotted using 2θ against χ (azimuth), using the detector calibration. In the middle is the fitted model for the data and on the right are the residuals between the data and the model.

Quantum oscillation and superconductivity study of the layered Weyl semimetal WTe2 under pressure

Wenyan Wang[1], Jianyu Xie[1], Wei Zhang[1], Xinyou Liu[1], King Yau Yip[1], Yuen Chung Chan[1], Kwing To Lai[1], Swee Goh[1]
[1]*Department of Physics, The Chinese University of Hong Kong, Shatin, Hong Kong, China*

Novel Superconductors 2, July 27, 2023, 14:00–16:00

We investigate the electronic properties of transition metal dichalcogenides WTe_2 under pressure. WTe_2 starts to superconduct at ~30 kbar. At 35 kbar, Tc is about 0.95 K. To figure out the relationship between the pressure-induced superconductivity and Fermi surface, we conduct Shubnikov–de Haas quantum oscillation measurements. At ambient pressure, four dominant peaks are observed, whose frequencies are 97 T, 134 T, 150 T and 172 T respectively. By applying pressure, these frequencies and the associated effective masses increase, suggesting the expansion of Fermi surfaces accompanied with enhanced electron-electron correlation. Moreover, we observe a high frequency at ~2000 T and extract a relatively large effective mass $m*$ of 1.8 m_0 at 35 kbar. The enhanced correlation under pressure revealed by our quantum oscillation study provides new information on understanding the pressure-induced superconductivity in WTe_2.

Superconductivity observed in yttrium lutetium ternary hydrides

Mr. Zhongyan Wu[1], Dr. Dongzhou Zhang[2], Dr. Changyong Park[3], Dr. Jaeyong Kim[1]
[1]Department of physics, Institute for high pressure, Hanyang university, Seoul, South Korea, [2]Hawaii Institute of Geophysics & Planetology, University of Hawaii Manoa, Honolulu, United States, [3]High Pressure Collaborative Access Team, X-ray Science Division, Argonne National Laboratory, Lemont, United States

Hydrides 4, July 26, 2023, 14:00–16:15

Although the routinely discovered high superconducting critical temperature (Tc) hydrides such as H3S, LaH10 and CaH6 have shown a promising route to achieve higher Tc, the requirements of extremely high-pressure conductions to synthesise those poly hydrides limit the worldwide researchers to reproduce and reach a consensus. By introducing a new element into binary hydrides, ternary hydrides show capability to reduce the stable pressure while maintain high Tc in both theory and experiment. Inspired by recent experimental high Tc discovery in binary hydride (e.g., 243 K in YH9, 70 K in Lu4H23) and theoretical prediction for room-temperature superconductivity in lutetium substituted clathrate hexahydrides under moderate pressure, we studied the superconductivity in yttrium lutetium ternary hydrides. The alloys were first prepared through induction melting method and the hydride samples were synthesised by laser heating of ammonia borane above 120 GPa. The results of the structure and zero resistance drop in yttrium lutetium ternary hydride with different compositions will be presented.

Observation on Physical Properties of nitrogen-doped lutetium hydrides under pressures below 30 GPa

Bin Li[1], Lei Sun[1], Young Jay Ryu[2], Dongzhou Zhang[3], Sungkyun Park[4], Soonjae Moon[1], Jaeyong Kim[1]

[1]Department of Physics, Institute for High Pressure, Hanyang University, Seoul, South Korea, [2]Center for Advanced Radiation Sources, The University of Chicago, Chicago, America, [3]Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, Honolulu, America, [4]Department of Physics, Pusan National University, South Korea

Hydrides 3, July 25, 2023, 14:00–16:00

The most recent report* that Nitrogen/Hydrogen-doped Lutetium (Lu) has sparked a tremendous interest in replicating the results. We synthesised the Lu hydrides by varying the composition ratio of N2/H2 from 1 % to 3% and investigated their structure and transport characteristics at a pressure below 30 GPa. Initially, the blue colour was noticed in our synthesised sample under ambient conditions; however, there was no noticeable colour changes other than becoming faintly transparent throughout the compression up to 30 GPa. The presence of two Fm3m hydrides with lattice constants of a = 5.01 Å and a = 4.76 Å was found by synchrotron XRD measurement at 2 GPa. Furthermore, our electrical resistivity studies showed no indication of superconductivity down to 10 K in the pressure range of up to 30 GPa. However, an anomaly of drop in resistance without zero resistance at 109 K under 25.9 GPa was observed. With further compression to 30 GPa, the optimised metallic behaviour became more significant. Further up-to-date findings pertaining to this system will be presented.

*Nathan Dasenbrock-Gammon et al., Evidence of near-ambient superconductivity in a N-doped lutetium hydride, Nature vol.65 244 (2023)

Complex electronic and magnetic properties in Fe4O5

Xiang Li[1,2], Denis Vasiukov[3], Georgios Aprilis[1], Sergey Yaroslavtsev[1], Elena Bykova[4], Efim Kolesnikov[2], Müller Susanne[1,2], Hu Tang[5], Anthony Lanati[2], Paul Pangritz[2], Arno Rohrbach[2], Davide Comboni[1], Michael Hanfland[1], Aleksandr Chumakov[1], Stephan Klemme[2], Carmen Sanchez-Valle[2], Leonid Dubrovinsky[5], Ilya Kupenko[1,2]

[1]European Synchrotron Radiation Facility, Gronoble, France, [2]Institute for Mineralogy, University of Münster, Münster, Germany, [3]Department of Physics, Lund University, Lund, Sweden, [4]Institute of Geosciences, University Frankfurt, Frankfurt , Germany, [5]Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, Germany

Electronic Transitions 1, July 26, 2023, 16:30–18:30

Investigations of iron oxides greatly contributed to condensed matter physics. For example, magnetite, the oldest-known mixed-valence oxide, was shown to have a ‘metal-insulator’-type transition when cooled below ~ 120 K, named later as the ‘Verwey’ transition after its discovery. This transition is linked to the formation of the linear Fe-site distortions called ‘trimerons’, which are three iron ions with one shared electron [1].

It is natural to expect to find some astonishing physical phenomena in other mixed-valence oxides. Therefore, the discovery of unconventional stoichiometries in an iron-oxygen system with a mixed valence of iron atoms such as Fe4O5 and Fe5O6 motivated the investigation of their physicochemical properties. The investigations of electronic structures of the novel oxides, although very scarce, indeed found some remarkable features. For instance, on cooling below ~150 K and 275 K at ambient pressure, Fe4O5 and Fe5O6 undergo unusual Verwey-type charge-ordering transitions similar to the one in magnetite [2, 3]. High pressure showed to tune the ambient-pressure charge-ordering pattern [4]. Moreover, the theoretical calculations indicate that Fe4O5 undergoes a series of site-selective spin transitions at high pressure [5]. Yet, the magnetic properties and structure details of Fe4O5 under extreme conditions have not been experimentally investigated and confirmed, although this information is crucial for understanding the interplay of iron ions in Fe4O5.

We will present our investigation on the pressure and temperature dependence of the electronic, magnetic and structural properties of Fe4O5 by means of Synchrotron Mössbauer Source spectroscopy and Single-Crystal X-ray diffraction in laser-heated diamond anvil cells up to 135 GPa and 1200 K. Particularly, we will show the role of interplay between Fe2+ and Fe3+ in determining these properties. The potential implications for other complex oxides systems will also be discussed.

[1] M. S. Senn, J. P. Wright, J. P. Attfield, Nature 481, 173–176 (2012).
[2] S. V. Ovsyannikov, M. Bykov, E. Bykova, et al., Nat. Chem. 8, 501 (2016).
[3] S. V. Ovsyannikov, M. Bykov, S. A. Medvedev, et al., Angew. 132, 5681 (2020).
[4] S. V. Ovsyannikov, M. Bykov, E. Bykova, et al., Nat. Commun. 9, 4142 (2018).
[5] A. Yang, Q. Qin, X. Tao, et al., Phys. Lett. A 414, 127607 (2021).

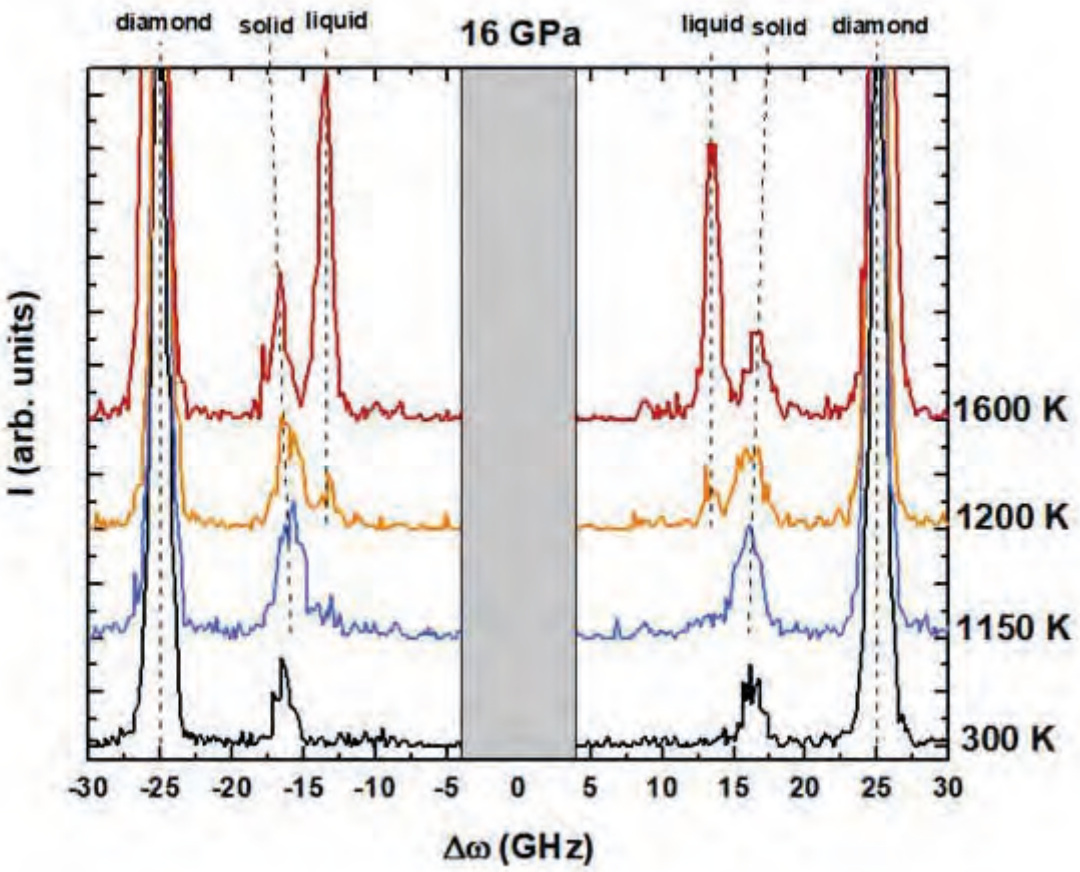
Phase diagram and sound velocity of ammonia from Brillouin scattering in the laser heated diamond anvil cell.

Bastien Guigue[1], Keevin Beneut[1], Sandra Ninet[1], Mandy Bethkenhagen[2], **Frédéric Datchi**[1]
[1]IMPMC, Sorbonne Université, CNRS and MNHN, Paris, France, [2]Lab. de Géologie de Lyon, ENS Lyon & Université de Lyon, Lyon, France

Molecular Compounds, July 25, 2023, 10:15–12:15

Ammonia has a significant abundance in the outer solar system and, together with water and methane, is thought to be a major component of the ice layer of giant planets and satellites. Depending on the size of these bodies, the pressure (P) at the bottom of the ice layer may range from a few to several hundreds of GPa, which makes the knowledge of the properties of these ices over a broad range of P-T conditions important input for modelling the icy planets. Of particular interest is the superionic solid at high P-T, whose large electrical conductivity may play an important role in the generation of the planet magnetic fields. This phase, suggested by theoretical calculations [1,2], was experimentally established to exist in NH3 above 57 GPa-710 K [3]. So far however its physical properties and melting point are poorly constrained by experiment. We report here on Brillouin and Raman scattering experiments on ammonia samples in the range 15-55 GPa and up to 3500 K. The latter were made possible by the construction of a new spectroscopic bench for Brillouin and Raman scattering in the laser heated DAC. In this setup, a CO2 laser (λ=10.6 μm) is used to heat the sample, while Brillouin and Raman spectra are obtained by excitation with a 514 nm CW laser. Temperature is determined by the thermal emission of the sample collected by reflective optics to avoid chromatic aberrations. Melting of solid ammonia is clearly detected in the Brillouin spectra up to 55 GPa-3300 K thanks to the large contrast in sound velocity between solid and liquid ammonia (Figure). The transition from molecular to superionic ammonia (α-SI phase) is detected at 37 GPa and about 2000 K along the melting line. Furthermore, we find no evidence for the existence of a second superionic phase of ammonia (γ-SI) with fluid-like elastic response as recently claimed [4]. The experimental results will be compared to new ab-initio MD calculations of SI ammonia in the same P-T range.

[1] C. Cavazzoni et al, Science 283, 44 (1999).
[2] M. Bethkenhagen et al, J. Chem. Phys. 138, 234504 (2013).
[3] S. Ninet et al, Phys. Rev. Lett. 108, 165702 (2012).
[4] T. Kimura and M. Murakami, Proc. Natl. Acad. Sci. 118, 14 (2021)


diamond
solid
liquid
16 GPa
liquid
solid
diamond
1600 K
1200 K
1150 K
300 K
I (arb. units)
-30
-25
-20
-15
-10
-5
0
5
10
15
20
25
30
Δω (GHz)

Metastable liquid-like CO2 confined in a mesoporous Metal-Organic Framework at high-pressure

Francesco Capitani[1], Vi Le Hanh[1], Anna Celeste[3], Pierre Fertey[1], Gabriela Blanita[4], Claudia Zlotea[2]
[1]Synchrotron SOLEIL, Saint-Aubin, France, [2]ICMPE, Thiais, France, [3]Stanford University, Stanford, United States, [4]NIRDMT, Cluj-Napoca, Romania

Multifunctional Materials, July 24, 2023, 10:15–12:15

Metal–Organic Frameworks (MOFs) are porous hybrid materials where metallic ions or clusters are interconnected by organic ligands. Their porous nature translates into a large internal surface area available [1]. Among MOFs, mesoporous frameworks, with their pore size between 2 and 50 nm, allow unprecedented functionalization as the confinement of large molecules and even metallic nanoparticles inside the pores, already at ambient conditions [2].

The large voids in the framework and the presence of guests could affect the mechanical stability of these materials when submitted to external stimuli as pressure, temperature and gas adsorption. This stimulated several works at high-pressure mainly on microporous (pore size < 2nm) MOFs [1].

In the last years, we focused instead on mesoporous MOFs, in particular MIL-101(Cr) which has pore sizes around 3 nm. We studied MIL-101 under pressure using diamond anvil cells (DACs), with different kinds of pressure transmitting media (PTM) fluid and solid [3, 4]. We showed that the intrinsic mechanical stability of the pristine framework is accessible only with the solid medium and is limited by a pressure-induced amorphization occurring below 0.4 GPa. We then demonstrated that high-pressure can foster the insertion of a fluid PTM, made of large polymers, inside the giant pores, thus creating a composite material with a higher bulk modulus and shifting the crystal-to-amorphous transition to higher pressure by more than one order of magnitude. This motivated us to verify whether a mesoporous MOF, as MIL-101, could be a platform to host a molecular liquid as CO2 confined in nanometric pores. We mainly employed two complementary synchrotron techniques at the synchrotron SOLEIL, X-ray diffraction and infrared spectroscopy to obtain a complete picture of such a complex system under pressure.

In this talk, we will show that the structural stability of MIL-101 is affected by the presence of liquid CO2, shifting the amorphization pressure to higher values, suggesting that the pores are thus filled by CO2, as also found in zeolites with much smaller pores [5]. The presence of CO2 inside the pores is corroborated by the IR combinations bands of CO2 and the OH vibration of the hydroxyl group of MIL-101, indicating host-guest interaction. Moreover, both IR spectra and XRD patterns above the known solidification pressure of bulk CO2 (around 1 GPa), show a coexistence of signals typical of liquid and solid CO2 [6, 7]. This can be explained by a picture where solid CO2 is outside the MOF acting as PTM and liquid-like CO2 is confined inside the nanometric pores. The liquid signals are still present up to 11 GPa, indicating that nanoconfined liquid-like CO2 is metastable over a large pressure range compared to the phase diagram of bulk CO2.

[1] F.-X. Coudert, Chem. Mater. 27, 1905 (2015)
[2] A. Malouche et al., J. Mater. Chem. A 5, 23043 (2017)
[3] A. Celeste et al., JACS 142, 15012 (2020)
[4] A. Celeste et al., ACS Appl. Nano Mater. 5, 3, 4196 (2022)
[5] J. Haines et al., J. Am. Chem. Soc. 132, 8860–8861 (2010)
[6] R. Lu et al., Phys. Rev. B 52, 3985 (1995)
[7] Datchi et al., Phys. Rev. B 94, 014201 (2016)

Electrical and thermal conductivity of iron at Earth's core conditions from ab initio simulations

Uwe Kleinschmidt[1], Martin French[1], Gerd Steinle-Neumann[2], Ronald Redmer[1]
[1]Universität Rostock, Institut für Physik, Rostock, Germany, [2]Bayerisches Geoinstitut, Universität Bayreuth, Bayreuth, Germany

Secular Evolution of the Earth, July 25, 2023, 10:15–12:15

We use ab initio simulations based on density functional theory to calculate the electrical and thermal conductivity of solid iron in face-centred cubic and hexagonal phases at high pressures and temperatures up to Earth's core conditions. Both our electrical and thermal conductivities increase systematically with density and reasonably follow the Wiedemann-Franz law, in particular at low temperatures. The fcc phase shows systematically larger conductivity values than the hexagonal phase. We also calculate the components of the conductivity tensors in the hexagonal iron phase and find an anisotropy by comparing the zz component and the basal plane components xx and yy. This anisotropy effect has been reported in previous publications [1] which showed comparable results. In comparison to experiments our calculations [2] do not support the trend towards density-independent thermal conductivity observed in recent measurements [3]. Our electrical conductivity values lie in between the wide spectrum of experimental results and show good agreement with reanalysed experimental data provided by Lobanov and Geballe [4].

[1] K. Ohta et al., Front. Earth Sci. 6, 176 (2018).
[2] U. Kleinschmidt et al., Phys. Rev. B 107, 085145 (2023)
[3] Z. Konôpková et al., Nature (London) 534, 99 (2016).
[4] S. S. Lobanov, Z. M. Geballe, Geophys. Res. Lett. 49, e2022GL100379 (2022)

Ab initio simulations for the ion-ion structure factor of warm dense matter in the hydrodynamic limit

Maximilian Schörner[1], Hannes Rüter[2], Martin French[1], Ronald Redmer[1]
[1]University of Rostock, Rostock, Germany, [2]The Centre for Physics of the University of Coimbra, Coimbra, Portugal

Computational Methods, July 25, 2023, 10:15–12:15

It has recently become possible to resolve ion dynamics at X-ray free electron laser facilities [A. Descamps et al., Sci. Rep. 10, 14564 (2020)] by measuring the dynamic ion-ion structure factor (DSF) via scattering experiments. In this work, we study the DSF of warm dense aluminium and copper in large-scale simulations using neural network interatomic potentials trained on density functional theory predictions. Following earlier work on water and hydrogen [B. Cheng and D. Frenkel, Phys. Rev. Lett. 125, 130602 (2020)], we investigate the convergence to the hydrodynamic model in the macroscopic limit for aluminium and show how these insights can be used to extract the adiabatic speed of sound and ionic thermal conductivity [M. Schörner et al., Phys. Rev. B 105, 174310 (2022)]. The results are discussed and compared with experimental data when available. Using copper as a test case, we apply these techniques to make predictions for the DSF and speed of sound in a typical shock compression experiment [M. Schörner et al., Phys. Rev. B 106, 054304 (2022)].

Synergetic Effect of High Pressure and Temperature Leading to Remarkably Enhanced CO2 Adsorption Capacity of ZIF-8

Miss Shan Jiang[1], Miss Jingyan Liu[1], Dr. Jiwen Guan[1], Professor Yining Huang[1], **Professor Yang Song**[1]
[1]Western University, London, Canada

Molecular Compounds, July 25, 2023, 10:15–12:15

Metal-organic frameworks (MOFs) and zeolitic imidazolate frameworks (ZIFs) are promising porous materials for adsorption and storage of greenhouse gases, especially CO2. In this study, guided by the CO2 phase diagram, we explore the adsorption behaviour of solid CO2 loaded with ZIF-8 framework by heating the sample under high pressures, resulting in a drastic improvement in the CO2 uptake. The behaviour of CO2 under simultaneous high temperature (T) and pressure (P) conditions is directly monitored by in situ FTIR spectroscopy. The remarkable enhancement in CO2 adsorption capability observed can be attributed to the synergetic effect of high T and P: high temperature greatly enhances the transport property of solid CO2 by facilitating its diffusion into the framework; high pressure effectively modifies the pore size and shape via changing the linker orientation and creating new adsorption sites within ZIF-8.

Antiferroelectric Pnma phase: The Missing Element to understand Morphotropic Phase Boundary lead-free Na1/2Bi1/2TiO3 based piezoceramics

Manuel Hinterstein[1], Thomas Hansen[2], Patrick Hermet[3], Julien Haines[3], **Jerome Rouquette**[3]
[1]Karlsruhe Institute of Technology (KIT), Haid-und-Neu Straße 7, 76131 Karlsruhe, Germany, [2]Institut Laue Langevin, 71 Avenue des Martyrs, 38000 Grenoble, France, [3]ICGM Universite de Montpellier, 1919 Route de Mende, cc043, 34095 Montpellier cedex5, France

Perovskites, July 27, 2023, 10:15–12:15

Na1/2Bi1/2TiO3 (NBT) perovskite (ABO3) based piezoceramics are of great interest due to their role as an end member of lead-free substitutes to replace the commercially dominant PbZr1-xTixO3. NBT exhibits two phase transitions with decreasing temperature: from Pm-3m paraelectric structure to tetragonal P4bm ferro(ielectric) and then rhombohedral R3c/Cc phase. With increasing pressure, NBT is found to transform from R3c/Cc phase to the CaTiO3-type structure (Pnma) which was proposed to be responsible for the disorder on Bi-atoms. Here, we report high-pressure neutron diffraction combined with density functional perturbation theory (DFT) calculations on (Na1/2Bi1/2TiO3)0.93-(BaTiO3)0.05-(K0.5Na0.5NbO3)0.02 piezoceramics which was chosen as i) it shows the P4bm structure at ambient temperature and ii) it exhibits optimal piezoelectric properties with a morphotropic phase boundary between the tetragonal P4bm and the R3c space groups.

The calculated full phonon dispersion relations obtained at the GGA level on a model Na1/2Bi1/2TiO3 compound clearly show three instabilities and support a P1 triclinic ground state structure. With increasing pressure, the tetragonal phase shows a first transition to the R-3c structure at about 2 GPa and then transforms to antiferroelectric ordered Pnma form close to 5 GPa. Large atomic displacement parameters (ADPs) for A-site perovskite atoms in the tetragonal phase are definitely associated to the high-pressure antiferroelectric symmetry whereas strong ADPs in the R-3c phase linked to density functional based calculations suggest a weakly polar P1 phase. The existence of this antiferroelectric state permits to understand disagreements about the average structure and based on group theory, validates the phase transition sequence in P-T space.

Investigation of environment and substrate roles on high pressure tuning of graphene properties

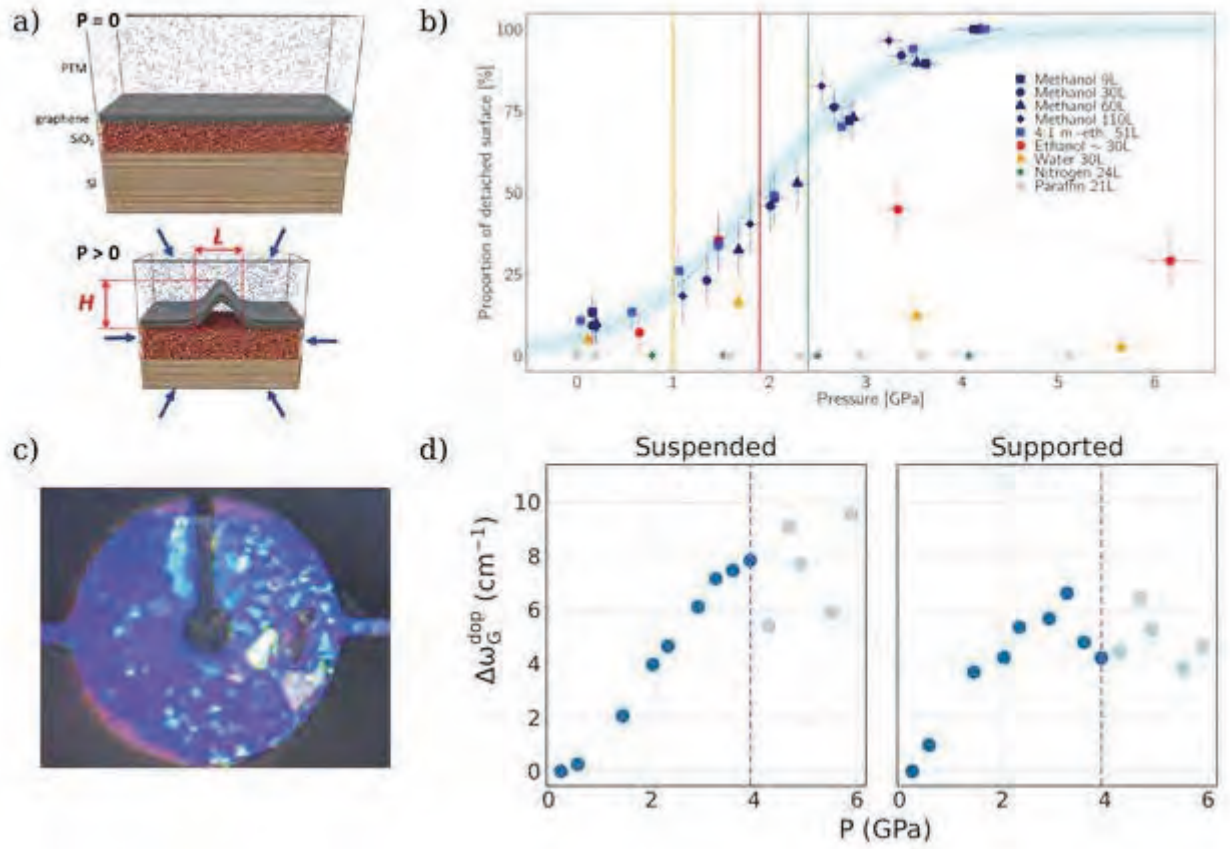
Riccardo Galafassi[1], Alfonso San Miguel[1], Fabien Vialla[1], Rajaji Vincent[1], Ian Rodriguez Do Amiral[2]
[1]Institut Lumière Matière, Université de Lyon, Villeurbanne, France, [2]Departamento de Física, Centro de Ciencias, Universidade Federal Do Cearà, Fortaleza, Brazil

Nanoscale Systems, July 24, 2023, 16:30–18:30

Environment play a central role in the properties of 2D materials. Due to their mono or few atoms thickness the majority of the atoms in those materials are in contact with the surrounding environment. Their mechanical and chemical properties are subjected to the influence of strain, charge injection and chemical bondings introduced by the neighbouring materials [1-3]. Moreover, the necessity of supporting the 2D material on a substrate leads to its central role in the properties of those materials. Applying pressure on 2D materials drew interest for the capability of acting on the environment and the substrate giving access to a tool for continuously tune the 2D material's properties [3,4,5]. In addition to that, the application of pressure is promising for the development of novel composite materials as well as for interesting applications in various fields such as tribology and straintronics.

We propose here innovative studies focussed on the use of pressure as a mean of tuning the environment-graphene and substrate-graphene interaction. In a first published work [6] we study wrinkle formations of few-layer graphene on SiO2/Si substrates. A universal behaviour, independent on the number of graphene layers, is found, leading to counter-intuitive result of complete detachment of the sample from the substrate applying pressure above ~4GPa. This behaviour is environment dependent as it is favoured by the use of alcohol and alcohol mixtures as pressure transmitting media (PTM). On the other hand, using paraffin and inert gasses as PTM led to no wrinkling nor detachment effects with pressure. On a second work we focussed on the further comprehension of the role of the substrate on 2D materials. We conducted pressure dependent studies on partially suspended bilayer samples. Using Raman spectroscopy as a primary tool, we compared the sample behaviour in the two regions and found major differences between the suspended and supported samples. In particular, using a mixture of methanol and ethanol as PTM, we obtained higher rates of charge transfer on the suspended regions compared to the supported ones.

[1] Meyer, J. et al., The structure of suspended graphene sheets., Nature 446, 60–63 (2007)
[2] C. Bousige et al., Nano Letters 2017 17 (1), 21-27
[3] A. Forestier et al., The Journal of Physical Chemistry C, 2020 124 (20), 11193-11199
[4] J. Nicolle, Nano Lett. 2011, 11, 3564–3568
[5] D. Machon, J. Raman Spectrosc. 49, 2017, 121– 129
[6] I.R. Amaral, A. Forestier, A. Piednoir, R. Galafassi et al., Carbon 185, 2021, 242-251


a)
P = 0
PTM
graphene
SiO_2
Si
P > 0
L
H
b)
Proportion of detached surface [%]
Pressure [GPa]
Methanol 9L
Methanol 30L
Methanol 60L
Methanol 110L
4:1 m-eth 51L
Ethanol ~ 30L
Water 30L
Nitrogen 24L
Paraffin 21L
c)
d)
Suspended
Supported
$\Delta\omega_G^{dop}$ (cm^{-1})
P (GPa)

Novel ammonia hydrates in the mid-mantle layers of icy (exo)planets

Anshuman Mondal[1], K Mohrbach[1,2], P Liermann[2], T Fedotenko[2], C Sanchez-Valle[1]
[1]Institut für Mineralogie, Universität Münster, 48149 Münster, Germany, [2]Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany

Outer Planets and Exoplanets 2, July 26, 2023, 16:30–18:30

Ices of Ammonia (NH3), Water (H2O) and mixtures thereof are major components in the interior of Solar ice giants and likely in thousands of newly discovered mini-Neptune exoplanets. These ices can display ionic and superionic behaviour at extreme conditions (>10 GPa and 900 K) that can be responsible for unusual magnetic fields detected for instance in Neptune [1, 2, 3]. Understanding the structure and physical properties of these hot compressed ice phases at relevant high pressure(P)-temperature(T) conditions are thus key to accurately model the internal structure and dynamics of large icy bodies. Experimental studies over the last two decades have largely focused on pure H2O and NH3 ices, while the behaviour of ice phases in binary systems at relevant P-T conditions still remains poorly understood. It is currently unknown whether planetary conditions could stabilise other ammonia hydrates than the well-known low-temperature stoichiometric forms– ammonia dihydrate (ADH, NH3:H2O = 1:2), ammonia monohydrate (AMH, NH3:H2O = 1:1) and ammonia hemihydrate (AHH, NH3:H2O = 2:1) [4]. Here we investigate the high P-T behaviour of ice phases in the NH3-H2O system using a combination of resistively heated dynamic diamond anvil cells (RhdDAC, [5]) and double-sided laser-heated diamond anvil cell (LHDAC) experiments and synchrotron X-ray diffraction. An H2O-rich ammonia mixture with 32 wt% NH3 (NH3:H2O = 1:2) was chosen as a starting material in order to resemble the cosmo-chemical abundance (NH3:H2O = 1:7) [6]. Samples were pressurised at room temperature to form a mixture of ice VII and NH3-rich ammonia hemihydrate (AHH-II) [7] before the high-temperature experiments. Our time-resolved high P-T X-ray diffraction studies result in the identification of several phase transitions in the ammonia hemihydrate phase up to 26 GPa and 800 K. Above this temperature, a novel ammonia hydrate phase with body-centred cubic (bcc) crystal structure forms by the reaction of H2O ice and the high-pressure AHH (DMA) phase. The new phase carries more H2O than any of the known ammonia hydrates as estimated from linear mixing of NH3 and H2O (Ice VII) phase volumes. These findings will thus be crucial to understand the internal structure of the outer mantle in icy planetary bodies and will in terms help to interpret the available geophysical observations [3, 8].

[1] W. B. Hubbard, Science 214: 145 (1981).
[2] V. N. Robinson and A. Hermann, J. Phys. Condens. Matter 32, 184004 (2020).
[3] J. J. Fortney & N. Nettelmann, Space Sci. Rev. 152: 423 (2010).
[4] J. S. Kargel, Icarus 100, 556 (1992).
[5] Méndez et al., Rev. Sci. Instrum. 91, 073906 (2020).
[6] M. Asplund et al. Annu. Rev. Astron. Astrophys. 47, 481 (2009).
[7] C. W. Wilson et al., J. Chem. Phys. 142, 094707 (2015).
[8] R. Helled et al., Astrophys. J. 726, 15 (2010).

Overview of beamline 16-ID-B of the High-Pressure Collaborative Access Team at the Advanced Photon Source

Jesse Smith[1], Yue Meng[1], Eric Rod[1], Rich Ferry[1], Curtis Kenney-Benson[1], Arunkumar Bommanavar[1]
[1]*HPCAT, X-ray Science Division, Argonne National Laboratory, Lemont, United States*

Facility Development 1, July 24, 2023, 16:30–18:30

HPCAT's beamline 16-ID-B at the Advanced Photon Source is one of just a few dedicated extreme conditions beamlines in the world which benefits from both a high energy electron storage ring and an undulator source. The available high flux of high energy photons is well-suited to studying weak-scattering materials; this weak scattering can be the result of minute sample volumes at ultrahigh pressure and/or low-Z materials. Micron-scale focusing provides exceptional spatial resolution, allowing detailed transmission and diffraction mapping of the heterogeneous sample chamber; this heterogeneity can arise from the sample material itself and/or from the extreme pressure gradients encountered in ultrahigh pressure applications. With the addition of high-efficiency, high-frequency imaging detectors, researchers can introduce time-dependence – either indirectly as a research tool or directly as an experimental parameter – using what would traditionally be considered static high-pressure apparatus. The exceptional beamline characteristics, together with extensive supporting apparatus and laboratory facilities, provide researchers with a uniquely powerful tool for addressing some of the most challenging problems in extreme conditions research.

We briefly describe the various beamline optics, components, and apparatus that facilitate micro-X-ray diffraction in the diamond anvil cell at pressures ranging from ambient pressure up to several hundred gigapascal, at temperatures ranging from liquid helium up to several thousand Kelvin, and at time scales ranging from static down to about a millisecond. We present several examples of users' research which highlight the capabilities of the beamline. Finally, we explore the future outlook of 16-ID-B in the context of the APS Upgrade, which will bring the APS into the era of the latest-generation storage ring, characterised by the multi-bend achromat. This upgrade will ensure HPCAT's diverse, international user community continues to have access to state-of-the-art experimental platforms for studying materials at extreme conditions.

Revealing pressure induced electronic phase transitions at extreme conditions

Igor Abrikosov[1]
[1]*Linköping University, Linköping, Sweden*

Electronic Transitions 2, July 25, 2023, 14:00–16:00

Extreme compression affects the electronic structure of materials and may lead to electronic phase transitions (EPT), a qualitative change of the electronic structure of a material, which may occur without a transition into a different crystallographic phase. Insulator-to-metal transitions (IMT) and the topological changes of the Fermi surface for valence electrons, the so-called electronic topological transition (ETT), represent well-known examples of the EPTs. Though capturing the EPTs in high-pressure experiments is a non-trivial task, it can be efficiently solved when theory is engaged. We briefly review state-of-the art techniques for electronic structure calculations, emphasizing novel approaches that allow for proper account of vibrational excitations and many-electron effects, essential at extreme conditions [1-3]. Discussing non-conventional types of EPTs, like the electronic transitions in hcp Os compressed to ~1 TPa [4], site-selective IMT in Fe2O3 [5] and inverse pressure-induced IMT in TiPO4 [6], we demonstrate that combining the experiments with advanced theoretical simulations greatly enhances the opportunity to study pressure induced electronic transitions.

[1] D. Laniel, et al., Nature Commun. 13, 6987 (2022).
[2] E. Koemets, et al., Phys. Rev. Lett. 126, 106001 (2021).
[3] A. N. Rudenko, et al., Phys. Rev. B. 105, 205135 (2022).
[4] L. Dubrovinsky, et al., Nature 525, 226–229 (2015).
[5] E. Greenberg, et al., Phys. Rev. X 8, 031059 (2018).
[6] H. J. M. Jönsson, et al., Phys. Rev. B 99, 245132 (2019).

Development of strength and texture in hexagonal Fe-Si-C alloy at planetary cores conditions

Efim Kolesnikov[1], Ilya Kupenko[1,2], Arno Rohrbach[1], Stephan Klemme[1], Jasper Berndt[1], Xiang Li[1], Susanne Müller[1], Hanns-Peter Liermann[3], Carmen Sanchez-Valle[1]
[1]University of Münster, Institute for Mineralogy, Münster, Germany, [2]ESRF, Grenoble, France, [3]DESY Photon Science, Hamburg, Germany

Cores of Terrestrial Planets, July 24, 2023, 14:00–16:00

The observed density of planetary cores is lower than expected for a pure iron-nickel alloy at corresponding conditions. Therefore, the cores of terrestrial planets should be composed of iron-nickel alloyed with some lighter elements. These elements should be abundant in the solar system, siderophile, and compatible with iron at high-pressure high-temperature conditions. Si and C comply with these requirements and are plausible planetary core constituents. Seismic observations of the Earth's inner core revealed anisotropy of seismic wave propagation. For instance, compressional waves travel 1-3% faster along the polar axis compared to waves traveling in the equatorial plane. One of the hypotheses of the origin of the anisotropy is the plastic deformation and development of textures in inner-core materials. We studied the yield strength and anisotropy of a Fe-2 wt % Si-0.4 wt % C alloy at high-pressure high-temperature conditions to compare its properties with those observed in the Earth's core. The experiments were conducted by radial X-ray diffraction technique coupled with resistively heated diamond anvil cells that acted as a deformation apparatus. We performed experiments up to 122 GPa pressure with temperatures exceeding 1100 K. The strength of the Fe-Si-C alloy is higher than the strength of pure Fe and Fe-Si alloys. Our results show lower anisotropy of sound-wave velocities in hexagonal Fe-Si-C alloy compared to the seismic observations. We detected the change in main texture orientation upon compression from [0001] to $[1\bar{1}00]$ and nearby to $[1\bar{2}1\bar{0}]$ in Fe-Si-C alloy. In this presentation, we will discuss the dominant mechanisms of plastic deformation, responsible for these observations, and the overall effects of carbon and silicon on the strength and anisotropy of hexagonal iron alloys in planetary cores.

The Metallic Hydrogens: Reflectance, Electrical Conductance, and Metastability

Professor Isaac Silvera[1], Dr. Wellington Ferreira[1], Dr. Morten Moeller[1], Mr. Kiran Linsuain[1], Dr. Jing Song[1], Professor Ashkan Salamat[2], Professor Ranga Dias[3]

[1]Lyman Laboratory of Physics, Harvard University, Cambridge, United States, [2]Department of Physics and Astronomy, University of Las Vegas, Las Vegas, United States, [3]Department of Physics and Astronomy, University of Rochester, Rochester, United States

Hydrogen, July 25, 2023, 10:15–12:30

Metallic hydrogen (MH) can be produced in two ways under pressure: either static pressurization at low temperatures to transition from the molecular solid to the atomic metallic phase predicted by Wigner and Huntington, or by heating a sample pressurised either statically or dynamically, to produce liquid MH. This presentation is focused on the Wigner-Huntington transition to MH. We first discuss techniques that enabled us to achieve pressures of order 500 GPa in conventional diamond anvil cells and study the properties of the MH. In one experiment MH was confirmed by reflectance measurements in the near IR and fit to a Drude free-electron model. Reducing the pressure on MH demonstrated that it was metastable, but not down to zero pressure, where it definitely had transformed back to the molecular phase. Zero-point energy or zero-point motion is an important consideration for metastability. Due to its substantially lower zero-point energy, metallic deuterium may be metastable down to zero pressure and experiments are ongoing to study its insulator-metal transition and metastability. In another set of experiments the electrical conductivity of hydrogen was measured with a 4-lead Kelvin geometry. In one pressurization, MH was produced at a pressure just under 500 GPa as measured by the shift of the Raman active phonon in the stressed part of the diamond culet. A broad transition to zero resistance, starting at about 270 K, was observed. These experiments are ongoing with an eventual goal of measuring the Meissner effect to establish superconductivity.

HYDROMET: A new facility to study hydrogen embrittlement of materials at up to 2 kbar H2-pressure

Stefan Klotz[1], Louis Amand[1], Eddy Lelièvre-Berna[2], Burkhard Annighöfer[3]
[1]Impmc, Sorbonne University, Paris, France, [2]Institut Laue Langevin, Grenoble, France, [3]Laboratoire Léon Brillouin, Saclay, France

Instrumentation and Techniques 1, July 26, 2023, 10:15–12:15

Hydrogen will play a major role in a future “green” (carbon-free) energy economy: It is the most abundant element in universe, it is the cleanest fuel one can imagine since it produces only water, and it can be stored in large quantities and transported over large distances. One of the most serious handicaps is its reaction with construction materials: In contact with H2, most steels (even stainless steels) undergo serious embrittlement which degrades massively their mechanical properties and leads to serious safety issues [1-3]. Here we present a facility which allows a systematic investigation of H-embrittlement of materials under H2 pressure in the kbar-range, an area where there is currently only little experimental data available. The systems consist of a 3 kbar gas vessel which incorporates a traction machine allowing to measure stress-strain relations on test samples which are under typically 2 kbar hydrogen gas pressure. The principal aim is to study high tensile steels and alloys which are relevant to high pressure research and potential candidates for hydrogen-storage and handling facilities. Technical details and the experimental protocol will be presented, as well as results on a series of steels and alloys currently used in high pressure research. An outlook to complementary analytical tools for the study of the post-mortem specimens will be discussed, such as X-ray diffraction, scanning election microscopy and nano-scale secondary ion mass spectroscopy (SIMS).

In situ X-ray diffraction of TATB on NIF

Dr. Samantha Clarke[1], Damian Swift[1], Martin Gorman[1], Michelle Marshall[2], Saransh Soderlind[1], Joel Christianson[1], Jon Eggert[1], Raymond Smith[1], Sorin Bastea[1], Lara Leininger[1], Lawrence Fried[1]
[1]Lawrence Livermore National Laboratory, Livermore, United States, [2]Laboratory for Laser Energetics, U. of Rochester, Rochester, United States

Developments at XFELs & Lasers, July 24, 2023, 14:00–16:00

We have performed in situ X-ray diffraction measurements of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) on NIF using the TARget Diffraction In Situ (TARDIS) diagnostic. TATB targets were shocked between 60 and 140 GPa and in situ diffraction was performed to determine the solid carbon reaction products produced under these conditions. VISAR was used to determine the sample pressure during the time of the X-ray exposure.

This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Grant No. DE-NA0003856 and performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 and 18-SI-004. LLNL-ABS-848002

Simulating Shock Compression with Ephemeral Data Derived Potentials.

Peter Cooke[1], Dr Chuck W Witt[1], Mr Pascal Thomas Salzbrenner[1], Dr Lewis J Conway[1,2], Prof Chris J Pickard[1,2]

[1]*Department of Materials Science & Metallurgy, University Of Cambridge, Cambridge, United Kingdom,*
[2]*Advanced Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba, Sendai, 980-8577, Japan*

Computational Methods, July 25, 2023, 10:15–12:15

Dynamic compression techniques have allowed new and interesting materials to be probed at extreme pressures. However, the transient nature of the pulse limits the information that can be extracted from a given experiment. Simulations can provide a useful tool to aid interpretation of this experimental data, but capturing the full complexity of the experiment requires large system sizes and timescales of nano-seconds, all at a quantum mechanical level of accuracy. Classical simulations using data derived potentials have been shown to maintain this 'quantum accuracy' at a fraction of the computational cost, allowing much larger length and timescales to be explored. We present results from the recently developed ephemeral data derived potential (EDDP) approach that has been integrated into the LAMMPS simulation package. Using a range of example systems, we demonstrate that the EDDPs are a versatile tool for fast and accurate simulations at high pressure.

X-ray diffraction and laser-driven ramp-compression of iron at TPa pressure

Federica Coppari[1], R Smith[1], S Singh[1], T Duffy[2], J Eggert[1], A Lazicki[1], M Millot[1]
[1]Lawrence Livermore National Laboratory, Livermore, United States, [2]Princeton University, Princeton, United States

Outer Planets and Exoplanets 1, July 26, 2023, 10:15–12:15

Laser-driven dynamic compression has enabled the study of material properties and equations of state at unprecedented extreme conditions. By carefully designing the laser pulse shape (i.e. laser power vs time), one can compress and heat the sample to a specific state, allowing the investigation of a wide range of pressures and temperatures. Specifically, “ramp”-compression can be used to reach extreme pressure conditions keeping the material in the solid state, by minimizing the entropy (and therefore temperature) increase associated with shock propagation. The combination of laser-driven compression and X-ray diagnostics allows us to probe these extreme pressure-temperature states in situ, providing a unique picture of the transformations taking place in high-energy-density matter with important applications for high pressure materials science, geophysics and planetary science. Structural probes, such as X-ray diffraction (XRD) have been developed at large laser facilities to investigate phase transitions and material properties at the nanosecond time scale.

In this talk, I will present new results from X-ray diffraction and ramp-compression experiments of iron up to 1 TPa. The data reveal that the hexagonal-closed packed (hcp) structure (one of the high-pressure polymorphs that form at pressures higher than ~13 GPa) is observed and allow us to determine the iron density up to these extreme compressions.

This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344

New HDCM and HDMM for Advanced Spectroscopy, Microscopy and Time-resolved XRD at HPCAT 16-ID-D and 16-ID-E Beamlines

Changyong Park[1], Paul Chow[1], Yuming Xiao[1], Eric Rod[1], Curtis Kenney-Benson[1], Rich Ferry[1], Arun Bommannavar[1], Maddury Somayazulu[1], Nenad Velisavljevic[1,2]
[1]Argonne National Laboratory, LEMONT, United States, [2]Lawrence Livermore National Laboratory, LIVERMORE, United States

Next Gen Synchrotrons, July 25, 2023, 14:00–16:00

The APS-U source will deliver substantially brighter and more coherent beams to downstream experimental stations, hence enabling techniques based on a finer focused beam with improved flux-density and orders of magnitude improved beam coherence. HPCAT's downstream end stations, 16-ID-D and 16-ID-E, are planning to utilise these new capabilities aiming at developing advanced spectroscopy, sub-micron resolution microscopy, and time-resolved XRD techniques. To achieve these goals, delivering a highly coherent beam with maximum thermal and mechanical stabilities is essential. We are preparing to have a new horizontally deflecting double crystal monochromator (HDCM) and a horizontally deflecting double multilayer monochromator (HDMM) in series in the 16-ID-C optical hutch for that purpose.

A series of new techniques will be enabled in both the 16-ID-D and 16-ID-E stations. In addition to existing Inelastic X-ray Scattering (IXS), Nuclear Resonance Scattering (NRS), and X-ray Emission Spectroscopy (XES) techniques at the 16-ID-D beamline, a new high-throughput XES von Hamos spectrometer based on the ~1% bandwidth HDMM beam at fixed energy about 11 keV and X-ray Absorption Spectroscopy based on the high-resolution energy scanning HDCM (4.8 – 45 keV) will be developed. In the 16-ID-E end station, we will develop 2D scanning probe X-ray Diffraction Imaging (XDI) with a sub-micron focused beam, grain Bragg Coherent Diffraction Imaging (g-BCDI) for polycrystalline materials, and time-resolved XRD (t-XRD) for fast pressure- and temperature-ramp experiments. These XRD based techniques are compatible with each other in terms of instrumental requirements so that they can be developed on an integrated experimental table. The new techniques will be fully utilizing the APS-U source properties, i.e., enabling nearly diffraction-limited focusing with pre-figured elliptical mirror optics, roughly 1000 times enhanced coherent intensities, and improved flux further boosted by DMM's 1% bandwidth, respectively. In this presentation, we describe the key specifications of the new monochromators and the mode of operations for the multiple featured techniques.

Acknowledgement:
HPCAT operations are supported by DOE-NNSA's Office of Experimental Sciences.
The Advanced Photon Source is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

Pressure-induced phase transition and bandgap decrease in semiconducting Na3Bi(IO3)6

Robin Turnbull[1], Akun Liang[1], Javier González-Platas[2], Dequan Jiang[3], Yonggang Wang[3], Catalin Popescu[4], Plácida Rodríguez-Hernández[2], Alfonso Muñoz[2], Jordi Ibáñez[5], Daniel Errandonea[1]

[1]University of Valencia, Spain, [2]University of La Laguna, Spain, [3]Center for High Pressure Science and Technology Advanced Research, Beijing, China, [4]ALBA Synchrotron, Spain, [5]Geosciences Barcelona (GEO3BCN-CSIC), Spain

Synthesis and Properties of Novel Materials 2, July 26, 2023, 10:15–12:15

Metal iodates exhibit a range of interesting physical properties due to their pseudo-layered crystal structure and lone electron pairs associated with their constituent iodine atoms. The pressure evolution of the properties of metal iodates is often extremely non-linear and it has been a focus of investigation in our group over recent years[1]. In this contribution we report a combined experimental/theoretical high-pressure study of $Na_3Bi(IO_3)_6$ under compression to 11.2 Ga at ambient temperature[2]. This compound has been shown to exhibit a highly intriguing crystal structure with one-dimensional BiI_6O_{18} chains[3]. Through a combination of single-crystal and powder synchrotron X-ray diffraction, optical absorption measurements and ab initio density functional theory calculations we unambiguously show a first-order pressure-induced phase transition at around 9.5 GPa new crystalline structure. The triclinic (P-1) to triclinic (P1) phase transition was investigated by DFT calculations, which found the β-phase to be more stable above 9.25 GPa, in excellent agreement with experiment. The phase transition is also characterised by an indirect → indirect electronic bandgap decrease of approximately 0.1 eV as measured by absorption spectroscopy (3.44(1) → 3.32(1) eV) due and a pressure induced increase in the average I-O bond length. The pressure evolution of the crystal lattice parameters and isothermal compressibility tensor of the ambient pressure phase of $Na_3Bi(IO_3)_6$ are also reported, which reveal highly anisotropic compressibility and a bulk modulus of 30.4(7) GPa.

Polymorphism of Luminescent Materials at High-Pressure and Why Crystal Orientation Matters

Dr hab. Anna Makal[1], Dr Daniel Tchoń[2], Róża Jastrzębska[1]
[1]University Of Warsaw, Faculty Of Chemistry, Warsaw, Poland, [2]Lawrence Berkeley National Laboratory, Berkeley, United States

Instrumentation and Techniques 1, July 26, 2023, 10:15–12:15

Solid state luminophores make inviting targets for high-pressure structural studies owing to their sensitivity to molecular and crystalline environment. Application of quasi-hydrostatic pressure can serve as a means to modify crystalline environment in a controllable manner or induce phase transitions. As a result, applied pressure can modify and regulate chemical bonding, intermolecular interactions and derived physicochemical properties, such as UV-vis absorption (manifested as sample color) [1] or emission wavelength and efficiency [2].

Unfortunately, experiments performed at high pressure in a diamond anvil cell (DAC) yield inherently biased intensities and incomplete datasets. The lack of completeness alone may impede space group determination, render solution of a crystal structure or determination of absolute configuration impossible, and conceal or misrepresent fine details such as disorder or unusual charge density distribution (Fig. 1). While data completeness is less of an issue in a regular crystal system, where abundance of symmetry elements allows for the retrieval of almost all unique reflections with satisfactory redundancy, the majority of interesting organic and organometallic materials tend to crystallise in lower-symmetry systems (like monoclinic) or transform to low-symmetry phases at higher pressures. The fact that sample orientation in a DAC can improve reciprocal space coverage is generally acknowledged throughout the high-pressure crystallographic community [3,4]. However, the extent to which data completeness can be improved by proper sample placement and how much can actually be gained by it has not been systematically investigated until recently.

Here I will present examples where carefully planned in-house experiments and controlled sample orientation allowed to study pressure-induced, symmetry-lowering phase transitions in luminescent organic [5] and organometallic gold(I) based materials. Effective sample orientation and careful data processing has ensured over 90% coverage even for the monoclinic system and enabled access to complete systematic extinction patterns. As a consequence, space groups could be properly determined far all investigated phases, resulting in unrestrained structure refinements and detailed description of subtle second order phase transitions occurring in these materials.

[1] Nogueira, B. A., Castiglioni, C.; Fausto, R., (2020). Communications Chemistry, 3, 2399–3669.
[2] Tchoń, D., Trzybiński, D., Wrona-Piotrowicz, A., Makal, A., (2019). CrystEngComm, 21, 5845–5852.
[3] Dziubek, K., Katrusiak, A., (2002). Defect Diffus. Forum, 208-209, 319-322.
[4] Dawson, A., Allan, D.R., Parsons, S., Ruf, M., (2004). J. Appl. Cryst., 37, 410-416.
[5] Tchoń, D., Makal, A., (2021). IUCrJ, 8, 1006-1017.

AM would like to acknowledge financial support from Polish National Science Centre OPUS grant No. DEC-2021/41/B/ST4/02760 and computational grants from PLGrid (amakalhp5, plgmakahp6).

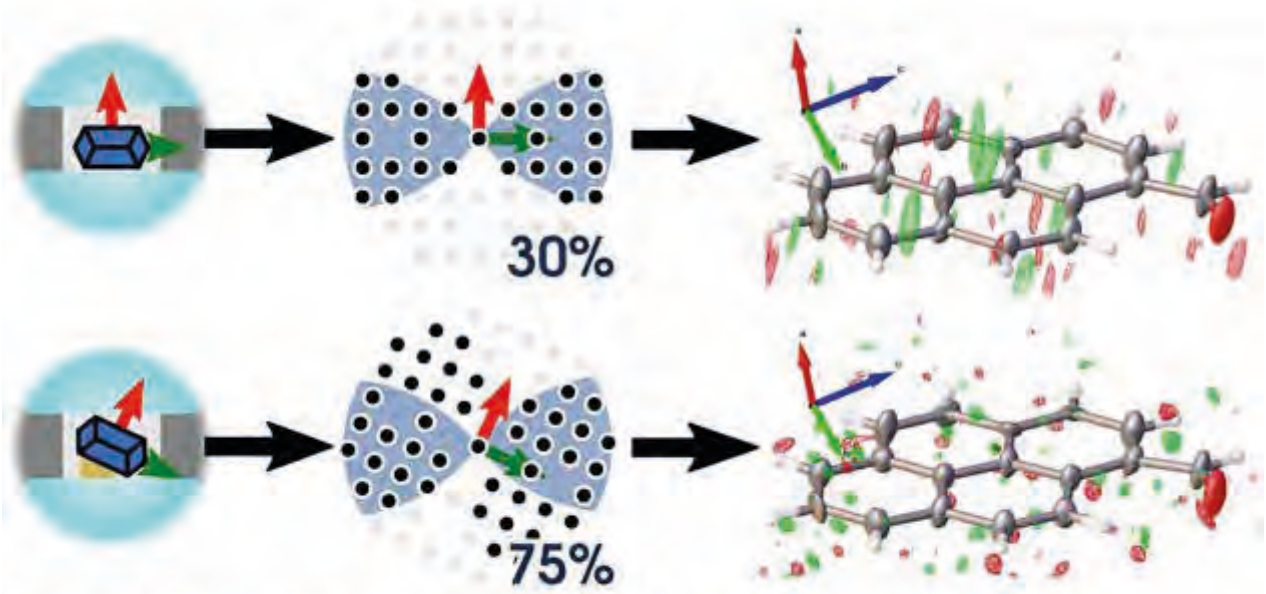


Figure 1. The crystal orientation in a DAC affects attainable data completeness, molecular geometry the residual density map.

Response of a few-layer graphene to high shear stress

Professor Alexander Soldatov
[1]*Center for High Pressure Science, State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, China*

Nanoscale Systems, July 24, 2023, 16:30–18:30

Graphene has been in the focus of materials research over a decade due to the superior physical properties it exhibits. Yet its behavior under high pressure and shear stress still not well understood. We conducted an in-situ Raman study of a few-layer graphene in powder form under high pressure and shear stress in a rotational diamond anvil cell. The recovered from high pressure samples were characterised by HRTEM and multi-wavelength Raman. Spectral mapping revealed high inhomogeneity of the Raman spectra across the sample: a minor change in the spectra in the centre vs very high increase of defect concentration (D-band intensity) on the sample periphery. Remarkably, the graphene structure was totally ruined in between, where certain combination of shear- and normal stress was reached. We interpret the data in terms of specificity of shear stress distribution in the pre-compressed sample. Our results provide deeper insight into the structural transformation of graphene exposed to different type of stress and demonstrate that shear stress at certain level may become the factor limiting performance (or even causing damage) of the stress sensors based on this strongest material.

Phase diagram of hot dense superionic ice probed by synchrotron X-ray diffraction.

Gunnar Weck[1]
[1]*CEA DAM DIF, Arpajon, France*

Ice, Water and Clathrates, July 24, 2023, 10:15–12:15

Water exhibits a complex phase diagram, with a large diversity of structures built from tetrahedral arrangements between hydrogen-bonded water molecules. Above 3 GPa, ice structures are based on body-centred cubic (bcc) oxygen sublattice. Upon heating, the hydrogen bond weakens and ice is expected to transform into a superionic (SI) phase in which a rigid oxygen sublattice coexists with mobile protons. Since its prediction in 1988 [1], this exotic form of water has garnered considerable attention as it could play a major role in the peculiar magnetic field of Uranus and Neptune. After more than twenty of theoretical investigation, first experimental reports of superionic conduction in water ice was obtained from transport and optical measurements [2]. However, due to the challenging P-T conditions and its highly reactive nature, experimental information's on SI ice remain scarce and contradictory.

We will present a detailed structural study of water ice up to 200 GPa and 2500 K. We have performed synchrotron X-ray diffraction measurements on water samples in diamond anvil cells under resistive laser, CO2 or YLF heating [3,4,5]. This allowed us to identify two new ice phases, of bcc and fcc structure, and to determine their stability field. Moreover, by finely probing their P-T evolution, we were able to confirm the SI character of these dense and hot phases and identify the first-order nature of the transition between insulating and superionic ices. Our observations will be compared to other recent experiments and computer simulations, and an experimental phase diagram will be proposed.

[1] P. Demontis, R. LeSar, and M. L. Klein, Phys. Rev. Lett. 60, 2284 (1988)
[2] M. Millot, S. Hamel, J. R. Rygg, P. M. Celliers, G. W. Collins, F. Coppari, D. E. Fratanduono, R. Jeanloz, D. C. Swift, J. H. Eggert, Nature Physics. 14, 297–302 (2018).
[3] J.-A. Queyroux, J.-A. Hernandez , G. Weck, S. Ninet, T. Plisson S. Klotz,G. Garbarino, N. Guignot, M. Mezouar, M. Hanfland, J.-P. Itié , and F. Datchi, Phys. Rev. Lett. 125, 195501 (2020)
[4] G. Weck, J-A. Queyroux, S. Ninet, F. Datchi, M. Mezouar, and P Loubeyre, Phys. Rev. Lett.
[5] A. Forestier, G. Weck, S. Ninet, F. Datchi, G. Garbarino, O. Marie, M. Mezouar , P. Loubeyre, in preparation

Structural transitions and electride properties in the phase diagram of magnesium

Dr Sabri Elatresh[1], Dr Stanimir Bonev[2]
[1]King Fahd University (KFUPM), Dhahran, Saudi Arabia, [2]Lawrence Livermore National Laboratory, Livermore, United States

Computational Studies of Elements, July 26, 2023, 10:15–12:15

The phase diagram of magnesium has gained significant attention, because of its structural properties, electride formation, and melting behaviour. In this study, we utilise a structure prediction method based on the liquid state and combined with first-principles calculations, to re-examine the solid phase stability of magnesium at high pressures. Additionally, analysis of various solid Mg structures will be discussed.

Acknowledgment: This work supported by King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia, Deanship of Scientific Research through Project No. SR211002. The work at LLNL was performed under the auspices of the U.S. DOE, Contract No. DE-AC52-07NA27344.

PBE-GGA predicts the B8↔B2 phase boundary of FeO at Earth's core conditions

Dr. Zhen Zhang[1], Dr. Yang Sun[1,2], **Prof. Renata Wentzcovitch**[1]
[1]Columbia University, New York, United States, [2]Iowa State University, Ames, United States

Phase Diagrams – Ionic Systems, July 24, 2023, 10:15–12:15

FeO is a crucial component of the Earth's core, and its thermodynamic properties are essential to developing more accurate core models. It is also a notorious correlated insulator in the NaCl-type (B1) phase at ambient conditions. It undergoes two polymorphic transitions at 300 K before it becomes metallic in the NiAs-type (B8) structure at ~100 GPa. Although its phase diagram is not fully mapped, it is well established that the B8 phase transforms to the CsCl-type (B2) phase at core pressures and temperatures. Here we report a successful ab initio calculation of the B8↔B2 phase boundary in FeO at Earth's core pressures. We show that fully anharmonic free energies computed with the PBE-GGA coupled with thermal electronic excitations reproduce the experimental phase boundary within uncertainties at P > 255 GPa, including the largely negative Clapeyron slope of –52 MPa/K. This study validates the applicability of a standard DFT functional to FeO under Earth's core conditions and demonstrates the theoretical framework that enables complex predictive studies of this region.

Acknowledgement:
Research supported by DOE Grant DE-SC0019759 and NSF Grant EAR-1918126.

Tunnelling and Andreev spectroscopy studies on H3S

Feng Du[1]
[1]*Max Planck Institute for Chemistry, Mainz, Germany*

Hydrides 4, July 26, 2023, 14:00–16:15

High-temperature conventional superconductivity in hydrogen-rich compounds at high pressures, first discovered in H3S1 has been developed and comprehensively studied in many experimental and theoretical works. Despite the high-pressure conditions, which severely limit the number of available experimental techniques, some basic characteristics of H3S and other hydride-family superconductors have been established, such as London penetration depth and coherence length2-4. However, determination of the superconducting gap, a microscopic manifestation of the superconductivity is a big challenge for high-pressure experiments.

Here we developed the planar tunnelling junction technique at high pressures and demonstrated the evidence of superconductivity in hydrides by electronic transport spectroscopy. We studied H3S, LaH10 as well as pure sulphur under high pressure up to ~200 GPa. We observed superconducting tunnelling behaviours and Andreev reflections below the critical temperature Tc and determined the superconducting gap value and the gap symmetry. These results as well as the temperature and magnetic field dependence of the superconducting gap can be described in the framework of BCS theory. Our results elucidate the superconducting mechanism in hydrides from a microscopic point of view.

[1] A. P. Drozdov et al., Nature 525, 73 (2015)
[2] V. S. Minkov et al., Nat Commun 13, 3194 (2022)
[3] F. Capitani et al., Nature Phys 13, 859–863 (2017)
[4] S. Mozaffari et al., Nat Commun 10, 2522 (2019)

Acoustic wave velocities in Mars' mantle minerals

Frederic Bejina[1], Caroline Bollinger[1], Misha Bystricky[1], Pascal Munsch[1], Matthew Whitaker[2,3], Man Xu[4], Tony *Yu[4], Yanbin Wang[4], Haiyan Chen[2,3]*
[1]IRAP, CNRS, University Toulouse III, Toulouse, France, [2]Department of Geosciences, Stony Brook University, Stony Brook, United States, [3]Brookhaven National Laboratory, Upton, United States, [4]Center for Advanced Radiation Sources, The University of Chicago, Chicago, United States

Mantles of Terrestrial Planets, July 27, 2023, 14:00–16:00

With the successful landing of a seismometer (SEIS) at the surface of Mars (Mars InSight mission), the interior structure of the red planet is now better constrained. However, these advances raise further questions as mineralogical models of the interior of Mars are debated. Mineral physics experiments conducted at high temperature and pressure (HT/HP) are essential to accurately measure the physical properties of the materials that potentially constitute the Martian mantle. In particular the thermoelastic parameters of possible mantle mineral phases are needed to interpret the seismic data and construct accurate models of mineralogical composition and structure of the Martian upper mantle.

We will present our results on the measurements of elastic properties of representative minerals from Mars' mantle. The experiments were performed on synthetic aggregates of olivine and of pyroxene under HP-HT in large volume presses installed at beamlines X17B2 (NSLS, Brookhaven National Lab., Upton NY, USA) and 13-ID (APS, Argonne National Lab., Chicago IL, USA). Equations of state and sound wave velocities were determined by coupled synchrotron X-ray diffraction and ultrasonic interferometry. Implications for the mineralogical composition of the upper mantle of Mars will be discussed.

Exploring phase diagrams, structures and properties at high resolution at ID06-LVP.

Wilson Crichton[1]
[1]*ESRF – The European Synchrotron, Grenoble, France*

Facility Development 2, July 27, 2023, 14:00–16:00

The ESRF's large-volume press beamline, ID06LVP, has been in User operation for 10 years (e.g. Guignard & Crichton, 2015). It complements the ESRF's already wide-ranging extreme conditions portfolio by offering, primarily, in situ angle-dispersive diffraction-based experimentation with a multi-anvil device that operates in one-and two-stage modes. Through use of independent anvils, both normal compression, with high degrees of triaxiality, and deformation data collections are possible. In the EBS configuration, it operates with continuous acquisition in pressure, temperature, time space through use of a custom-built CdTe detector, allowing for rapid assessment of phase diagrams, reactions (and rates) and, under static conditions, sufficiently resolved data for structure solution and refinement. Ancillary techniques often supplement the primary diffraction measurements (conductivity, resistivity, ultrasound, &c); thus, providing the complementarity of transport and physical properties measurements required by materials exploration in solid-state physics, chemistry and geosciences. In this presentation, we highlight the evolution of the main design features of the instrument during this period of continuous User operation. We will give an overview of the current operational status as part of the ESRF's EBS and expectations for future technologies. During these, we will draw-upon data and examples from in-house testing and User operation to illustrate features and the typical uses from various fields of research.

Hydrogen molecules in competition with superconductivity

Graeme J Ackland[1], Sebastiaan van der Bund, Miriam Marques, Miriam Pena Alvarez, Miguel Martinez Canales, Peter Cooke
[1]*University of Edinburgh, Edinburgh, United Kingdom*

Hydrides 2, July 24, 2023, 16:30–18:30

55 years have passed since Ashcroft laid out the principles of hydrogen-based superconductivity. The basic idea is simple: the high frequencies associated with light atoms will give strongly-bound Cooper pairs which survive to high temperatures. The practical difficulty is that this pairing is in competition with a more prosaic one: covalent bonding.

In pure solid hydrogen, extreme pressures are required to break the molecules. It has recently become clear that one can reduce the necessary pressure by alloying to form hydrides, and the challenge has shifted to determining which are the most promising candidates. Binary alloys have been exhaustively studied by electronic structure calculations and BCS theory, which can typically predict Tc to within 50%. However, the combinatorix involved for tertiary alloys makes comprehensive searches, theoretical of experimental, impractical.

Going from material to Tc provides little insight for why high pressure seems to be necessary, and which materials will yield high Tc: the two record-breaking hydrides, of sulphur and lanthanum, come from very different parts of the periodic table, and their atomic hydrogen fraction – inferred from calculation – are very different at H3S and LaH10.

Here we approach the problem from the opposite direction – rather than calculating superconductivity, we investigate the principles involved in disrupting covalent bonding. We start by demonstrating that covalent bonding is a meaningful concept inside high pressure solids. We show how materials such as LaH10 exhibit competition between molecular and atomic hydrogen, and how the atomic structures are favoured by high electron density, by temperature and by confinement of atomic hydrogen in interstices. We also show that zero-point motion can have a significant contribution to breaking bonds, providing a severe challenge to calculations.

The work also illustrates how density functional theory calculations follow the octet rule in chemistry to surprisingly high temperatures: that precursors to atomic-metallic hydrides typically contain enough H- ions to compensation for the cation charge, with remaining hydrogen forming molecules which break symmetry in static relaxation calculations but are short-lived enough that the symmetry is restored at higher temperature.

See e.g. https://arxiv.org/abs/2303.01441

High-pressure synthesis of light lanthanide dodecaborides (RB_{12}) : Synthesis condition, valence fluctuation and bulk moduli

Dr. Hitoshi Yusa[1], Prof. Fumitoshi Iga[2], Dr. Hiroshi Fujihisa[3]
[1]National Institute for Materials Science, Tsukuba, Japan, [2]Institute for Quantum Beam Science, Ibaraki University, Mito, Japan, [3]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

Nitrides, Borides and Carbides 1, July 24, 2023, 14:00–16:00

Light lanthanide dodecaborides (RB_{12}, R = Ce, Pr, Nd, and Eu) were synthesised from a stoichiometric mixture of hexaborides (RB_6) and boron using a laser-heated diamond anvil cell at high temperature under high pressure. Due to the lanthanide contraction, it is expected that the crystallization of RB_{12} with lower atomic number will require a high pressure to stabilise the UB_{12}-type face centered cubic (fcc) structure. The NdB_{12} and PrB_{12} could be synthesised under 28 and 35 GPa, respectively, as expected. Contrary to the expectations, cerium dodecaboride (CeB_{12}) crystallises at 26 GPa, which is significantly lower than that required to synthesise the heavier praseodymium dodecaboride (PrB_{12}). The XRD data clearly indicates that the a-axis of fcc CeB_{12} is exceptionally short compared with the systematic relationship among the other lanthanide dodecaborides. XANES spectra of the recovered samples shows the valence of the cerium in CeB_{12} was assumed to be Ce3.3+, suggesting a valence fluctuation [1]. The valence fluctuation reduces the cationic mean radius and lattice parameters, and thus also reduces the synthesis pressure. On the other hands, the synthesis pressure of EuB_{12} (22 GPa) is somewhat higher than the expected pressure (ca. 14 GPa). Probably, the low valence state of europium (Eu2+) in EuB_6, used as a starting material, could require excessive pressure to incorporate europium cation into the RB_{12} structure.

The change of polyhedral coordination style from a truncated cube in RB_6 to a truncated octahedron in RB_{12} and associated shortening of the R−B bond length result in an increase in bulk modulus and hardness. The bulk moduli of dodecaborides (B_0 = 205–220 GPa) are approximately 20% larger than those of hexaborides despite the reduction in density. The hardness calculated by DFT methods [2] indicates high hardness of RB_{12} (Hv ~ 38 GPa) as compared to RB_6 (Hv ~ 23 GPa). Both bulk modulus and hardness are not so dependent on the cation type in RB_{12}. Therefore, the structural rigidity arises from the evolution of boron cluster from B_6 octahedron in RB_6 to B_{12} cubo-octahedron in RB_{12}.

[1] H. Yusa, F. Iga, and H. Fujihisa, Inorg. Chem., 61, 2568-2575 (2022).
[2] Y. Tian, B. Xu, and Z. Zhao, Int. J. Refract. Met. Hard Mater., 33, 93-106 (2012).

Use of FEA for temperature gradient determination inside a high-pressure sample assembly

Vili Grigorova[1], Michael Howie[1], Benedict Heinen[2], Oliver Lord[2], Simon M. Clark[1]
[1]Macquarie University, Macquarie Park, Australia, [2]University of Bristol, Bristol, United Kingdom

Computational Methods, July 25, 2023, 10:15–12:15

High-pressure experiments are essential for studying materials under extreme conditions. Experimental data on the thermal expansion of crustal and mantle materials can be used to constrain the Earth's adiabatic geotherm. The density of minerals is also crucial in modelling the mineralogy of the deep Earth. When combined with experimental investigations of high-temperature dislocation and creep recovery, grain growth, and boundary lattice diffusion, experimental data can aid in determining kinetic processes that contribute to the generation, implementation, and evolution of magmatic bodies. These findings are critical for the interpretation of geophysical data. Furthermore, high-pressure experiments offer a wide range of conditions that are optimal for synthesizing new materials, such as superconductors and superhard materials.

Accurate temperature measurement is crucial for understanding the behaviour of materials under high pressure. In the laboratory, temperature is typically measured using a thermocouple and pressure is determined through a fixed-point calibration method. Both methods have considerable uncertainties. For example, thermocouples are usually placed outside the sample to avoid chemical reactions, which can introduce uncertainty due to temperature gradients.

Finite element analysis (FEA) is a powerful computational tool that can simulate the response of complex structures to external factors. It is based on the finite element method, which can model small changes in the object in response to changing conditions. In this study, we used FEA to model the temperature distribution inside high-pressure sample assemblies of various volumes. We used the finite element method to model the response of the samples to changing conditions and the resulting temperature distribution inside the assemblies.

Our FEA simulations showed that we could accurately calculate the temperature distribution inside high-pressure sample assemblies. This computational technique provides information about the average temperature and the temperature gradient within the sample. We found that FEA was a cost-effective and efficient alternative to traditional methods of temperature gradient measurement. In addition, FEA allows rapid optimization of a sample assembly to give a more uniform temperature distribution with considerable savings in both coat and time.

The use of FEA has the potential to revolutionise the way high-pressure experiments are conducted. By providing a faster, more accurate, and cost-effective way to measure temperature, FEA could lead to new discoveries in the field of materials science. However, there are still limitations to the use of FEA, such as the need for accurate material properties and assumptions about the heat transfer mechanisms. To further enhance the accuracy of the FEA models, future research endeavours may entail conducting measurements of the thermal conductivity, specific heat, and density changes under varying pressure and temperature conditions.

Molecular dynamics study of thermally-activated plastic transition in Ammonia Hemihydrate under intense pressure

Niccolo Avallone[1], Leon Andriambariarijaona[3], Simon Huppert[1], Philippe Depondt[1], Riccardo Spezia[2], Frederic Datchi[3], Sandra Ninet[3], Fabio Finocchi[1]
[1]INSP – Sorbonne University, Paris, France, [2]LCT – Sorbonne University, Paris, France, [3]IMPMC – Sorbonne University, Paris, France

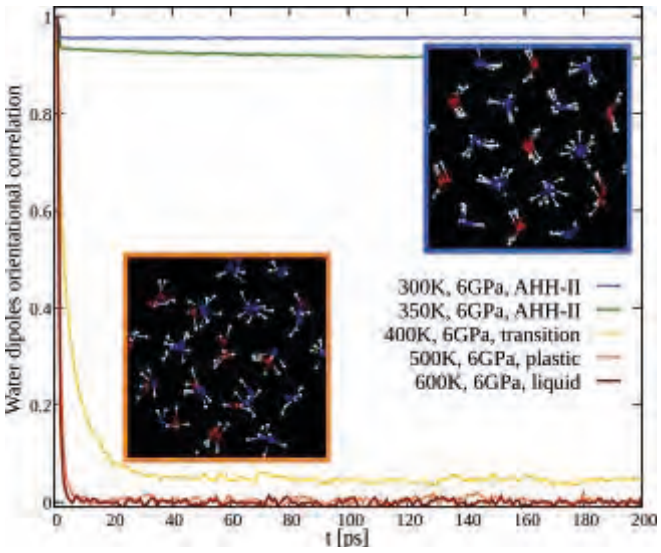
Molecular Compounds, July 25, 2023, 10:15–12:15

Ammonia hydrates are the simplest systems with mixed oxygen-nitrogen hydrogen bonds. They present a interesting variety of solid phases when compressed to extreme pressures. These conditions are coherent with the interior of giant iced planets, such as Uranus and Neptune. It has been shown that ammonia hydrates form different mixtures, depending on the respective concentrations. Ammonia MonoHydrate (AMH) is a candidate for the composition of iced planets. Nevertheless, AMH forms a different mixture, namely Ammonia HemiHydrate (AHH), when compressed to 3.5GPa at room temperature [1]. Various studies have shown the existence of two solid phases between ~3GPa and ~29GPa at room temperature, namely molecular, monoclininc phase-II (AHH-II) and a Disordered Molecular Alloy (AHH-DMA) [2] [3]. Moreover, numerous plastic and superionic phases are predicted for very high pressures at room temperature [4].

The AHH phase diagram in the range 0-30GPa and 300K-600K has been recently explored in detail via Raman and infrared spectroscopy, and X-ray diffraction [5]. Two new solid phases were highlighted in the region where only AHH-DMA was previously observed. Both phases present a bcc structure and they differ in the type of disorder: plastic at high temperature and static disorder at higher pressures. This updated experimental phase diagram inspired our theoretical investigation. We conducted molecular dynamics simulations via the TinkerHP package between 300K and 600K, and pressures range between 2GPa and 18GPa. In order to speed up the calculations, we use the flexible OPLS-all atoms force field for the ammonia molecules, coupled with a SPC flexible model for the water molecules. Using GPU architecture, we were able to simulate systems up to 132k atoms, as long as several tens of nanoseconds per trajectory. Classical Langevin molecular dynamics simulations (both in NVT and NPT ensembles) were analysed. In addition, Nuclear Quantum Effects were included via Adaptive Quantum Thermal Bath and Path Integral Molecular Dynamics [6].

The large dimensions of the system allowed the computation of structure factors with high k-resolution, to be directly compared with experimental X-ray diffraction, in order to determine the bulk structure of the different solid phases. Moreover, we reproduced with remarkable precision the phase transition lines, determining the transition temperatures and pressures, free from finite-size effects. Finally, we computed dynamical observables, such as molecular dipole orientational correlations, diffusion coefficients and hydrogen bonds lifetimes. Thus, we are able to show the predicted plasticity and static disorder of the new phases from a microscopical point of view and explain the mechanism underling the ordered-plastic phase transition.

[1] C. W. Wilson et al., 2012, J. Chem. Phys. 136, 094506 https://doi.org/10.1063/1.3686870
[2] C. W. Wilson et al., 2015, J. Chem. Phys. 142, 094707 https://doi.org/10.1063/1.4913684
[3] C. Ma et al., 2012, RSC Adv., 2, 4920-4924 https://doi.org/10.1039/C2RA01156E
[4] V. N. Robinson and A. Hermann, 2020, J. Phys.: Condens. Matter 32 184004 https://doi.org/10.1088/1361-648X/ab68f7
[5] L. Andriambariarijaona PhD Thesis, 2020, unpublished https://www.theses.fr/en/s266539
[6] S. Huppert et al., 2022, Appl. Sci. 12, 4756. https://doi.org/10.3390/app12094756


Water dipoles orientational correlation
t [ps]
300K, 6GPa, AHH-II
350K, 6GPa, AHH-II
400K, 6GPa, transition
500K, 6GPa, plastic
600K, 6GPa, liquid

Non-random fluid mixtures, present and future: the case of methane and water

Ciprian Pruteanu[1], Victor Naden Robinson[3], Sandro Scandolo[2], Ali Hassanali[2], Graeme Ackland[1], John Loveday[1]

[1]Centre for Science at Extreme Conditions, School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom, [2]Abdus Salam International Centre for Theoretical Physics, Trieste, Italy, [3]Department of Earth and Planetary Science, University of California, Berkeley, Berkeley, United States

Ice, Water and Clathrates, July 24, 2023, 10:15–12:15

Binary fluid mixtures have been at the core of thermodynamics and chemistry from the beginning of the fields, driven largely by interests in distillation and beverage production. Interests have evolved since then, with nowadays methane-water mixtures holding a privileged position among binary mixtures. Apart from both components being abundant on and inside our planet, and throughout the Solar System, they are a model system of non-random mixing, where one component (water) preferentially forms bonds (H-bonds). This turns methane-water mixtures into the first building block for our current understanding of hydrophobic and hydrophilic interactions, dictating behaviours ranging from convection and properties of planetary bodies (Neptune, Titan) to cell wall formation and protein folding.

A few years ago, in a series of studies we have found that the solubility of methane in water increases with pressure, from almost fully immiscible (<1 mol %) up to 1.3 GPa to an almost 1:1 mixture (40 mol %) at 2 GPa. To elucidate the reasons behind this entirely unforeseen change, we have employed coupled neutron diffraction measurements and long-term large-system ab initio molecular dynamics calculations. These revealed that despite the increase in methane's solubility water retains an almost intact H-bond network (97 % bonded in comparison to pure water), which is also complemented by methane experiencing a 3-fold increase in its dipole moment (~10 % that of water).

In this talk we will discuss several key aspects to be considered when dealing with such non-random mixtures and how to mitigate against the artefacts that may be introduced. Such artefacts can lead to both false positives and false negatives, and so lead to a deeply inaccurate description of binary systems and their properties. We will discuss in detail the impact of chosen system size and geometry, for both real-space structure extraction methods (Reverse Monte Carlo – Empirical Potential Structure Refinement) and purely computational ones, such as classical and ab initio molecular dynamics simulations.

Finally, we aim to provide some hope for the future, and discuss a novel methodology that blends coherently real space data refinement methods for disordered systems with Density Functional Theory-based calculation, allowing the data to steer the calculations directly and these in turn to adjust on-the-fly the atomic and molecular models and properties with which the data is fitted. Such a method would ensure a coherent and accurate description of disordered systems like single and multi-component glasses and fluids from the atomic level up to the bulk, macroscopic one.

Effect of surface tension on the ferropericlase morphology of the Earth's lower mantle

Dr Amrita Chakraborti[1], Dr Hongzhan Fei[1], Dr Artem Chanyshev[1], Prof. Yu Nishihara[2], Dr Noriyoshi Tsujino[3], Dr Marcel Thielmann[1], Prof. Dr. Tomo Katsura[1]
[1]University Of Bayreuth, Bayreuth, Germany, [2]Ehime University, Japan, [3]Spring 8 synchrotron, Japan

Mantles of Terrestrial Planets, July 27, 2023, 14:00–16:00

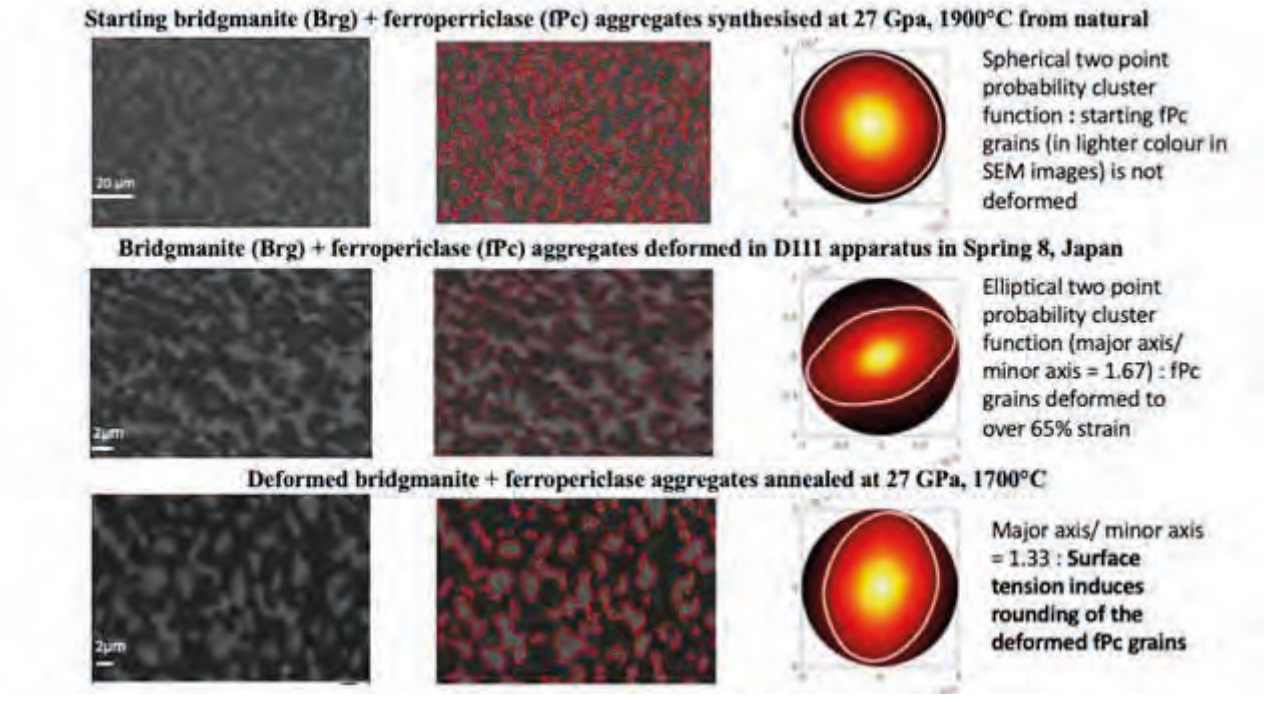
Understanding the rheology of the lower mantle of the earth is crucial for our understanding of the evolution of the earth. However, not much is known about the rheology because of the high pressures, temperatures and very large total strains involved.

The lower mantle is mainly composed of bridgmanite (80%) and ferropericlase (20%). Thus, bridgmanite should ideally control lower mantle viscosity because of its larger fraction (Load bearing framework model). However, geological time scales create large total strains that can interconnect ferropericlase grains (interconnected weak layers model)– this would make ferropericlase morphology the controlling factor. The viscosity of the lower mantle would differ by orders of magnitude depending on which model is relevant and therefore, this is a very important question for our understanding of the Earth.

But, in inferring the ferropericlase morphology in the lower mantle, a very important factor to consider is the surface energy which would lead to the aspect ratio of the grains approaching unity over time. In this work, the reduction of the aspect ratio of the deformed ferropericlase grains is called rounding.

We have studied the morphology of ferropericlase grains deformed under high pressure-temperature-high total strain conditions in the D111 apparatus. Then the grains were annealed under different P-T conditions commensurate to the lower mantle. The elongation and then rounding of the grains was statistically evaluated using a two-point probability cluster function.their morphology was again examined using a two point probability cluster function.

This work settles the question whether Load bearing framework model or Interconnected weak Layers model is the correct approach for the Earth's lower mantle.



Revised Phase Diagram of Methane

Dr. Miriam Pena-Alvarez[1], Mengnan Wang[1], Ross T. Howie[1], Eugene Gregoryanz[1,2,3]
[1]Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom, [2]Chinese Academy of Sciences, Hefei, China, [3]Center for High Pressure Science and Technology Advanced Research (HPSTAR), Shanghai, China

Other Molecular Systems, July 27, 2023, 10:15–12:15

Methane plays an important role in fundamental and applicable sciences. Also, it is present in outer Solar planets such as Uranus and Neptune, as well as in the deep Earth, where its state is determined by pressures and temperatures. Therefore, the high-temperature -- high-pressure phase diagram of methane is of fundamental importance to many fields of physics, chemistry, planetary and geological sciences. As the simplest hydrocarbon, CH4 adopts a rich variety of crystal structures that have been extensively studied in a wide pressure and temperature range. (1-4) However, compared to other simple molecular solids its phase diagram and the relationship between solid phases and fluid states is surprisingly not that well established. (5-10)

By combining the high-pressure high-temperature techniques with Raman spectroscopy we have studied the phase diagram of methane up to 40 GPa and 1200K, illustrating the complexity and (meta)stability of its phases. Our results indicate that there are two triple points between the solid and liquid states. Interestingly, we find that the P-T boundaries of the different phases are path dependent, so we will discuss their kinetics, formation and (meta)stability. More importantly, we demonstrate that the melting curve changes slope at one of the triple points and melting happens at temperatures considerably higher than previously thought.

[1] Bini, R., et al., JCMP, 103, (1995): 1353-1360.
[2] Maynard-Casely, H. E., et al., JCP, 133, (2010): 064504.
[3] Bykov, M. et al., PRB 104, (2021): 184105.
[4] Bini, R., et al., PRB, 55, (1997): 14800.
[5] Naumova, A., et al. JPCC 123, (2019): 20497-20501.
[6] Conway, Lewis J., and Hermann A., Geosciences 9, no. 5 (2019): 227.
[7] Hazen, R. M., et al., APL 37, (1980): 288-289.
[8] Abramson, Evan H. HPR, 31, (2011): 549-554.
[9] Yagi, T. , and Hiroto S., Proc. Jap. Aca, 66, (1990): 167-172.
[10] Lobanov, S. S., et al. Nat. Comm.4, (2013): 2446.

M. P.-A. acknowledges UKRI- FLF Mrc-Mr/T043733/1.
R. T. H. acknowledges 948895 “MetElOne”.

Microscopic theory of colour in lutetium hydride

Sun-Woo Kim[1], Lewis J. Conway[1,2], Chris J. Pickard[1,2], G. Lucian Pascut[3], Bartomeu Monserrat[1]
[1]University Of Cambridge, United Kingdom, [2]Tohoku University, Japan, [3]Stefan Cel Mare University, Romania

Hydrides 3, July 25, 2023, 14:00–16:00

Nitrogen-doped lutetium hydride has recently been proposed as a near-ambient conditions superconductor. Interestingly, the sample transforms from blue to pink to red as a function of pressure, but only the pink phase is superconducting. Subsequent experimental studies have failed to reproduce the superconductivity but have confirmed the existence of pressure-driven colour changes. However, these colour changes appear in different sequences and at different pressures depending on the experiment, with observed colours including blue, pink, red, violet, and orange. Given the relationship between colour and superconductivity, understanding colour changes in nitrogen-doped lutetium hydride may hold the key to clarifying the possible superconductivity in this compound. Here, we describe a full microscopic theory of colour in lutetium hydride. We find that hydrogen-deficient LuH_2 is the only phase which exhibits colour changes under pressure consistent with experimental reports, with a sequence blue-violet-pink-red-orange. We also find that the concentration of hydrogen vacancies controls the precise sequence and pressure of colour changes, rationalising seemingly contradictory experiments. Nitrogen doping also modifies the colour of LuH_2 but it plays a secondary role compared to hydrogen vacancies. Therefore, we propose hydrogen-deficient LuH_2 as the key phase for exploring the superconductivity claim in the lutetium-hydrogen system. Finally, we find no phonon-mediated superconductivity near room temperature in the pink phase.

Strong-correlation effects in high-pressure rare-earth superhydrides

PhD Student Siyu Chen[1], Yao Wei[2], Evgeny Plekhanov[2], Samuel Poncé[3], Bartomeu Monserrat[1], Cedric Weber[2]

[1]TCM Group, Cavendish Laboratory, University Of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom, [2]Theory and Simulation of Condensed Matter (TSCM), King's College London, The Strand, London, United Kingdom, [3]Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Chemin des Étoiles 8, B-1348 Louvain-la-Neuve, Belgium

Hydrides 1, July 24, 2023, 10:15–12:15

Rare-earth superhydrides have recently attracted considerable attention in condensed matter physics due to their high-temperature superconductivity at extreme pressure. It has long been known that rare-earth metals have highly localised electrons which can lead to non-trivial strongly correlated interactions between them. However, such interactions are rarely included in the first-principles studies of rare-earth superhydrides due to the complexity of their high-pressure phases. In this work, we propose a novel approach that combines dynamical mean-field theory with the finite displacement method to study both electrons and phonons in strongly-correlated materials on an equal footing. This allows us to investigate the role of electron correlations on the superconducting critical temperatures. We demonstrate the effectiveness of our new method using two prototypal lanthanide superhydrides: LaH10 and CeH9. Our findings indicate that the dominant correction to the critical temperature of LaH10 comes from the correlation-driven changes to its phonon spectrum, while the dominant correction in the CeH9 case is from the renormalization of its electron structure under the strongly correlated interactions. The resulting changes in superconducting critical temperatures can be as high as 50 K. Overall, our approach provides a new avenue for investigating physical properties related to electron-phonon coupling in strongly correlated materials, providing new insights into high-temperature superconductivity.

Material properties of matter in Saturn's interior from ab initio simulations

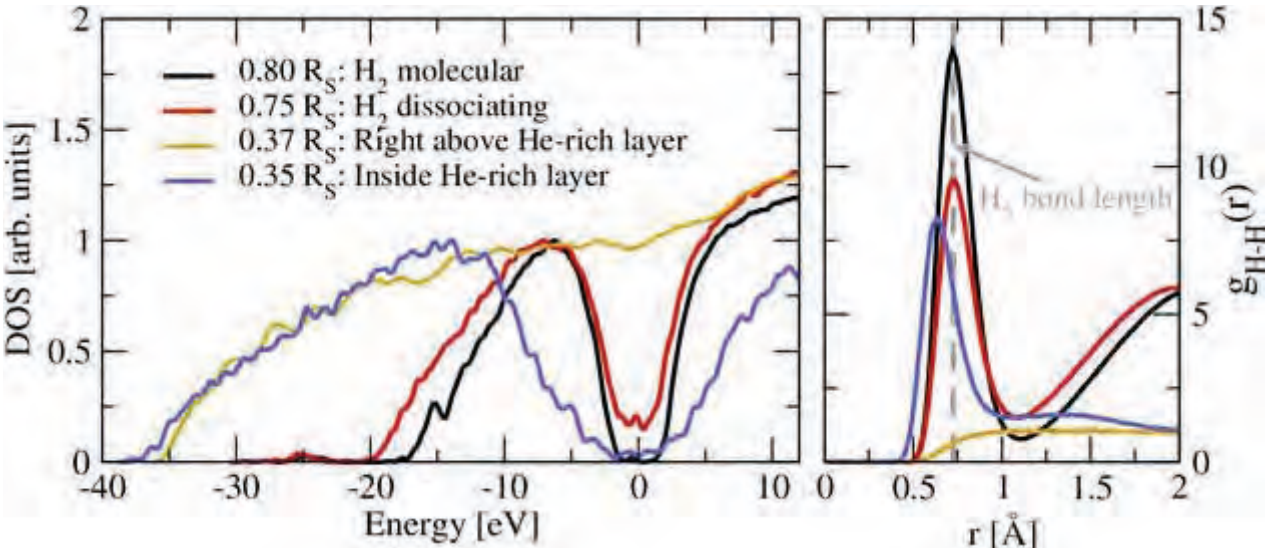
Dr. Martin Preising[1], Dr. habil. Martin French[1], Dr. Christopher Mankovich[2], Dr. Francois Soubiran[3], Prof. Dr. Ronald Redmer[1]
[1]University of Rostock, Germany, [2]California Institute of Technology, Pasadena, United States, [3]Commissariat à l'énergie atomique et aux énergies alternatives, Arpajon, France

Outer Planets and Exoplanets 2, July 26, 2023, 16:30–18:30

Calculation of material properties from ab inito simulations along Jupiter [1] and Brown Dwarf adiabats [2] have been subject of earlier studies. However, accurate models of Saturn's interior are still very challenging. A recent study by Mankovich and Fortney on Jupiter and Saturn models was based on a single physical model [3] which predicts a strongly differentiated helium distribution in Saturn's deep interior, resulting in a helium-rich shell above a diffuse core.

We focus on the calculation of material properties of matter at P-T conditions along the Saturn model proposed by Mankovich and Fortney. The dissociation of hydrogen as well as the onset of the helium-rich layer have profound impact on material properties: Dissociation of hydrogen triggers the metallization of the hydrogen sub-system and the band gap of the system closes. However, helium is still an insulator under all the conditions of the model [4,5]. The onset of the helium-rich layer in the deep interior therefore again changes the properties of the mixture: Molecular hydrogen dominates the outer atmosphere, followed by a layer of mainly metallic hydrogen in the interior, followed again by a layer of helium-dominated insulating material above the core. We present results on thermodynamic and transport properties of a hydrogen-helium-water mixture that closely resembles the element distribution of the Saturn model. We discuss implications of the results on our understanding of Saturn's interior and evolution.

[1] French et al., Astrophys. J. Suppl. Ser., 202, 5 (2012).
[2] Becker et al., Astron. J., 156, 149 (2018).
[3] Mankovich and Fortney, Astrophys. J., 889, 51 (2020).
[4] Monserrat et al., Phys. Rev. Lett., 112, 055504 (2014).
[5] Preising and Redmer, Phys. Rev. B, 102, 224107 (2020).



Neutron scattering study of SrCu2(BO3)2 under high pressure

Mohamed Zayed[1], Ellen Fogh[2]
[1]Carnegie Mellon University in Qatar, Qatar, [2]Laboratory for Quantum Magnetism. École Polytechnique Fédérale de Lausanne, Switzerland

Magnetic Materials 1, July 24, 2023, 10:15–12:15

We present a series of high-pressure elastic and inelastic neutron scattering experiments on the quantum magnet SrCu2(BO3)2. This material is of considerable importance for our understanding of frustrated magnetism as, at low pressure, it realises the exactly solvable Shastry-Sutherland lattice. With coupling parameters close to critical values, it can be pressure-tuned, and we exhibit several novel phases. We also discuss the technical challenges of these high-pressure neutron scattering experiments.

Observation of A15-type LaH~6 at Moderate Pressures

Dr. Israel Osmond[1], Dr. Mikhail Kuzovnikov[1], Dr. Tomas Marqueño[1], Ms. Mylaine Holin[1], Dr. Ross Howie[1,2], Dr. Eugene Gregoryanz[1,2,3], Dr. Miriam Pena-Alvarez[1]
[1]Centre For Science At Extreme Conditions, Edinburgh, United Kingdom, [2]Center for High Pressure Science and Technology Advanced Research (HPSTAR), Shanghai, China, [3]Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Hefei, China

Hydrides 3, July 25, 2023, 14:00–16:00

Recent discoveries of high-temperature superconductivity in metallic hydride compounds at megabar pressures[1,2] have raised the possibility that this traditionally low temperature phenomenon can exist at room temperature. Despite showing evidence for superconductivity at record high temperatures, the extreme pressures necessary to synthesise such compounds provide significant experimental challenges in a field where any claimed superconductivity in such compounds is heavily disputed. Rare-earth hydrides have previously been shown to possess a diverse set of structures that can exist upon laser heating where many structures of varying stoichiometries may be present and remain to be well characterised.

In this work, we experimentally study the formation of La-H compounds at pressures below 100 GPa in a diamond-anvil cell. Clear evidence is shown for the synthesis of A15-type LaH~6 at pressures above 75 GPa. While absent from previous published predicted phases of the La-H system, this phase is in excellent agreement however with prior experimental work above 100 GPa[3] and is observed to be stable upon decompression down to at least 48 GPa. Such measurements raise the possibility that highly symmetric superhydride phases in a system with record critical temperatures may exist down to low or ambient pressure and merit significant future study.

Acknowledgements:
M. P.-A. acknowledges the support of the UKRI Future leaders fellowship Mrc-Mr/T043733/1. We acknowledge the PETRA III synchrotron for allocating beamtime at P02.2 under the proposal I-20221042 and beamline scientist Nico Giordano for assisting our experiments.

[1] A. P. Drozdov, P. P. Kong, V. S. Minkov, S. P. Besedin, M. A. Kuzovnikov, S. Mozaffari, L. Balicas, F. F. Balakirev, D. E. Graf, V. B. Prakapenka, E. Greenberg, D. A. Knyazev, M. Tkacz & M. I. Eremets “Superconductivity at 250 K in lanthanum hydride under high pressures” Nature 569, (2019)

[2] P. Kong, V. S. Minkov, M.A. Kuzovnikov, A. P. Drozdov, S. P. Besedin, S. Mozaffari, L. Balicas, F. F. Balakirev, V. B. Prakapenka, S. Chariton, D. A. Knyazev, E. Greenberg & M. I. Eremets “Superconductivity up to 243 K in the yttrium-hydrogen system under high pressure” Nature Comm. 12 (2021)

[3] D. Laniel, F. Trybel, B. Winkler, F. Knoop, T. Fedotenko, S. Khandarkhaeva, A. Aslandukova, T. Meier, S. Chariton, K. Glazyrin, V. Milman, V. Prakapenka, I. A. Abrikosov, L. Dubrovinsky & N. Dubrovinskaia “High-pressure synthesis of seven lanthanum hydrides with a variability of hydrogen content” Nat. Comm. 13 (2022)

Experimentally observed and computationally confirmed electronic topological transition in cadmium

Jasmine Hinton[1], Daniel Schacher[1], Wonseok Lee[3], G. Alexander Smith[1], Emily Siska[1], Changyong Park[4], Scott K. Cushing[3], Craig P. Schwartz[1], Keith V. Lawler[1], Ashkan Salamat[1]
[1]University of Nevada, Las Vegas, Las Vegas, United States, [2]Nevada Extreme Conditions Laboratory, Las Vegas, United States, [3]California Institute of Technology, Pasadena, United States, [4]Advanced Photon Source, Argonne National Lab, Lemont, United States

Electronic Transitions 1, July 26, 2023, 16:30–18:30

It has long been believed that Cd has an electronic topological transition (ETT) at less than 5 GPa; however, determining if and where this phase transition occurs has been an ongoing challenge due to the difficulty in observing such mechanisms. An ETT is characterised by a non-continuous change of the topology of the Fermi surface and is tied to behaviors like superconductivity or giant magnetoresistance. Structural probes, including X-ray diffraction, have a particularly difficult time characterizing ETTs; structural discontinuities that sometimes occur in correlation to an ETT can be due to other factors such as non-hydrostaticity. Here, using X-ray absorption spectroscopy, we experimentally confirm an electronic topological transition between 0 and 1 GPa and show a technique to understand these phase transitions. Projections of the excitons onto the electronic density of states calculations show that the change in experimentally observed XAS is due to the ETT, and not due to another structural change.

Integrated Neutron Diffractometer at Extreme Conditions (INDEC) at China Spallation Neutron Source (CSNS)

Professor Yusheng Zhao[1,2], Dr. Songbai Han[2], Dr. Jinlong Zhu[2], Dr. Liping Wang[2], Professor Tianjiao Liang[3], Dr. Le Kang[3]

[1]Eastern Institute for Advanced Study, China, [2]Southern University of Science and Technology, China, [3]China Spallation Neutron Source, China

Facility Development 1, July 24, 2023, 16:30–18:30

As one of the cornerstone research platforms within the Shenzhen Material Genome Large-Scale Facilities project, INDEC has been designated as Beamline BL-15 at CSNS and is currently under construction by the Southern University of Science and Technology (SUSTech) and CSNS. The beamline is expected to be commissioned in early 2024, with neutron diffraction and imaging as its primary techniques in conjunction with various sample environments under extreme conditions.

The main design parameters of INDEC are as follows: 1) the d-spacing range (90° detector in the single frame mode): 0.5 – 5 Å; 2) the resolution: $\Delta d/d \leq 0.6\%$ (90° detector); and 3) the neutron flux at the sample position: $> 5 \times 10^6$ n/s/cm^2 @ 100 kW. The extreme sample environments include: 1) high-pressure (P) and temperature (T) [P (max) = 20 GPa, T (max) = 1300 K); 2) low-T and high magnetic field [B (max) = 9 T, T (min) = 4 K]; and 3) high-P percolation (pore pressure ≤ 150 MPa, confining pressure ≤ 200 MPa, deviatoric stress ≤ 300 MPa, and sample temperature: $270\ K \leq T \leq 370\ K$). A suite of pressure devices, such as true triaxial multi-anvil press, piston cylinder, P-E cell, gas/liquid high-P cell, portable cubic press, and ZAP cell, etc., will be used to provide extreme P-T conditions and the flexibility of switching experimental systems between the portable and transferable devices. INDEC is augmented by simultaneous multi-mode in situ measurements for physical parameters such as mechanic, thermal, acoustic, optical, and electrical properties under extreme conditions.

INDEC will provide scientists with a new venue to carry out frontier interdisciplinary research under comprehensive extreme sample environments of high pressure, high/low temperature, and/or high magnetic field. It is expected to have a positive impact on the basic science research in physics, chemistry, materials science, energy science, and earth and planetary sciences, and therefore create ample opportunities for new discoveries in science and technology.

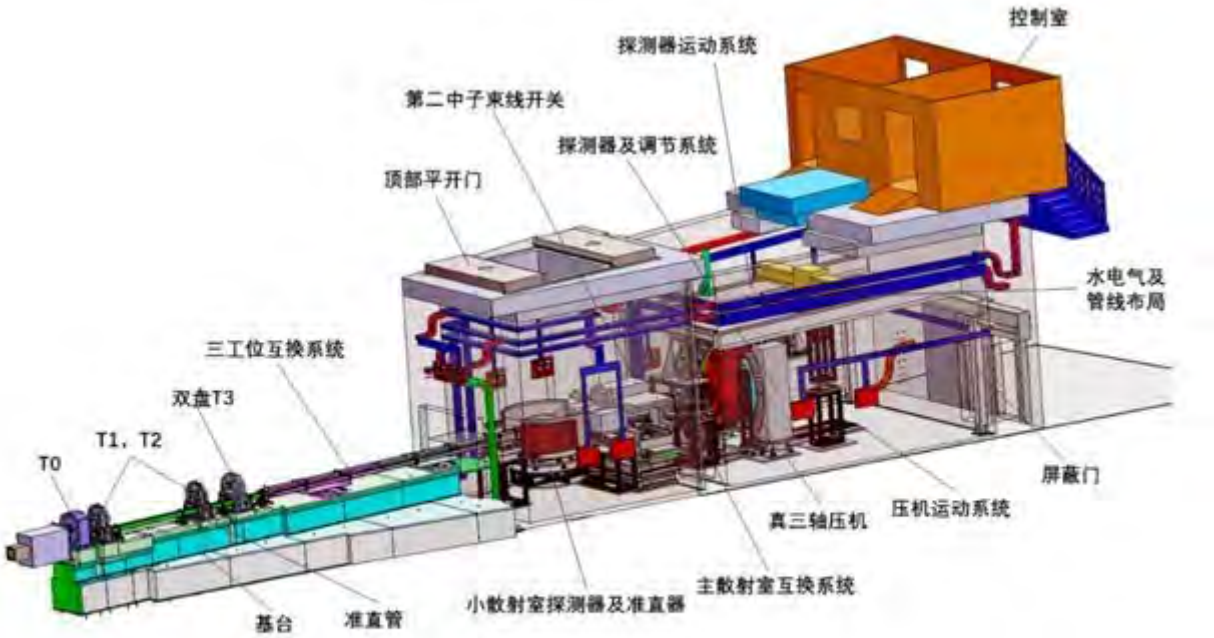


Figure 1. Schematics of the Integrated Neutron Diffractometer at Extreme Conditions (INDEC) at CSNS.

Layered redox processes of post-giant impact Earth, simulated and probed by European-XFEL

Dr. Jinhyuk Choi[1], Dr. Taehyun Kim[1], Dr. Yoonah Bang[1], Ms. Seohee Yun[1], Ms. Jeongmin Lee[1], Ms. Heehyeon Sim[1], Mr. Yeonhak Jung[1], Dr. Rachel Husband[2], Dr. Hanns-Peter Liermann[2], Dr. Heinz Graafsma[2], Dr. Torsten Laurus[2], Dr. Stephan Stern[2], Dr. Cornelius Strohm[2], Prof. Huijeong Hwang[3], Dr. Mungo Frost[4], Dr. Siegfried Glenzer[4], Prof. Stewart McWilliams[5], Dr. Bernhard Massani[5], Dr. Orianna Ball[5], Dr. Matthew Duff[5], Dr. James McHardy[5], Prof. Malcolm McMahon[5], Dr. Elena Bykova[6], Dr. Saiana Khandarkhaeva[6], Dr. Maxim Bykov[7], Dr. Leon Andriambariarijaona[8], Dr. Guillaume Fiquet[8], Dr. Sandra Ninet[8], Dr. Karen Appel[9], Dr. Valerio Cerantola[9], Dr. Anand Dwivedi[9], Dr. Zuzana Konôpková[9], Dr. Motoaki Nakatsutsumi[9], Dr. Jolanta Sztuk-Dambietz[9], Dr. Monica Turcato[9], Dr. Carsten Bähtz[10], Dr. Stella Chariton[11], Dr. Vitali Prakapenka[11], Dr. Hyunchae Cynn[12], Dr. Eric Edmund[13], Dr. Alexander Goncharov[13], Dr. Nicolas Jaisle[14], Dr. Guillaume Morard[14], Prof. Jaeyong Kim[15], Ms. Lan Anh Nguyen[15], Mr. Zhongyan Wu[15], Prof. Clemens Prescher[16], Prof. Ronald Redmer[17], Prof. Yongjae Lee[1]

[1]Department of Earth System Sciences, Yonsei University, Seoul, South Korea, [2]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany, [3]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology (GIST), Gwangju, South Korea, [4]High Energy Density Science Division, SLAC National Accelerator Laboratory, Menlo Park, United States, [5]School of Physics and Astronomy (SUPA), and Centre for Science at Extreme Conditions (CSEC), University of Edinburgh, Edinburgh, United Kingdom, [6]University of Bayreuth, Bayreuth, Germany, [7]Mathematisch-Naturwissenschaftliche Fakultät – Institut für Anorganische Chemie, Universität zu Köln, Köln, Germany, [8]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris, France, [9]European XFEL, Schenefeld, Germany, [10]Radiation Physics / High Energy Density, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany, [11]Consortium for Advanced Radiation Sources, The University of Chicago, Chicago, United States, [12]Physical & Life Sciences, Lawrence Livermore National Laboratory (LLNL), Livermore, United States, [13]Earth and Planets Laboratory, Carnegie Institute for Science, Washington D. C., United States, [14]Université Grenoble Alpes, Université Savoie Mont Blanc, CNRS, IRD, Université Gustave Eiffel, Grenoble, France, [15]Department of Physics, Hanyang University, Seoul, South Korea, [16]Institute of Earth and Environmental Sciences, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany, [17]Institut für Physik, Universität Rostock, Rostock, Germany

Secular Evolution of the Earth, July 25, 2023, 10:15–12:15

The incorporation of volatile elements, such as hydrogen, into the iron core is a crucial factor influencing the complex evolution of the Earth, from their solid interiors to their atmospheres and magnetospheres. The incorporation of hydrogen into the metallic core, in particular, is thought to determine the physical and chemical properties of the core and adjacent regions of lower mantle. In this study, we have investigated the reactions between volatile elements and iron to gain insights into the magma ocean conditions driven by the Moon-forming impact (MFI), which is believed to have dictated the last stages of the evolution of the Earth. We have conducted two different radiative-heating methods using a high-brilliance X-ray free electron laser (XFEL) and an infrared laser, on pre-compressed mixtures of iron and H2O (Fe-O-H system), in order to simulate mixed state of foreign iron from the impactor and original volatiles of the proto-Earth, under the syn- and post-giant impact conditions. Our experiments show that when the iron is compressed at 8.1(1) GPa, near 200 km depth in the magma ocean, and heated up to ~38,000 K, it reacts with H2O to form ferrous oxide (FeO) and hydrides (γ-FeHx), which transform gradually to ε-FeHx below 12.1(1) GPa, i.e., 305 km depth, under the XFEL pump at 2.2 MHz repetition. Similarly, under infrared laser-heating up to ~1,700 K at 50.4(1) GPa, i.e., near 1,255 km depth in the magma ocean, the iron reacts with H2O to form FeO, hydrides (ε-FeHx and FeH2), and hydroxides (ε-FeOOH), which remain stable down to 30 GPa, i.e., near 750 km depth. These findings suggest the possible existence of redox boundaries in the magma ocean near 200–305 km and 750–1,255 km depths, where the reaction products from the Fe-O-H system change and the amount of hydrogen incorporation into the iron increase correlatively with pressure. The Fe(III)/Fe(I) ratios calculated from the quantitative analysis using the Rietveld method decreased with increasing pressures, from 1.01(1) at 10.7(1) GPa via 0.89(1) at 30.2(1) GPa, down to 0.32(1) at 50.4(1) GPa. These results suggest that under higher pressures, not only the incorporation of hydrogen into the iron is more favorable, but the iron prefers more reduced state.

A case study for X-ray imaging at high pressure and temperature

Bernhard Massani[1], Stewart McWilliams[1], Rachel Husband[2,4], Daniel Campbell[3], Hanns-Peter Liermann[2], Daniel Sneed[3], Konstantin Glazyrin[2], Timofey Fedotenko[2], Thea Engler[2], Johannes Hagemann[2], Zsolt Jenei[3], Earl O'Bannon[3]

[1]The University Of Edinburgh, Edinburgh, United Kingdom, [2]DESY, Hamburg, Germany, [3]LLNL, Livermore, USA, [4]EuXFEL, Schenefeld, Germany

Phase Diagrams – Molecular Systems, July 27, 2023, 14:00–16:00

Our understanding on how opaque materials respond to extreme compression and high temperatures heavily relies on X-ray techniques. While X-ray diffraction is a powerful approach, some properties such as viscosity are experimentally not accessible with such approaches. Other techniques more suitable for this kind of measurement, like X-ray imaging, has been widely applied in extreme pressure and temperature conditions using multi-anvil presses, but obtaining sufficient space and time resolution for similar experiments using diamond anvil cells, at commensurately higher pressure and temperature conditions, have been challenging.

We present recent developments in synchrotron X-ray imaging at the ECB beamline at PETRA III, DESY used in combination with laser heated DAC methods. Simultaneous X-ray imaging and diffraction allows for deeper insight in properties of materials under high pressure as well as the direct correspondence of phase transition diagnostics. We present a case study in the laser-heated diamond anvil cell showing detection of solid-solid and solid-liquid transitions and explore how X-ray imaging can be used to determine viscosity of opaque melts under pressure.

Dynamic Optical Pyrometry of Static High-Pressure Targets under X-ray Free Electron Laser Radiation

Orianna Ball[1], R. Stewart McWilliams[1], Zuzana Konopkova[2]
[1]University Of Edinburgh, Edinburgh, United Kingdom, [2]European XFEL, Schenefeld, Germany

Developments at XFELs & Lasers, July 24, 2023, 14:00–16:00

Pyrometric temperature measurements [1, 2] are central to determining the temperature in very high temperature (T>1000 K) static compression experiments, particularly in laser-heated diamond-anvil cell applications. Pulsed X-ray irradiation, from a hard X-ray free electron laser (XFEL), can also drive samples under static compression to high temperatures [3], to explore conditions previously difficult to achieve using conventional optical laser techniques, while adding in the possibility to use X-ray probing (e.g. diffraction). However, while long proposed [4], the application of pyrometric temperature measurements to X-ray heated matter has never been demonstrated. Here we report time-resolved, direct measurements of temperature using spectrally-resolved streaked optical pyrometry (SOP) of X-ray and optical laser-heated states at the High Energy Density (HED) instrument of the European XFEL. Dynamic temperatures above 1500 K are measured continuously from thermal emission at 450–850 nm, with time resolution on the order of nanoseconds for 1 -200 μs streak camera windows. A collection of typical experiments will be discussed to explore the possibilities and complications of time dependent temperature measurements using optical emission at XFEL sources. These studies investigate the response of matter under hard X-ray irradiation with MHz pulse repetition rates, with targets including zero-pressure foils free-standing in air and in vacuo, and high-pressure samples compressed in diamond anvil cell multi-layer targets. A range of further possibilities for optical measurements of visible light in X-ray laser experiments using streak optical spectroscopy are also explored, including for study of X-ray induced optical fluorescence, which often appears as background in thermal radiation measurements. We establish several scenarios where combined emissions from multiple sources are observed and discuss their interpretation. Challenges posed by using X-ray lasers as non-invasive probes of sample state are addressed.

[1] G. Weck, V. Recoules, J-A. Queyroux, F. Datchi, J. Bouchet, S. Ninet, G. Garbarino, M. Mezouar and P. Loubeyre, Phys. Rev. B, 2020, 101, 14106
[2] A. Dewaele M. Mezouar, N. Guignot, and P. Loubeyre, Phys. Rev. Lett., 2010, 104, 255701
[3] J. Meza-Galvez, N. Gomez-Perez, A. Marshall, A. L. Coleman, K. Appel, H. P. Lier-mann, M. I. McMahon, Z. Konopkova, and R. S. McWilliams, Journal of Applied Physics, 2020, 127, 195902
[4] E. Principi, C. Ferrante, A. Filipponi, F. Bencivenga, F. D'Amico, C. Masciovecchio, and A. D. Cicco, Nuclear Instruments and Methods in Physics Research Section A, 2010, 621, 643–649

Acknowledgments: O.B.B. acknowledges support from the Scottish Doctoral Training Program in Condensed Matter Physics (CM-CDT).

Measurements of melting and pressure calibration at extreme pressure

Yingwei Fei[1]
[1]*Carnegie Institution for Science, Washington, United States*

Outer Planets and Exoplanets 1, July 26, 2023, 10:15–12:15

The fast-past discovery of exoplanets and novel materials at high pressure challenge experimentalists to expand the pressure-temperature range to probe material properties under extreme conditions. We have been developing various high-pressure techniques to extend the P-T range and optimise sample volume for synthesis and characterization. Using Sandia's Z-facility, we have determined the melting temperature of MgSiO3 at 500 GPa along Hugoniot by direct shock compression of dense bridgmanite. The densities of silicate liquid were measured up to 1250 GPa, which would provide critical constraints for modeling the density profile of hot super-Earths. In parallel, we have routinely extended density measurements of solids to multi-megabar pressures using optimised toroidal diamond anvils by in situ synchrotron X-ray diffraction. The equations of state of MgO, NaCl, tungsten, gold, platinum, and iron will be compared to check self-consistency of pressure scales. For large-volume synthesis, we utilise large sintered-diamond cubes (up to 25.4mm) to optimise sample volume, including synthesis of large bridgmanite samples for shockwave experiments. New configuration of assembly is designed to reach simultaneous pressure and temperatures over 32 GPa at 3000 K in the multi-anvil press with relatively large sample and stable heating that has been used to simulate deep magma ocean. These advances have greatly enhanced our ability to investigate internal structure of super-Earths and differentiation of early Earth.

Na-W-H and Na-Re-H ternary hydrides at high pressures

Dr. Tomas Marqueno[1], Dr. Mikhail Kuzovnikov[1], Dr. Ross T Howie[1], Dr. Israel Osmond[1], Mrs. Hannah Shuttleworth[1], Dr. Eugene Gregoryanz[1], Dr. Miriam Pena-Alvarez[1]
[1]*Center for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom*

Hydrides 2, July 24, 2023, 16:30–18:30

The quest for novel high temperature superconductors has prompt the study of binary metal-hydrogen systems at high temperatures, leading to the discovery of superhydrides such as LaH10 or H3S [1, 2]. Nevertheless, these compounds are found at pressures beyond the Mbar, which hinders the possibility of obtaining superconductive materials at room conditions [5]. Conversely, experimental studies have shown that hydrogen-rich ternary compounds can be synthesised at modest high pressures and be recovered near ambient conditions [3, 4]. In addition to this, recent theoretical studies have predicted the existence of high Tc superconductivity in alkaline-transition metal ternary hydrides under compression [6].

In our study we explored the polymorphism of ternary hydrides involving sodium and transition metals from the VI and VII group (rhenium and tungsten) at high pressures. Na-Re-H and Na-W-H compounds were synthesised at high pressures by employing diamond anvil cells and laser heating, which allowed to trigger chemical reactions. Synchrotron angle-dispersive powder X-ray diffraction measurements allowed determining the structures of the new compounds regarding their heavy atoms. These novel polyhydrides were studied under decompression, showing phase transitions to different structures, which were recovered at low pressures.

Acknowledgements:
M. P.-A. acknowledges the support of the UKRI Future leaders fellowship Mrc-Mr/T043733/1. R. T. H. acknowledges that the project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant Agreement No. 948895 "MetElOne"). The PETRA III synchrotron is acknowledged for allocating beamtime at P02.2 under the proposal I-20221042 and beamline scientist Nico Giordano for assisting our experiments. The authors also thank the European Synchrotron Radiation Facility (ESRF) for the beamtime at ID15B (proposal HC-5261) as well as Michael Hanfland, Gaston Garbarino and Samuel Gallego for their help.

[1] Drozdov, A.P., Kong, P.P., Minkov, V.S., Besedin, S.P., Kuzovnikov, M.A., Mozaffari, S., Balicas, L., Balakirev, F.F., Graf, D.E., Prakapenka, V.B. and Greenberg, E. Superconductivity at 250 K in lanthanum hydride under high pressures. Nature, 569(7757), pp.528-531, 2019.
[2] Drozdov, A. P., Eremets, M. I., Troyan, I. A., Ksenofontov, V., & Shylin, S. I. Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system. Nature, 525(7567), 73-76, 2015.
[3] Spektor, K., Crichton, W. A., Filippov, S., Simak, S. I., Fischer, A., & Häussermann, U. Na3FeH7 and Na3CoH6: hydrogen-rich first-row transition metal hydrides from high pressure synthesis. Inorg. Chem., 59(22), 16467-16473, 2020.
[4] Bronger, W., Gehlen, M., & Auffermann, G. Na3RhH6, Na3IrH6 und Li3IrH6, neue komplexe Hydride mit isolierten [RhH6] 3-und [IrH6] 3--Oktaedern. J. Alloys Compd., 176(2), 255-262, 1991.
[5] Lilia, B. et al. The 2021 room-temperature superconductivity roadmap. J. Phys. Condens. Matter, 34(18), 183002, 2022.
[6] Zhao, Y., Zhang, X., Li, X., Ding, S., Liu, Y., & Yang, G. Emergent superconductivity in K2ReH9 under pressure. J. Mater. Chem. C, 10(39), 14626-14632, 2022.

Probable origin of pressure-induced solid-state amorphization of SnI4

Prof. Dr. Kazuhiro Fuchizaki[1], Dr Hiroki Naruta[1], Dr Akio Suzuki[2], Dr Tomohiro Ohuchi[1]
[1]Ehime University, Matsuyama, Japan, [2]Tohoku University, Sendai, Japan

Other Molecular Systems, July 27, 2023, 10:15–12:15

SnI_4 has been known to undergo pressure-induced solid-state amorphization at about 15 GPa [1]. A series of our research has unveiled that this phenomenon is the tip of the iceberg regarding SnI_4's polyamorphic nature [2]. However, we are still unaware of how SnI_4 transforms from the ambient-pressure crystalline phase, CP-I, to the closed-packed crystalline phase, CP-III, via amorphization because the structure of the intermediate-pressure modification, CP-II, has not been solved yet [3]. More importantly, we should answer why CP-I is amorphised on compression. CP-I is a molecular crystal with which Am-II and Liq-II are associated as the metastable amorphous and stable liquid states [4]. An atomic crystal CP-III may melt to an atomic liquid phase whose metastable state could be the high-pressure Am-I formed due to molecular dissociation [2]. Thus, revealing the structure and the thermodynamic relationship around CP-II would remain a critical piece of the jigsaw puzzle.

This study aims to reveal SnI_4's structural variations above 5 GPa up to about 15 GPa, where the CP-I-to-CP-II transformation would be completed, thereby providing fundamental knowledge to consider thermodynamic reasoning of amorphization.

Instead of using a diamond-anvil cell, we recently approached the relevant pressure region using the CAESAR technique [5] with a multianvil press of DIA-6 type to attain better hydrostaticity. We used MAX80 installed in beamline NE5C, KEK-AR in Japan for in situ measurements in a 6–6 compression mode.

We first compressed SnI_4 at room temperature (RT) up to 15 GPa and then decompressed it along an isotherm at 533 K or 640 K down to ambient pressure. Along the paths, we identified two structures besides CP-I: Yatsugatake and 'unknown.' Yatsugatake transformed to 'unknown' at ~10 GPa on the return paths. The d-value distributions obtained through CAESAR measurements were used as the references for the structures. The diffraction pattern obtained at 533 K and 15.22 GPa exhibited partial crystalline features. From multiple systematic measurements performed between 5 and 10 GPa, we confirmed that Yatsugatake, found at RT and 15 GPa, survived until melting. The 'unknown' transformed to Yatsugatake at about 850 K, irrespective of pressure. Interestingly, a transformation from CP-I to 'unknown,' accompanied by a specific volume change, has a negative Clapeyron slope.

We speculate that Yatsugatake is CP-II and 'unknown' is a mixed state of CP-I and CP-II. The 'unknown'–Yatsugatake transition may be a kinetic one. We could give the thermodynamic basis for this speculation. The CP-I–CP-II boundary can thus have a negative slope. Because the boundary constitutes the melting curve of CP-I when extended to lower pressures, CP-I could be amorphised, just like ice Ih, when crossing the boundary upon compression.

[1] Y. Fujii et al., J. Phys. C 18, 789 (1985).
[2] K. Fuchizaki et al., J. Phys.: Condens. Matter 33, 365401 (2021).
[3] N. Hamaya et al., Phys. Rev. Lett. 79, 4597 (1997).
[4] K. Fuchizaki et al., J. Chem. Phys. 135, 091101 (2011).
[5] Y. Wang et al., J. Appl. Cryst. 37, 947 (2004).

High-pressure structural systematics of Dy compressed in a neon pressure medium.

Dr. Daniel Sneed[1], Dr. Earl O'Bannon III[1], Dr. Per Soderlind[1], Dr. Hyunchae Cynn[1], Dr. Zsolt Jenei[1]
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Static Studies of Elements 2, July 26, 2023, 16:30–18:30

Lanthanides have been the focus of many studies over the years, however the majority of these have been performed under nonhydrostatic conditions. One reason given for this has been the potential reaction with the pressure medium. In this talk I will present results from compression studies on Dy compressed in a soft Ne pressure medium, in which no reaction with Ne was observed up to ~185 GPa. These results show that Dy exhibits an interesting axial ratio response to pressure across its polymorphic landscape, which can be sensitive to hydrostatic conditions. Finally, I will discuss experimental and theoretical results suggesting a potential phase transition in Dy beyond the collapsed phase.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.

Studying high-Z material strength under high pressure at the National Ignition Facility

Hye-Sook Park[1], R. A. Austin[1], N. R. Barton[1], Y. -J. Kim[1], T. E. Lockard[1], B. A. Remington[1], G. Righi[1], R. E. Rudd[1], D. C. Swift[1], J. M. McNaney[1]
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Dynamic Studies of Elements, July 25, 2023, 10:15–12:15

Understanding the plastic deformation dynamics of materials under extreme conditions is of high interest to a number of fields, including meteor impact dynamics and advanced inertial confinement fusion. We infer the strength of samples at pressures up to 4 Mbar, strain rates of ~10^7 /s, and high strains (> 30%) by measuring the growth of Rayleigh-Taylor instabilities (RTI) under ramped compression. We use two methods to create a ramp drive that prevents the sample from shock-melting. The first method uses 800 kJ of laser energy to drive a 4-layer reservoir-gap configuration. The second method uses a direct drive with laser pulse shaping. The target package includes sinusoidal sample surface ripples that are used to infer the plastic flow stress of the material from a measurement of the Rayleigh-Taylor instability ripple growth. The ripple growth is measured by face-on high-energy X-ray radiography. We have studied Ta [1,2], Pb [3] and Pt samples at NIF. We are now studying the dynamic response of materials with implanted helium bubbles that simulate ageing by radioactive alpha decay. This paper will present the experimental results and compare them with various strength models.

[1] H. -S. Park et al., Phys. Rev. Lett, 114, 065502 (2015)
[2] B. A. Remington et al., PNAS, 116, 18233 (2019)
[3] A. Krygier et al., Phys. Rev. Lett, 123, 205701 (2019)

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Displacive Ferroelectricity Realised in a New A-site-ordered Quadruple Perovskite Synthesised at High Pressure

Dr. Jianfa Zhao[1], Prof. Runze Yu, Prof. Changqing Jin
[1]*The Institute of Physics, Chinese Academy of Sciences, Beijing, China*

Perovskites, July 27, 2023, 10:15–12:15

Perovskite and related compounds are the versatile host of functional materials. Various crystal structure sites can accommodate different type of ions (transition metals, alkali metals and/or alkaline earth metals) and lead to a plenty of exotic physical properties owing to the cross interplay and correlation of lattice, charge, spin, and orbital degrees of freedom. Pb-based perovskite demonstrate much more fascinating physical properties for the adding of the skip-valence electronic configuration and 6s2 stereo-chemically active lone pair effect. Here, we report a series of newly found Pb-based perovskite functional materials fabricated under high pressure and the investigation on their physical properties. Especially, we found a new A-site ordered perovskite PbHg3Ti4O12, which undergoes a transition from a centrosymmetric and paraelectric phase to a non-centrosymmetric and ferroelectric phase with a record high Curie temperature at 250 K. This is the only example so far showing ferroelectricity due to symmetry breaking phase transition in AA3B4O12-type A-site ordered perovskites and opens a direction to search for ferroelectric materials.

Acknowledgement: We would like to thank Professors Martha Greenblatt, Zhiwei Hu, and Liu-Hao Tjeng for collaboration.

[1] J. F. Zhao, J. C. Gao, C. Q. Jin, et al., Nat. Commun. 12, 747 (2021).
[2] J. F. Zhao, X. Wang, C. Q. Jin, et al., Chem. Mater. 34, 97 (2022).
[3] J. F. Zhao, S. C. Haw, C. Q. Jin, et al., Phys. Rev. B 107, 024107 (2023).
[4] X. B. Ye#, J. F. Zhao#, H. Das#, et al., Nat. Commun. 12, 1917 (2021).

A diamond anvil cell setup for dielectric measurements of aqueous and non-aqueous solutions up to 5 GPa and 1073 K

Kirill Vlasov[1], Jiang Jiang[2], Sven Friedemann[2], Jonathan Buhot[2], Oliver Lord[1]
[1]School of Earth Sciences, University Of Bristol, Bristol, United Kingdom, [2]School of Physics, University of Bristol, Bristol, United Kingdom

Instrumentation and Techniques 4, July 26, 2023, 16:30–18:30

The relative dielectric permittivity of water is a physical parameter crucial for understanding deep fluids inside Earth and other planets. Also known as the dielectric constant of water (εW), this property largely controls dissociation processes and the solubility of assorted chemical substances (Sverjensky et al., 2014). In the past, εW at the conditions corresponding to Earth's surface and upper crust was measured primarily by dielectric spectroscopy, yet such experiments proved to be quite challenging. There are no experimental data beyond 0.5 GPa (5 kb) and 823 K (Heger et al., 1980). With so little data available for H_2O, even less is known about the dielectric properties of various solutions at the conditions corresponding to deep planetary interiors.

We propose a novel method, allowing the determination of the dielectric constants of pure water and various aqueous and non-aqueous solutions up to 5 GPa and 1073 K. Resistively heated BX90-type diamond anvil cell (DAC) is utilised for pressure and temperature control, while the dielectric measurements are performed with the use of interdigitated microelectrodes deposited directly on top of the diamond culet (1000-600 μm). A microlithographic technique is employed to place the 150-300 nm thick tungsten and/or gold electrodes onto the culet. The interdigitated electrodes, with water in contact with the anvil, form a capacitor (i.e. this is a free space measurement). The dielectric properties of the system throughout the experiment are measured by a NEISYS frequency response analyzer (NOVOCONTROL Technologies GmbH & Co, Germany). The electrodes are insulated from the metal gasket (Fe, Re, Ir) by air plasma sprayed Al_2O_3 ceramics (Monitor Coatings Ltd., UK).

While this particular experimental design is tailored for dielectric spectroscopy, the method itself is suitable for much broader geoelectrochemical applications, including for example electrical conductivity measurements.

We present the experimental setup and initial results. We discuss the advantages and challenges of the approach as well as how the setup can be optimised in the future.

[1] Heger, K., Uematsu, M., & Franck, E. U. (1980). The static dielectric constant of water at high pressures and temperatures to 500 MPa and 550 °C. Berichte Der Bunsengesellschaft Für Physikalische Chemie, 84(8), 758–762. https://doi.org/10.1002/bbpc.19800840814
[2] Sverjensky, D. A., Harrison, B., & Azzolini, D. (2014). Water in the deep Earth: The dielectric constant and the solubilities of quartz and corundum to 60 kb and 1200 °C. Geochimica et Cosmochimica Acta, 129, 125–145. https://doi.org/10.1016/j.gca.2013.12.019

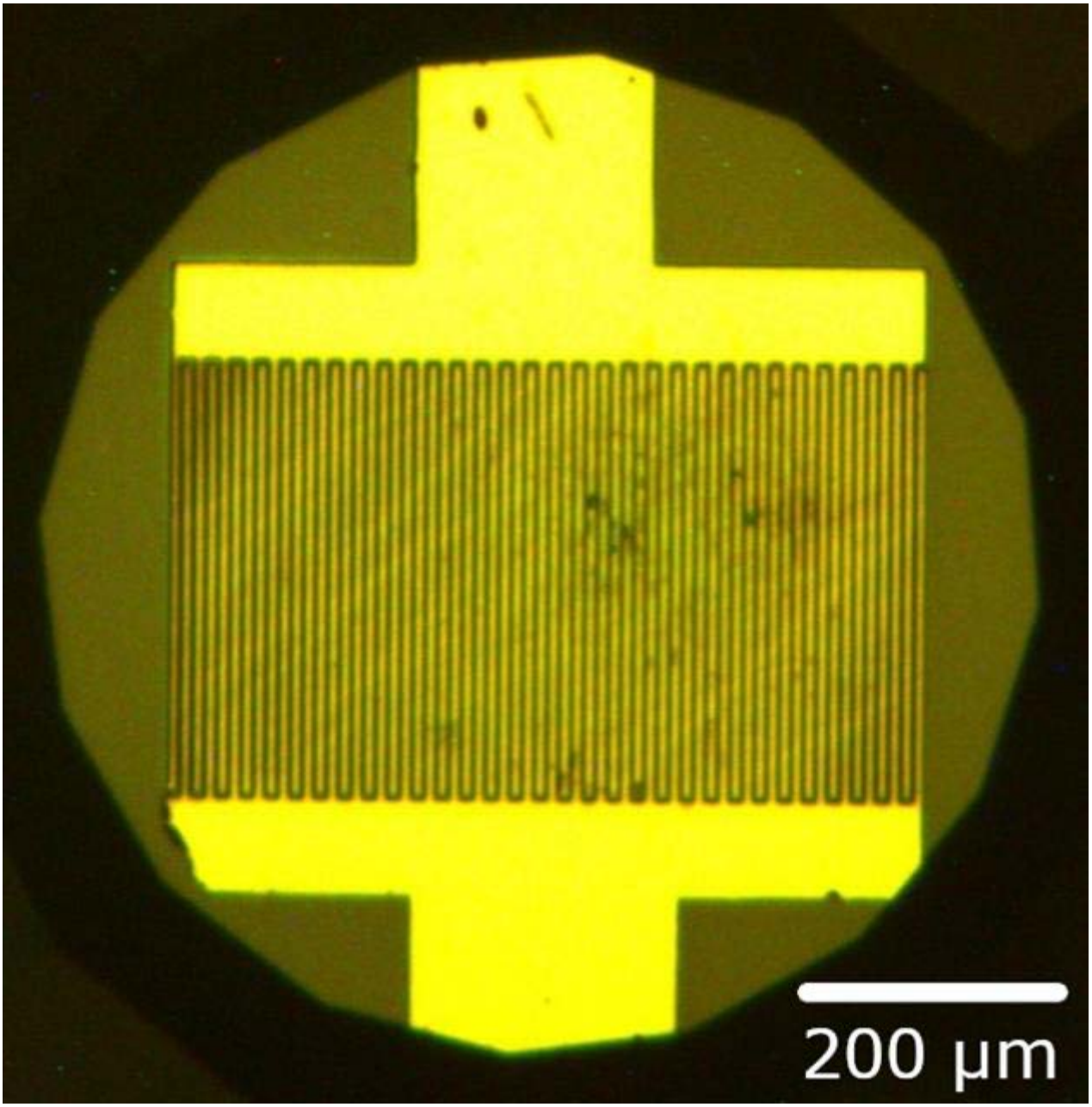


Figure 1. An interdigitated tungsten-gold electrode with 32 digits (5 µm width, 2 µm separation, 150 nm thickness) on an 800 µm diamond culet.

A Ferrotoroidic Candidate with Well-Separated Spin Chains Synthesised at High Pressure

Dr. Jun Zhang[1], Professor Xiancheng Wang[1], Professor Changqing Jin[1]
[1]*Institute of Physics Chinese Academy of Sciences, Beijing, China*

Synthesis and Properties of Novel Materials 2, July 26, 2023, 10:15–12:15

The search of novel quasi-1D materials is one of the important aspects in the field of material science. Toroidal moment, the order parameter of ferrotoroidic order, can be generated by a head-to-tail configuration of magnetic moment. It has been theoretically proposed that 1D dimerised and antiferromagnetic (AFM)-like spin chain hosts ferrotoroidicity and has the toroidal moment composed of only two antiparallel spins. Here, we report a ferrotoroidic candidate of Ba6Cr2S10 with such a theoretical model of spin chain. It was synthesised at high pressure of 6 GPa and systematically studied via structural, magnetic and the electric polarization measurements at ambient pressure. The structure consists of unique dimerised face-sharing CrS6 octahedral chains along the c axis. An AFM-like ordering at ~10 K breaks both space- and time-reversal symmetries and the magnetic point group of mm′2′ allows three ferroic orders in Ba6Cr2S10: (anti)ferromagnetic, ferroelectric, and ferrotoroidic orders. The investigation reveals that Ba6Cr2S10 is a rare ferrotoroidic candidate with quasi 1D spin chain, which can be considered as a starting point for the further exploration of the physics and applications of ferrotoroidicity.

Acknowledgements:
The authors are grateful to Manfred Fiebig and Nicola Spaldin for the helpful discussion about the ferrotoroidicity, Devashibhai T. Adroja, Ivan da Silva, Franz Demmel, Dmitry Khalyavin, Jhuma Sannigrahi, Hari S. Nair, Zhiwei Hu, Hong-Ji Lin, Ting-Shan Chan, Chien-Te Chen for the provision of experimental facilities and discussions about the magnetic structure, μSR and XAS.

[1] Zhang, J., Wang, X.C., Jin, C.Q., et al. A ferrotoroidic candidate with well-separated spin chains. Adv. Mater. 34, 2106728 (2022).
[2] Zhang, J., Wang, X.C., Jin, C.Q., et al. High-pressure synthesis, crystal structure, and properties of iron-based spin-chain compound Ba9Fe3Se15. Phys. Rev. Mater. 5, 054606 (2021).
[3] Zhang, J., Wang, X.C., Jin, C.Q., et al. The synthesis of a quasi-one-dimensional iron-based Telluride with antiferromagnetic chains and a spin glass state. Inorg. Chem. 59, 5377 (2020).
[4] Zhang J., Wang X.C., Jin C.Q., et al. Structure-spin-transport anomaly in quasi-1-dimensional Ba9Fe3Te15 under high pressure. Chin. Phys. Lett. Express Lett., 37, 087106 (2020).
[5] Duan, L., Wang, X.C., Jin, C.Q., et al. High-pressure synthesis, crystal structure and physical properties of a new Cr-based arsenide La3CrAs5. Sci. China Mater. 63, 1750 (2020).
[6] Zhang, J., Wang, X.C., Jin, C.Q., et al. Ba9V3Se15: a novel compound with spin chains. J. Phys.: Condens. Matter. 30, 214001 (2018).

Exploring hard X-ray free electron laser energy deposition through target imprinting

James McHardy[1], Christian Storm[1], Matthew Duff[1], Cameron Lonsdale[1], Simon MacLeod[2], Malcolm McMahon[1]

[1]The University of Edinburgh, Edinburgh, United Kingdom, [2]Atomic Weapons Establishment, Reading, United Kingdom

Developments at XFELs & Lasers, July 24, 2023, 14:00–16:00

The ultrashort duration (1-100 fs) pulses of hard X-rays (>10 keV) generated from X-ray free electron laser sources (XFELs), the brightest X-ray sources in the world, are capable of both creating and extremely probing energy dense states within the bulk of thick (>10 μm) irradiated matter. The hard X-rays can pass through several millimetres of diamond without significant energy loss and so at the European XFEL, these capabilities are being combined with the well-established diamond-anvil cell to provide new insight into pre-compressed matter under extreme high-pressure-temperature conditions [1,2]. The absorption of these photon rich pulses (>10^{10} photons per pulse) can generate temperatures of several eV in just a single pulse, however, the resulting state is highly dependent on the target absorption and thermal properties, the spatial focusing of the XFEL, and the energy dispersion in the target. Interpreting and understanding measurements in these experiments, particularly X-ray diffraction data, requires detailed knowledge of the beam energetics, spatial profile of the focal spot and interaction of the X-rays with the sample.

We have employed a simple target imprinting technique [3] using single XFEL pulses, to infer the both the incident energy on the target surface and the spatial distribution of the heating spot intensity. We compare the damage imprints generated from a consistent focal spot in a broad range of metal targets with atomic numbers ranging from 13 to 83 across variable target thicknesses and consider how the target properties affect the resulting thermodynamic state.

[1] Zastrau, U. et al. The High Energy Density Scientific Instrument at the European XFEL. J. Synchrotron Radiat. 28, 1393–1416, (2021).
[2] Liermann, H. P. et al., Novel experimental setup for megahertz X-ray diffraction in a diamond anvil cell at the High Energy Density (HED) instrument of the European X-ray Free-Electron Laser (EuXFEL). J. Synchrotron Radiat. 28, 688–706, (2021).
[3] Chalupský, J. et al. Spot size characterization of focused non-gaussian X-ray laser beams. Opt. Express 18, 27836–27845, (2010)

Unsplit superconducting and time reversal symmetry breaking transitions in Sr_2RuO_4 under hydrostatic pressure and disorder

Dr. Rustem Khasanov[1], Vadim Grinenko[2], Debarchan Das[1], Ritu Gupta[1], Bastian Zinkl[3], Naoki Kikugawa[4], Yoshiteru Maeno[5], Clifford Hicks[6], Hans-Henning Klauss[2], Manfred Sigrist[3]
[1]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, [2]Institute for Solid State and Materials Physics, Technische Universität Dresden, D-01069 Dresden, Germany, [3]Institute for Theoretical Physics, ETH Zurich, CH-8093 Zurich, Switzerland, [4]National Institute for Materials Science, Tsukuba 305-0003, Japan , [5]Department of Physics, Kyoto University, Kyoto 606-8502, Japan, [6]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

Novel Superconductors 2, July 27, 2023, 14:00–16:00

There is considerable evidence that the superconducting state of Sr_2RuO_4 breaks time reversal symmetry. In the experiments showing time reversal symmetry breaking its onset temperature, T_TRSB, is generally found to match the critical temperature, T_c, within resolution. In combination with evidence for even parity, this result has led to consideration of a d_xz ± id_yz order parameter. The degeneracy of the two components of this order parameter is protected by symmetry, yielding T_TRSB = T_c, but it has a hard-to-explain horizontal line node at k_z=0. Therefore, s± id and d ± ig order parameters are also under consideration. These avoid the horizontal line node, but require tuning to obtain T_TRSB = T_c.

In this work, to test whether the order parameter of Sr_2RuO_4 is of single- or composite-representation type we perform zero-field muon spin rotation/relaxation measurements on hydrostatically pressurised Sr_2RuO_4 and on La-doped Sr_2-yLa_yRuO_4. Both of these perturbations maintain the tetragonal symmetry of the lattice. If the order parameter has single-representation nature, T_TRSB will therefore track T_c. If the order parameter is of the composite-representation kind, with T_TRSB matching T_c in clean, unstressed samples through an accidental fine tuning, then perturbations away from this point should in general split T_TRSB and T_c, whether they preserve tetragonal lattice symmetry or not [1]. We have observed a clear suppression of T_TRSB at a rate matching the suppression of T_c. Our experimental results provide evidence in favour of single-representation nature of the order parameter in Sr_2RuO_4.

Figure 1 caption: Dependence of the time-reversal symmetry-breaking temperature T_TRSB on the superconducting transition temperature T_c for Sr_2RuO_4 [2,3]. The colored areas represents parts with preserved tetragonal lattice symmetry (hydrostatic pressure and disorder effects) and with orthorhombic distortions in the lattice (uniaxial pressure). The red solid line corresponds to T_TRSB = T_c. The dashed line is a guide to the eye.

[1] B. Zinkl and M. Sigrist, Phys. Rev. Research 3, L012004 (2021).
[2] V. Grinenko, D. Das, R. Gupta, B. Zinkl, N. Kikugawa, Y. Maeno, C. W. Hicks, H.-H. Klauss, M. Sigrist and R. Khasanov, Nat. Commun. 12, 3920 (2021).
[3] V. Grinenko, S. Ghosh, R. Sarkar, J.-C. Orain, A. Nikitin, M. Elender, D. Das, Z. Guguchia, F. Brückner, M. E. Barber, J. Park, N. Kikugawa, D. A. Sokolov, J. S. Bobowski, T. Miyoshi, Y. Maeno, A. P. Mackenzie, H. Luetkens, C. W. Hicks, and H.-H. Klauss, Nat. Phys. 17, 748 (2021)

Giant Exchange Bias Induced by Few Oersteds in a High-Pressure Stabilised Double Perovskite Y2NiIrO6

Zheng Deng[1], Jianfa Zhao[1], Yi Peng[1], Wenmin Li[1], Changqing Jin[1]
[1]*Institute of Physics, Chinese Academy of Sciences, Beijing, China*

Magnetic Materials 1, July 24, 2023, 10:15–12:15

Exchange bias (EB) effect has important applications in spintronic technologies such as spin valves and magnetic tunnel junctions in high-density storages and magnetic switching for logic devices. In a conventional EB bilayer, magnetic moments of the ferromagnetic layer are pinned by interfacial antiferromagnetic spins to obtain extra magnetic fields for rotating the whole moments. Such mechanism usually demands large cooling fields to obtain sufficient EB fields, adverse to the applications of EB based devices. It is crucial for applicability to obtain considerable exchange bias fields with minimum cooling fields.

Double perovskite is an excellent platform to explore exotic EB effects, owing to two different magnetic cations at B-site. High-pressure synthesis technique is widely used to stabilise the double perovskite structure. We synthesised an exchange bias effect in a double perovskite compound Y2NiIrO6 under 6 ~ 8 GPa and 1500 K for 2 hours. It shows long-range ferrimagnetic ordering below 192 K. The robust exchange bias appears at 170 K. It manifests a giant bias field of 1.1 T with a cooling field of only 15 Oe at 5 K. This fascinating exchange bias is attributed to the pinned magnetic moments by the combination of strong spin-orbit coupling on Ir, and antiferromagnetically coupled Ni- and Ir-sublattices. The pinned moments in Y2NiIrO6 are present throughout the full volume rather than those at the interface in conventional bilayers. Y2NiIrO6 requires the lowest cooling field to induce an equivalent exchange bias field in known single-phase materials, showing substantial potential for applications.

Acknowledgement: We would like to thank Professors Martha Greenblatt, Zhiwei Hu, Lunhua He, and Jirong Sun for collaborations.

[1] Z. Deng, M. Greenblatt, C. Q. Jin, et al., Advanced Materials 35, 2209759 (2023)
[2] J. Zhang, X. C. Wang, C. Q. Jin, et al., Advanced Materials 34, 2106728 (2022)
[3] J. F. Zhao, M. Greenblatt, C. Q. Jin, et al., Nat. Commun. 12, 747 (2021)
[4] Z. Deng, C. Q. Jin, M. Greenblatt, et al., Angew. Chem. Int. Ed. 59, 8240 (2020)
[5] W. M. Li, S. Uchida, C. Q. Jin, et al., PNAS 116, 12156 (2019)
[6] Z. Deng, C. Q. Jin, M. Greenblatt, et al., Chem. Mater. 30, 7047 (2018)

Overview of High-Pressure Collaborative Access Team (HPCAT) facility at the Advanced Photon Source at Argonne National Laboratory

Nenad Velisavljevic[1]
[1]Lawrence Livermore National Laboratory , Livermore, United States, [2]High pressure Collaborative Access Team, Advanced Photon Source, Argonne, United States

Facility Development 1, July 24, 2023, 16:30–18:30

Goal of HPCAT is to develop and implement synchrotron-based X-ray techniques that are coupled with diamond anvil cell (DAC), large volume press (LVP), and other platforms for studying materials at extreme pressure-temperature and strain rate conditions.

Comprised of four simultaneously operational beamlines HPCAT provides broad range of cutting-edge X-ray techniques, as well as complementary high-pressure support equipment. Over the years numerous high-pressure X-ray diffraction, X-ray spectroscopy, and X-ray imaging techniques have been developed and established for high pressure research through a robust national laboratory and university partnership, and broad national and international general user operations. Currently, HPCAT has two insertion device beamlines, one for diffraction and the other for spectroscopy, and two bending magnet beamlines, one for general purpose and the other for white-beam application. Our presentation will provide overview of HPCAT and some of the available online and offline techniques, as well as some of the recent experimental techniques being developed. Furthermore, we will also discuss plans for upgrades at HPCAT that will take place as part of the broader upgrade to the Advanced Photon Source (APS-U).

Superconductivity in carbon-boron clathrates

Mads Fonager Hansen[1], Bi Tiange[1], Timothy Strobel[1]
[1]*Carnegie Institution For Science, Washington, United States*

Novel Superconductors 2, July 27, 2023, 14:00–16:00

Conventional superconductivity research has become a significant part of high pressure in recent years, notably with the discovery of superconductivity in superhydrides at temperatures approaching room temperature. So far, these high transition temperatures are restricted to experiments in the mega bar range, and compounds have proven to be unrecoverable to ambient pressures. Searching for light element framework compounds that are recoverable to ambient pressure is thus an interesting avenue of research. One path to finding such materials is by utilizing the strong sp^3 bonds of carbon, that are essential to the strength of diamond. Using diamond-like bonding, the energetic barrier for meta stable high-pressure phases can be expected to be high enough to keep them in a meta stable phase at ambient pressure.

Recently, the first boron substituted carbon clathrate, SrB_3C_3, was synthesised, paving the way for a new class of clathrate materials [1]. This material has a superconducting transition temperature of 20 K at pressures of 40 GPa, and is predicted to show an increasing Tc, up to 30 K, when pressure is decreased to ambient conditions [2]. Furthermore, the isostructural compound LaB_3C_3 has also been experimentally realised, showing that it is indeed possible to substitute on the guest atom site [3]. The guest-host nature of these materials enables the tuning of properties, drastically enhancing Tc. Specifically, this class of materials has been predicted to display superconducting transition temperatures up to 88 K in the hypothetical compound $KPbB_6C_6$, among other structure candidates, that are predicted to have transition temperatures in excess of 50 K [4]. Hence, boron stabilised carbon clathrates represent a novel playground for conventional high temperature superconductivity.

In this talk we discuss the synthesis of novel meta stable boron stabilised carbon clathrates, utilizing high pressure and high temperature conditions, employed through laser heating in diamond anvil cells. Characterizing samples in these conditions poses a multitude of challenges and here we will discuss these challenges, and techniques that can allow us to address them. Here we focus on compounds that crystallise in the sodalite structure (Type-IIV clathrate) as these show high superconducting transition temperatures, increasing upon decompression. We will detail the synthesis and characterization of these materials and through an interplay between theoretical calculations and experimental evidence, show the superconducting properties and how we can tune these to increase the transition temperature.

[1] Zhu, L., et al. Sci. Adv. 6, eaay8361, (2020)
[2] Zhu, L., et al. Phys. Rev. Research 5, 013012, (2023)
[3] Strobel, T. A., Angew. Chem. Int. Ed., 60, 2877, (2021)
[4] Geng, N., et al. JACS 145 (3), 1696-1706, (2023)

Evidence of symmetry lowering in dense H2O-ice above 300 GPa

Ashkan Salamat[1], Zach Grande, Dean Smith, Oliver Tschauner, Jesse Smith
[1]*University of Nevada, Las Vegas, Las Vegas, United States*

Outer Planets and Exoplanets 1, July 26, 2023, 10:15–12:15

The observation of water-rich super Earths, along with direct measurements of the ice-giants and their orbiting celestial bodies that reside in our solar system has spurred a need to understand the behaviour of H_2O at the most extreme pressure and temperature scales. Breakdown of the hydrogen- to an ionic bond, superionicity, followed by major rearrangements of the crystal structure and metallic conductivity are the parameters proposed to control H_2O at these conditions. Here, we show that the body centred (bcc) O-sublattice of H_2O-ice persists from 1.26 up to 300 GPa at 300 K, thus shifting major structural rearrangements far beyond earlier estimates. Instead of an ionic bond, ice at 300 GPa exhibits non-symmetric O-H bond distances in an orthorhombic structure, derived from ice-VII. The phase boundary between bcc- and other arrangements of O exhibits a small negative slope, hence, between 200 and 300 GPa it is temperature-not pressure-driven and shifts the H-bonded to superionic transition to the shallow mantle of Neptune and Uranus.

High-throughput search and discovery of near-room temperature superconductors under extreme pressures

Taner Yildirim[1], Tianran Chen
[1]*National Institute of Standards and Technology, Gaithersburg, United States,* [2]*University of Tennessee, Knoxville, United States*

Hydrides 1, July 24, 2023, 10:15–12:15

Since the discovery of superconductivity in solid mercury, countless scientists have been searching for a material whose Tc exceeds room temperature. Despite intense research, only very recent observations of superconductivity at 200K in pressed H3S and 250-260 K in LaH10 at pressures near 200 GPa gave some hope that superconductivity at room temperature may be possible soon. However, the experimental study of these materials under extreme pressures is challenging, and the equilibrium structure of materials at these pressures is usually very different than those under ambient conditions. Hence, as a result, first-principles-based computational searches have become extremely important in predicting new materials and guiding high-pressure experimental measurements.

In this work, we have developed a super-efficient, fast, high-throughput method for searching high-Tc hydride superconductors. We introduce new "metrics" strongly correlated to electron-phonon solid coupling and Tc, but it is much quicker to calculate them. We have searched more than 100,000 binary hydride and metal-borates superconductors using our new method and discovered many new high-Tc systems. Among them, we report our prediction of high-temperature superconductivity at relatively low pressure in a novel binary metal hydride which may break the current record. A detailed mechanism of the superconductivity, phonons, electron-phonon coupling, anharmonicity, and abnormal Tc-pressure dependence will also be discussed.

Our work will significantly accelerate the discovery of new high-Tc conventional superconductors and give a detailed understanding of important factors that yield superconductivity near room temperature at extreme pressures.

Thermal Conductivity of Bridgmanite at Lower Mantle Conditions

Eric Edmund[1], R. S. McWilliams[2], Kara Brugman[1], James Badro[3], Carmen Sanchez-Valle[4], Alexander Goncharov[1], On Behalf of EuXFEL Proposal 3160
[1]Earth & Planets Laboratory, Washington, United States, [2]University of Edinburgh, Edinburgh, United Kingdom, [3]Institut de Physique du Globe de Paris, Paris, France, [4]Westfälische Wilhelms-Universität Münster, Münster, Germany

Secular Evolution of the Earth, July 25, 2023, 10:15–12:15

MgSiO3 perovskite (Bridgmanite) is the primary component of the Earth's mantle however the combined effect of pressure and temperature on its lattice thermal conductivity is poorly understood at the conditions of the lower mantle. As bridgmanite is likely the primary control on heat conduction in the lower mantle, establishing its thermal conductivity at relevant conditions is fundamental to the dynamics and thermal evolution of Earth's interior. Here we present novel measurements carried out at the European X-ray Free Electron Laser (EuXFEL) employing fast heating and serial X-ray diffraction in order to determine the thermal conductivity of end-member MgSiO3 alongside Fe- and Fe+Al-bearing bridgmanite at the conditions of the Earth's lower mantle. Our results establish the thermal conductivity of bridgmanite and constrain the effect of composition at these extreme conditions of pressure and temperature.

HP-HT hydrogenation of LaFeSi by decomposition of anthracene or borazane and study of the P,T phase diagram of the superconductor LaFeSiO1-δ

Pierre Toulemonde[1], Mads Fonager Hansen[1], Fabio Denis Romero[1], Christophe Lepoittevin[1], Murielle Legendre[1], André Sulpice[1], Andres Cano[1], Manuel Nunez Regueiro[1], Sophie Tencé[2], Jean-Baptiste Vaney[2], Philippe Boullay[3], Frederico Alabarse[4]
[1]Institut Néel, Grenoble Cedex 9, France, [2]ICMCB, Bordeaux, France, [3]CRISMAT, Caen, France, [4]Elettra Sincrotrone, Trieste, Italy

Novel Superconductors 2, July 27, 2023, 14:00–16:00

Since their discovery in 2008, pnictides (Pn = As, P…) and chalocgenides (Ch = Te, Se…) of iron superconductors now form a well-established class of unconventional superconductors, divided in different structural families and showing a critical temperature Tc up to 55 K in bulk materials [1]. This category has recently extended to other lamellar materials where the Pn/Ch atoms are replaced by crystallogenic elements: either with Ge in YFe2Ge2 (Tc ~ 2 K) [2] or Si in LaFeSiH (Tc ~ 10 K) [3].

In this work, we first explored a new way of hydrogenation of LaFeSi than the one used previously (heating at 250°C under 10-20 bar of H2) [4]. By using the decomposition of materials with high hydrogen density (anthracene or ammonia borane) at high pressure and moderate temperature in a large volume press, we were able to synthesise the superconducting tetragonal silicide LaFeSiH but also a new over-hydrogenated orthorhombic phase LaFeSiH1+x where superconductivity is suppressed.

In a second study, following our very recent discovery of the superconductor LaFeSiO1-δ, of Tc ~ 10 K [5], we probed its pressure [0 – 20 GPa] temperature [10 – 300 K] phase diagram by X-ray diffraction experiments at the Elettra synchrotron and electrical resistivity in the laboratory. While superconductivity seems enhanced at low pressure, two successive structural transitions (~5 GPa and ~8 GPa) have been highlighted.

[1] H. Hosono, K Kuroki, Physica C 514, 399 (2015).
[2] J. Chen et al., Phys. Rev. Lett. 125, 237002 (2020).
[3] F. Bernardini et al., Phys. Rev. B 97, 100504 (2018).
[4] M.F. Hansen et al., J. Alloy. Compd. 945, 169281 (2023).
[5] M.F. Hansen et al., npj Quantum Mater. 7, 86 (2022).

The densities and phase transformations of subducted hydrous oceanic crust up to the Earth's transition zone: Insights from in situ X-ray diffraction measurements

Dr. Anja Rosenthal[1,2], Dr. Wilson Crichton[1], Dr. Jean-Luc Devidal[3], Dr. Valentina Batanova[4], Dr. Valerie Magnin[4], Prof. Alexander Sobolev[4]
[1]European Synchrotron Radiation Facility, Grenoble, France, [2]Australian National University, Canberra, Australia, [3]Clermont Auvergne University, Clermont-Ferrand, France, [4]Université Grenoble Alpes, Grenoble, France

Phase Diagrams – Ionic Systems, July 24, 2023, 10:15–12:15

The detectability of large and small-scale mantle heterogeneities caused by remnants of former recycled oceanic crustal material (eclogite) by means of seismic velocities remains notoriously challenging [1-2]. Constraints of these important variables come chiefly from previously determined densities and elastic properties of eclogites [3-5].

This study refines the densities of eclogitic assemblages up to the transition zone and in a manner that will account for the effect of all compositional changes including changes of phase proportions along subduction paths into the Earth's deep mantle using in situ X-ray diffraction measurements.

We conducted experiments using an average altered oceanic basalt GA1 [6] + 3 wt.% H_2O from 3 up to 18 GPa at sub-solidus conditions along a subduction path using the large volume press at ID06, ESRF. We analysed major and minor elements of phase compositions by microprobe. Basalt transforms to eclogite >100 km depth during subduction [7]. Our experiments yield well-crystallised eclogitic assemblages of garnet + clinopyroxene + Ir ± coesite/stishovite ± phengite ± lawsonite ± vapour. Similar to previous studies [e.g. 3], the rise in garnet/clinopyroxene ratios with pressure is a consequence of the increased dissolution of clinopyroxene into garnet towards greater mantle depths. Similar to Irifune et al. [3], in this study, the determined lattice volume of eclogitic garnet at ambient pressure increases with increasing pressure and recovered garnets from highest pressures are least dense. The garnet/clinoyroxene proportion is largest contributor to the observed eclogitic density on the geotherm. Within this a more straight-forward description for the density of all eclogitic garnets encountered on our pressure-temperature path is highlighted for possible use as a barometer. Eclogite is between 3-6 % denser than mantle models PEM-C and PEM-O [8] up to 12 GPa, which develops into a zero-density contrast above 12 GPa in the transition zone. Using Anderson's seismic equation of state model [9] and our whole rock density, we obtain estimations of the bulk sound velocity, which are comparable to the measurements of Kono et al. [4]. Our high-pressure data are consistent with their ultrasound data for eclogites and, in addition, our seismic parameters are remarkably consistency with the seismic description of IASP91 [8] over the full pressure range of eclogitic assemblages studied.

The outcomes quantify fundamental constraints on the effects of continuously changing proportions, compositions and phase transformations in eclogite. They clarify the influence on density and buoyancy changes caused by the recycling of oceanic crust as part of the subducting slab in Earth's deep convecting mantle. The study is supported by MSCA-IF 898169 'ELASTIC' to AR.

[1] Bascou et al. (2001). Tectonophysics 342, 61-80.
[2] Tkalčic et al. (2009). Geophys J Intern 179, 425-443.
[3] Irifune et al. (1986). EPSL 77, 245-256.
[4] Kono et al. (2012) GRL 39, L24306, doi:10.1029/2012GL054009
[5] Ricolleau et al. (2010). JGR 115, B08202, doi:10.1029/2009JB006709
[6] Spandler et al. (2008) JP 49, 771-795.
[7] Green, Ringwood (1967). CMP 15, 103-190.
[8] Kennett, B.L.N. (1991) "IASPEI 1991 Seismological Tables." Bibliotech, Canberra, Australia, 167pp
[9] Anderson, D.L. (1967) Geophys J Intern 13, 1-3, 9-30.

High-pressure preference for low-density polymorphs

Prof. Andrzej Katrusiak[1], Dr Kinga Roszak[1]
[1]*Faculty of Chemistry, Adam Mickiewicz University, Poznań, Poland*

Molecular Compounds, July 25, 2023, 10:15–12:15

High-temperature polymorphs are intuitively connected with low-density polymorphs, but there are numerous exceptions indicating that this is not a general rule. For example, the transformation between the low-temperature low-density resorcinol polymorph α and high-temperature high-density polymorph β , the first structurally characterised polymorphs of organic compounds in the 1930s [1-3], contradicted the in generality of temperature-density relation. However, the pressure-density relation, that high-pressure phases must be more dense than the low-pressure ones, is usually considered a general one. Here we present new experimental evidence of the low-density phases in situ crystallised under the high-pressure conditions. Two new polymorphs β and γ of bis-3-nitrophenyl disulphide (3-NO2-PhS)2, when their crystallization triggered under high-temperature high-pressure conditions was driven by kinetic cooling of the sample in the diamonds-anvil cell, were recovered to ambient conditions and their structures determined by X-ray diffraction. Their density is significantly lower than that of polymorph α crystallised under the atmospheric conditions [4]. Most recently, we established that another well-known compound of DL-menthol displays a preference to form a new lower-density polymorph β when crystallised either in isothermal or isochoric conditions above 0.4 GPa [5]. These observations shed new light on the pressure-volume relations in condensed-matter physics.

[1] Robertson, J. M. The Structure of Resorcinol a Quantitative X-ray Investigation. Proc. Roy. Soc. London A 1936, 157, 79−99, DOI:10.1098/rspa.1936.0181
[2] Robertson, J. M.; Ubbelhode, A. R. A New Form of Resorcinol. Proc. Roy. Soc. London A 1938, 167, 122−−135, DOI:10.1098/rspa.1938.0123
[3] Safari, F.; Katrusiak, A. (2021). High-pressure polymorphs nucleated and stabilised by rational doping under ambient conditions. J. Phys. Chem. C 125, 23501–23509. DOI: 10.1021/acs.jpcc.1c07297
[4] Sobczak, S.; Ratajczyk, P.; Katrusiak, A. High-Pressure Nucleation of Low-Density Polymorphs. Chem. Eur. J. 2021, 27, 10769–10779. https://doi.org/10.26434/chemrxiv.13161956.v1.
[5] Roszak K.; Katrusiak A. Low-density preference of the ambient and high-pressure polymorphs of DL-menthol. IUCrJ 2023, 10, https://doi.org/10.1107/S2052252523002452.

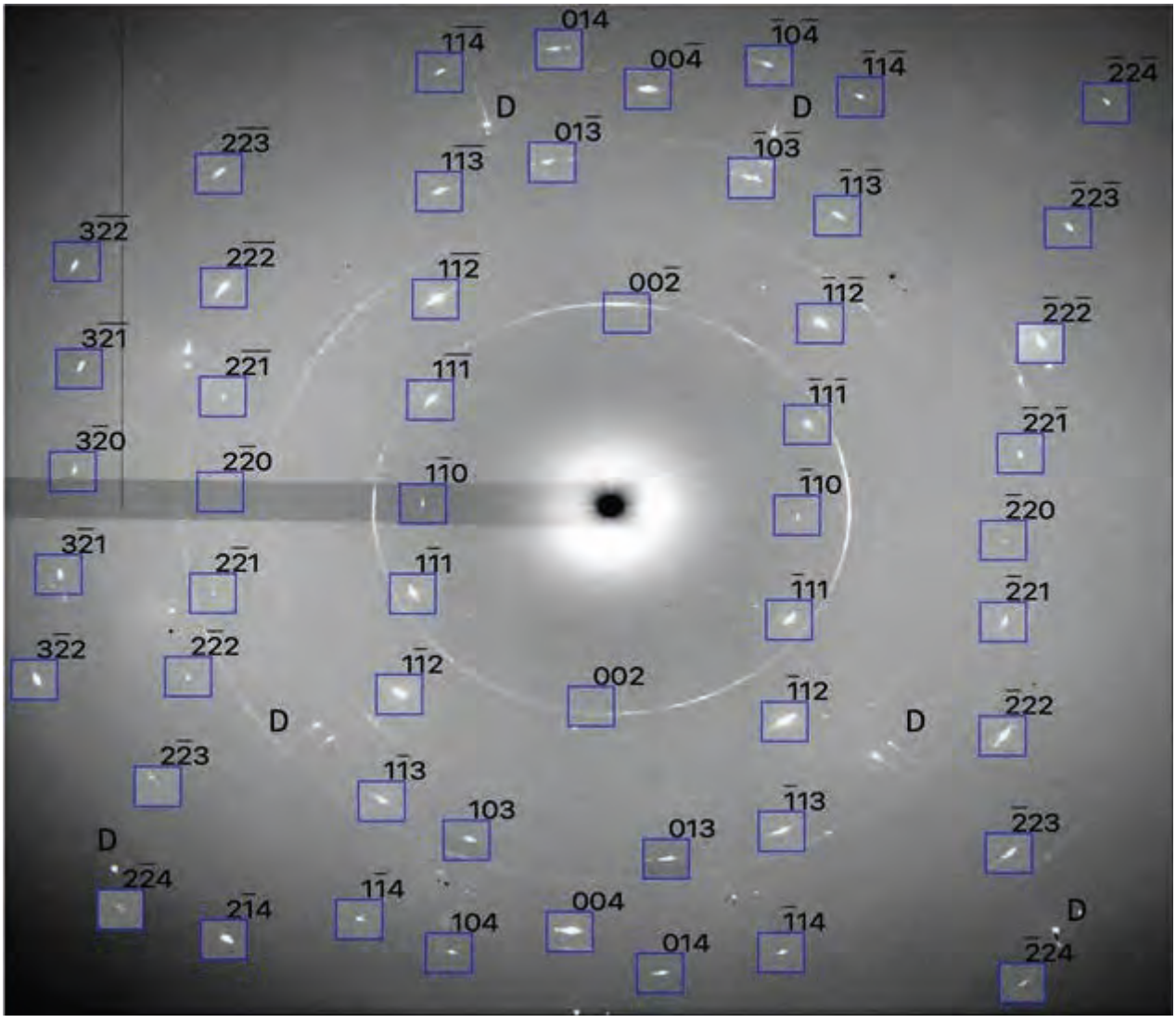
The Structure and Behaviour of Na-hP4 Up to 300 GPa

Christian Storm[1], Matthew Duff[1], James McHardy[1], Malcolm McMahon[1]
[1]*The University Of Edinburgh, Edinburgh, United Kingdom*

Static Studies of Elements 1, July 25, 2023, 14:00–16:00

Upon compression the alkali metals exhibit a marked departure from their simple free-electron nature at ambient conditions. Experimental and computational studies have found increasingly complex structures appearing under high pressures and temperatures, including localization of the valence electrons, forming non-nuclear maxima in the charge density, and incommensurate host-guest structures. Sodium (Na) is no exception to this trend, exhibiting a variety of low-symmetry phases with complex structures above 100 GPa, and a deep minimum in the melting curve at 300 K and 118 GPa. Above 125 GPa, Na adopts the incommensurate host-guest tI19 phase, which exhibits unusual and disordered chains within a crystallised lattice. At 200 GPa Na becomes an optically transparent insulator, with a wide band gap and fully localised valence electrons, as a result of strong band hybridisation.

We have used diamond anvil cells and X-ray diffraction methods to investigate the behaviour of the Na-hP4 phase up to 300 GPa, comparing its behaviour to the same hP4 phase previously observed in Rb. We present our structural analysis of single-crystal Na-hP4 at 200 GPa, including discussion on how the electride-nature of this phase can be investigated with X-ray diffraction methods. Using Rietveld refinements of the single-crystal data, we present experimental evidence that the Na-hP4 phase is indeed electride-like.



Towards the Understanding of Pressure-Induced Protein Phase Transitions

Professor Arvi Freiberg, Dr. Kõu Timpmann, Dr. Liina Kangur
[1]*University of Tartu, Tartu, Estonia*

Bio/Life Sciences and Soft Matter, July 26, 2023, 10:15–12:15

The thermodynamic parameters essential for supporting life are largely determined by the properties of proteins, with many of these parameters dependent on the precise structure of the proteins. Despite the well-documented denaturing effects of pressure on proteins, the exact nature of the structural changes involved remains largely unknown. To shed light on this issue, we investigated the destabilization of multiple Ca binding sites in cyclic LH1 light-harvesting membrane chromoprotein complexes from two Ca-containing sulphur purple bacteria using hydrostatic high-pressure perturbation spectroscopy. In this study, the Ca-saturated (native) and Ca-depleted (denatured) phases of these complexes were clearly distinguishable due to the much-shifted bacteriochlorophyll-a (BChl) exciton absorption bands, which served as innate optical probes. Our findings revealed that the pressure-induced denaturation of these complexes involved the failure of protein Ca-binding pockets and the concomitant breakage of hydrogen bonds between the pigment chromophores and the protein environment. This process was cooperative and irreversible, affecting all or most of the Ca-binding sites. The strong hysteresis observed in the spectral and kinetic characteristics of phase transitions along the compression and decompression pathways suggested an asymmetry in the relevant free energy landscapes and activation free energy distributions. Moreover, we determined that the phase transition pressure was approximately 1.9 kbar for the complexes from Thiorhodovibrio strain 970, based on the pressure dependence of biphasic kinetics observed over time periods ranging from minutes to 100 hours.

In addition, we investigated the denaturation of LH2 light-harvesting complexes from non-sulphur purple bacteria under high pressure. To better understand the structural changes involved, we used two different innate optical probes located in strategic positions within the complexes: BChl in the hydrophobic interior and tryptophan at the protein-solvent interfacial gateways to internal voids. We compared the naturally robust complexes of Thermochromatium tepidum with the pressure-sensitive complexes of mutant Rhodobacter sphaeroides. Our results revealed a firm correlation between the abrupt blue shift of the BChl exciton absorption, a known indicator of breakage of tertiary structure pigment-protein hydrogen bonds, and the quenching of tryptophan fluorescence, which is believed to result from further protein solvation. These effects were not observed in the reference complex. Although these findings might be interpreted as evidence for the governing role of hydration, our analysis of atomistic model structures of the complexes confirmed the critical role of the protein structure in the pressure-induced denaturation of the membrane proteins studied.

Superconductivity at 90 K in a lanthanum hydride film at 95 GPa

Mr Sam Cross[1]
[1]*University of Bristol, Bristol, United Kingdom*

Hydrides 4, July 26, 2023, 14:00–16:15

The discovery of superconductivity with a record critical temperature of 250 K at 180 GPa in LaH10 provided further progress towards room temperature superconductivity in hydrogen rich compounds [1,2]. Calculations predict a rich variety of hydride phases stabilised at megabar pressures [3], and recent experimental work has revealed the chemical and structural diversity amongst lanthanum hydrides across a wide pressure range [4]. In particular, the coexistence of multiple phases coupled with inhomogeneities induced by laser heating at high pressure hinders the isolation of a single superconducting phase, which remains an important experimental challenge for reliable study the superconducting properties. In this work, I present the formation of a superconducting lanthanum hydride sample at 95 GPa, synthesised via laser heating a lanthanum film with ammonia borane. Our X-ray Rietveld analysis demonstrates the presence of the recently discovered Pm-3n La4H23 structure [4]. In this sample, we observe a single transition at 90 K in resistance measurements, and suppression of Tc in magnetic field up to 12 T. In this talk I will outline our thin film synthesis techniques and the origin of the superconducting phase. This work further highlights the importance of exploring hydride phases at moderate pressures.

[1] A.P Drozdov et al., Nature 569, 528 (2019)
[2] Somayazulu et al., Physical Review Letters 122, 027001 (2019)
[3] Liu et al., PNAS 114, 6990 (2017)
[4] Laniel et al., Nature Communications 13, 6987 (2022)

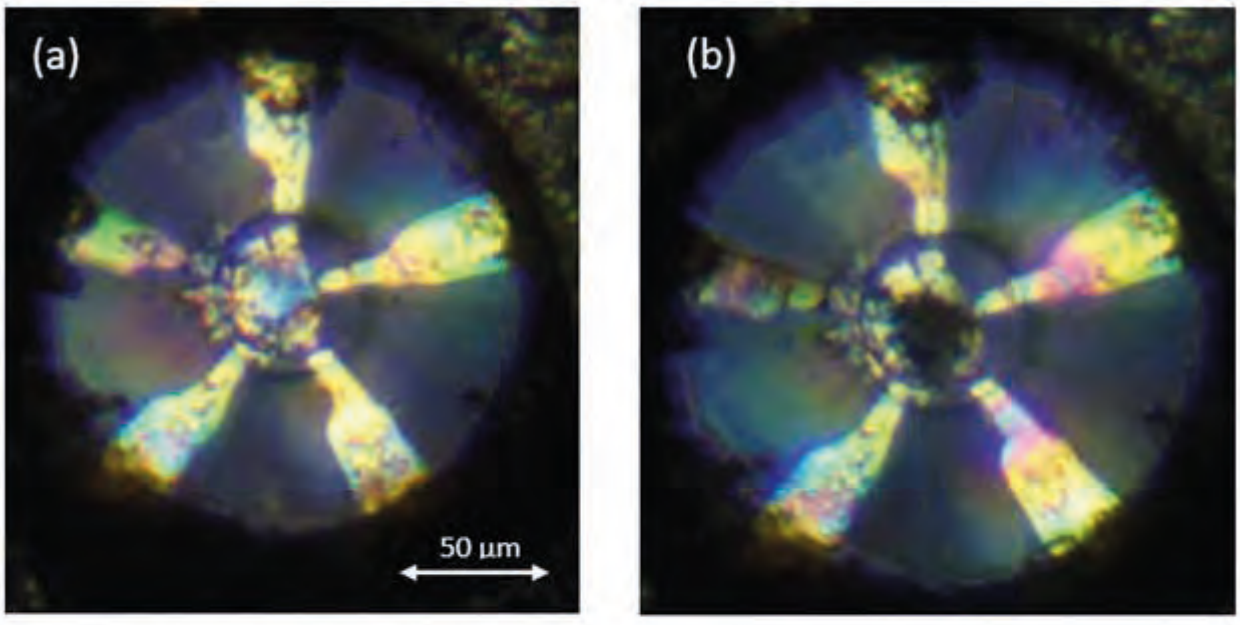


Fig.1(a): The lanthanum film loaded in a DAC with ammonia borane at 95 GPa before laser heating. Five electrodes make contact with the sample for resistivity measurements. Fig.1(b): The synthesised lanthanum hydride sample after laser heating.

First principles calculations of light element mixtures at planetary conditions

Professor Andreas Hermann[1], Dr Lewis Conway[1,2], Dr Umbertoluca Ranieri[1], Dr Ross Howie[1], Prof Chris Pickard[2]
[1]The University of Edinburgh, Edinburgh, United Kingdom, [2]University of Cambridge, Cambridge, United Kingdom

Outer Planets and Exoplanets 2, July 26, 2023, 16:30–18:30

The interiors of icy planets contain vast 'hot ice' mantle regions, which are the largest water reservoirs in planetary systems. Those regions are chemically very complex and while individual constituents (water, methane, ammonia) have been studied in great detail both computationally and experimentally, their mixtures are much less explored. As molecular mixtures allow for chemical changes that can drastically alter their properties, consequences for internal stratification, depth-density profiles, thermal and electrical conductivities can be qualitatively different from their constituents.

Here, we discuss some of our recent computational work on complex molecular mixtures at extreme conditions, including the methane-hydrogen phase diagram, in close collaboration with experimental syntheses and characterisations, and the structure of the full H-C-N-O quaternary chemical space near Neptune's core pressure conditions, as explored with unbiased crystal structure searching. Electronic structure analyses help uncover the rules that govern stability in complex chemical spaces. Molecular dynamics simulations are used to explore high-temperature states, including partial and full melting, and chemical reactivity. Planetary ice mixtures can exhibit properties not found in their constituting compounds, and the full complexity of these mixtures needs to be considered to arrive at a realistic picture of planetary interiors.

The phase transitions of CaSiO3 perovskite at extreme conditions

Dr Andrew Thomson[1,2], Dr Wilson Crichton[2], Dr Rong Huang[1], Dr Anja Rosenthal[2,3]
[1]University College London, London, United Kingdom, [2]The European Synchrotron (ESRF), Grenoble, France, [3]The Australian National University, Canberra, Australia

Mantles of Terrestrial Planets, July 27, 2023, 14:00–16:00

Calcium silicate perovskite (capv) is the third most abundant mineral in Earth's lower mantle. After entering phase assemblages at ~ 19-21 GPa [1] it constitutes ~ 5 to ~ 30 wt.% of ultramafic to mafic lower mantle assemblages respectively [2]. Additionally, it is commonly observed as mineral inclusions trapped within diamonds that are believed to have been exhumed from the transition zone and/or lower mantle, e.g. [3]. The crystal structure, phase transitions, elastic properties, and equation of state of CaSiO3 perovskite are, therefore, all of great significance for the interpretation of seismological data. Recent studies of capv's elasticity [4, 5] demonstrated that its seismic velocities were significantly slower than previous theoretical estimates such that, if present, it will be geophysically observable. Additionally, it was also observed that capv undergoes multiple elastically anomalous phase transitions as a function of increasing temperature (T) at mantle pressure (P) conditions [4]. However, estimates of the PT slope of capv's phase transitions are extremely variable [6], preventing their inclusion in geophysical models of the deep mantle.

We have performed high pressure experiments in the large volume press at beamline ID06-LVP of the ESRF. The experimental design was optimised to study the phase transitions occurring in capv, which involve extremely subtle variations in peak width and/or the appearance of new (but weak) superlattice peaks, at pressure conditions of 10-30 GPa. Low density amorphous gaskets were combined with B-doped polycrystalline diamond furnaces and MgO components to provide low and continuous background, with few Bragg reflections from the sample environment to complicate interpretation. Additionally, the sample detector distance and 2-theta diffraction range were set to achieve the highest resolution diffraction resolution possible. In combination this setup facilitated the unequivocal detection of superlattice peak appearances as well as the evolution of capv Bragg peaks during heating/cooling ramps as pressure was varied. Combined these observations are diagnostic of the crystallographic structure for capv. Results allow extrapolation of the PT conditions of capv's phase transitions, permitting interpretation of seismic observations from the lower mantle.

[1] Holland et al. (2013), JPet, 54(9), 1901-1920.
[2] Kesson et al. (1998), Nature, 393, 252-255.
[3] Nestola et al. (2018), Nature, 555, 237-241.
[4] Thomson et al. (2019), Nature, 572, 643-647.
[5] Greaux et al. (2019), Nature, 565, 218-221.
[6] Hirose et al. (2017) Science, 358, 734-738.

Boron-Stabilised Carbon Clathrates

Dr Timothy Strobel[1]
[1]*Carnegie Institution of Washington, United States*

Synthesis and Properties of Novel Materials 3, July 26, 2023, 16:30–18:30

Diamond, comprised of a tetrahedral network of covalent sp^3 C–C bonds, represents a remarkable material with superlative properties including hardness/strength, thermal conductivity, and electron mobility. Nevertheless, a surprisingly limited number of three-dimensional, carbon-based frameworks are known, despite a large body of theoretical predictions that suggest many energetically plausible allotropes.[1] While some extended sp_3 carbon-based compounds are known, most consist of heterodiamond structures with light-element substitutions (e.g., B, N, Si) in the diamond lattice. The realization of new three-dimensional carbon-based frameworks would unlock possibilities for novel superhard/strong materials while simultaneously enabling access to currently inaccessible changes in electronic structure. Indeed, novel forms of carbon and related compounds have been predicted to possess tensile and compressive strengths exceeding diamond [2], and to exhibit properties like high-temperature conventional superconductivity.[3]

Here, we provide an overview of our recent discoveries of boron-stabilised carbon clathrate compounds, which are three-dimensional (3D), sp^3 diamond-like materials comprised of polyhedral cages that trap guest atoms. The discovery of the first boron-stabilised carbon clathrate in the type-VII, bipartite sodalite structure [4] has been extended to a range of new guest elements including multi-guest combinations. Large variability in guest-dependent type-VII clathrate properties has been established, including materials that are semiconducting, metallic, superconducting, as well as those exhibiting ferroelectricity and ferromagnetism. [5-9] High-throughput computational screening has revealed new low-energy and thermodynamically stable type-I and type-II clathrates, as well as completely new 2D framework types. [9] We report here the experimental validation of new superhard clathrate compounds (Figure 1) and new clathrate-like structure types with structural confirmation by single-crystal X-ray diffraction, Raman spectroscopy and transmission electron microscopy measurements. [10] Strong covalent bonding allows for robust metastable persistence of these materials at ambient pressure, and boron-stabilised carbon clathrate frameworks thus represent a broad family of new diamond-like materials with tuneable properties relevant to structural materials and energy applications.

[1] Hoffmann, R., Kabanov, A.A., Golov, A.A., Proserpio, D.M., Angew. Chem. Int. Ed., 55, 10962 (2016).
[2] Blase, X., Gillet, P., San Miguel, A., Melinon, P., Phys. Rev. Lett., 92, 215505 (2004)
[3] Zipoli, F., Bernasconi, M., Benedek, G., Phys. Rev. B, 74, 205408 (2006)
[4] Zhu, L. Borstad, G.M., Liu, H., Guńka, P.A., Guerette, M., Dolyniuk,J., Meng, Y., Greenberg, E., Prakapenka, V.B., Chaloux, B.L., Epshteyn, A., Cohen, R.E., Strobel, T.A. Science Advances, 6, eaay8361 (2020).
[5] Strobel, T.A. Zhu, L., Guńka, P.A., Borstad, G.M., Guerette, M. Angew. Chem. Int. Ed., 133, 2913 (2021)
[6] Zhu, L., Strobel, T.A., Cohen, R.E., Phys. Rev. Lett., 125, 127601 (2020)
[7] Zhu, L. Liu, H., Somayazulu, M., Meng, Y., Guńka, P.A., Shiell, T.B., Kenney-Benson , C., Chariton, S., Prakapenka, V.B., Yoon, H., Horn, J.A., Paglione, J., Cohen, R.E., Hoffmann, R., Strobel, T.A. Phys. Rev. Research, 5, 013012 (2023).
[8] Geng, N., Hilleke, K.P., Zhu, L., Wang, X., Strobel, T.A., Zurek, E., J. Am. Chem Soc., 145, 1696 (2023)
[9] Strobel et al., In preparation (2023)
[10] Bi and Strobel, In preparation (2023)
[11] Strobel et al., In Preparation (2023)

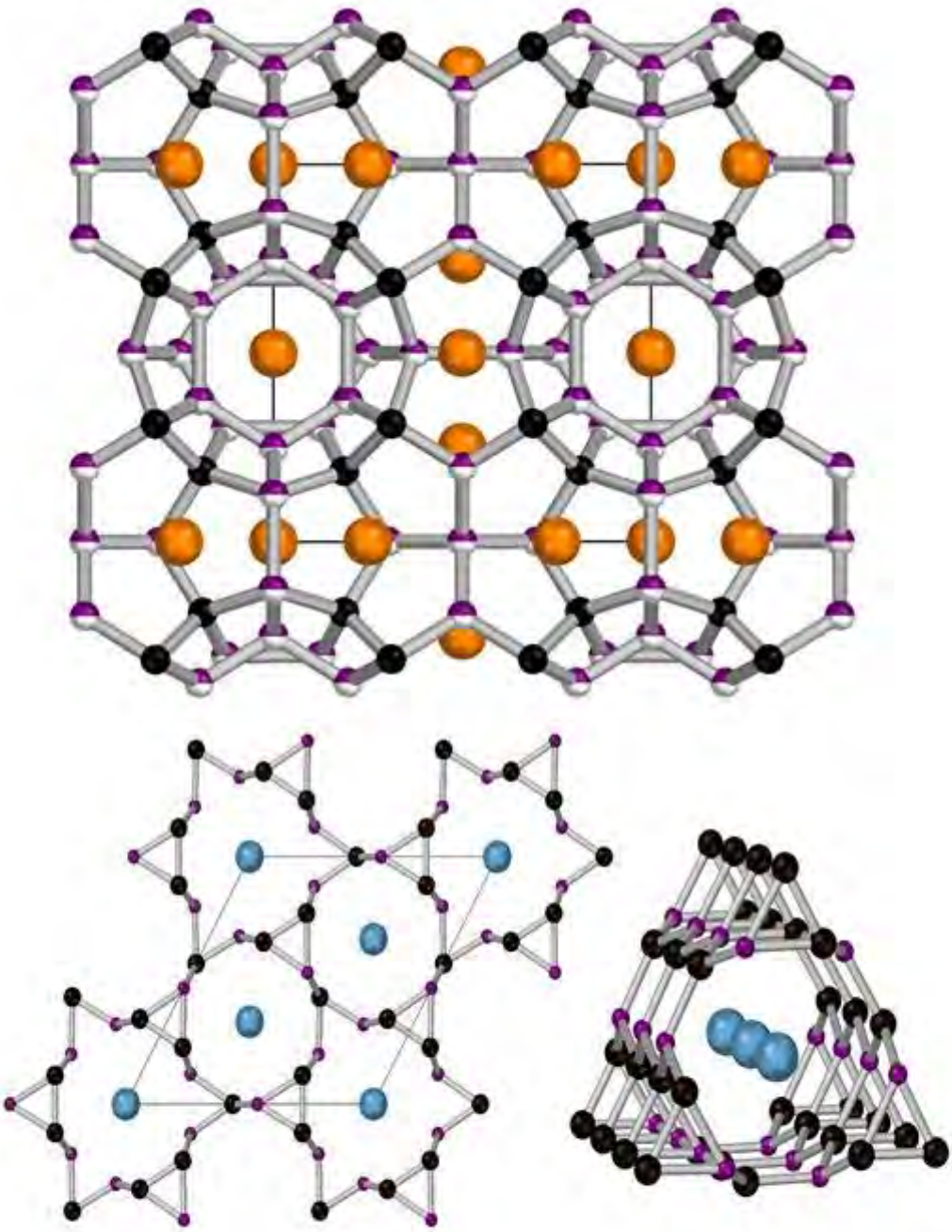


Figure 1. *Novel boron-substituted clathrate a clathrate-like structures discovered in this work.*

First principles calculations of liquid entropy

Stanimir Bonev[1], Kwangnam Kim[1]
[1]*Lawrence Livermore National Laboratory, Livermore, United States*

Computational Methods, July 25, 2023, 10:15–12:15

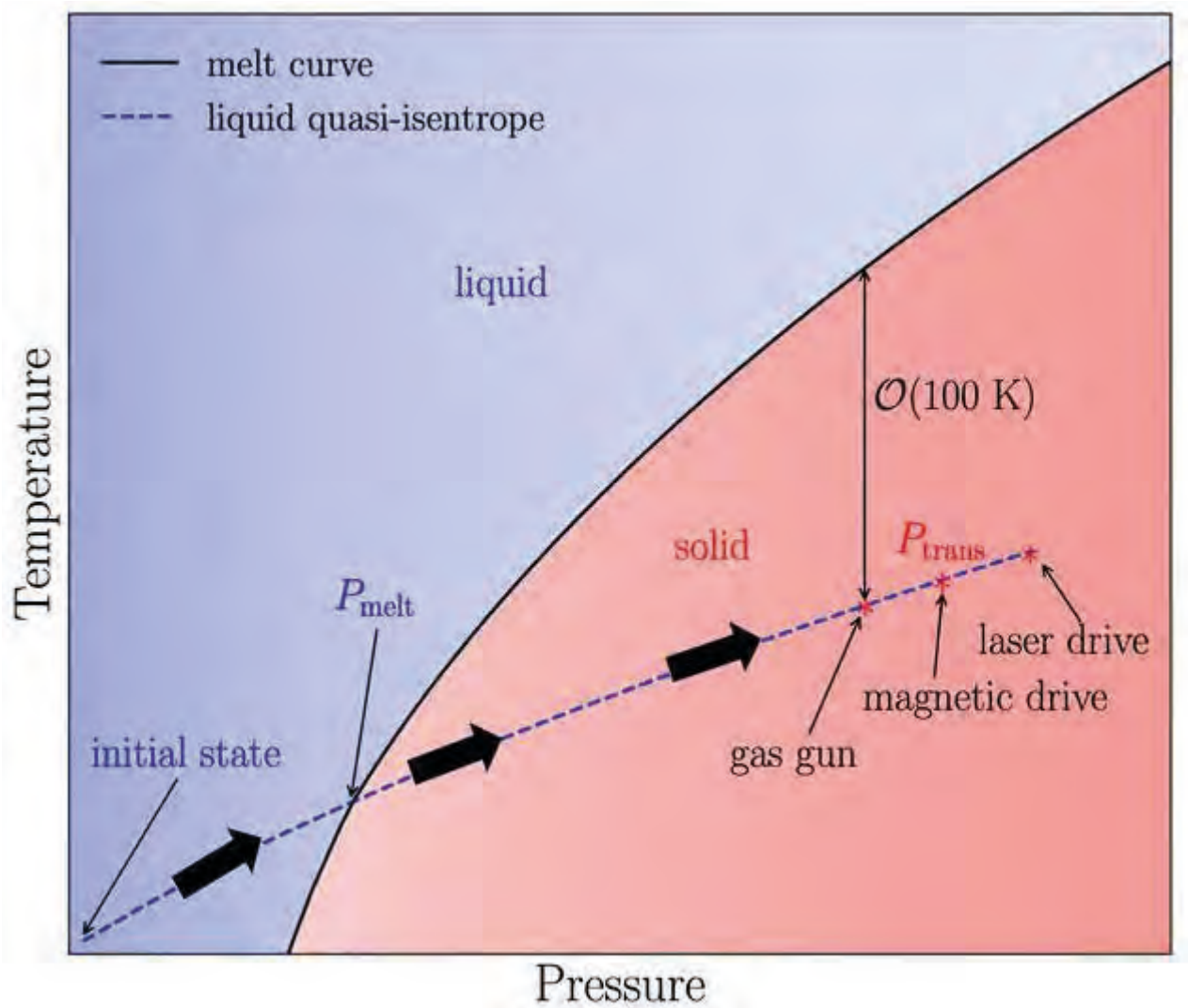
The ability to calculate accurately the entropy of liquids is essential for the theoretical construction of high-pressure phase diagrams. We present an approach for rapid computation of liquid entropy with controlled accuracy at the level of density functional theory (and possibly beyond). Application of the method to several systems, including Sn and LiF, and results for their melting lines will be presented as well.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

A scaling law for the onset of solidification at extreme undercooling

Jonathan Belof[1], *Philip Myint*[1], *Dane Sterbentz*[1], *Justin Brown*[2], *Brian Stoltzfus*[2], *Jean-Pierre Delplanque*[3]
[1]*Lawrence Livermore National Laboratory, Livermore, United States,* [2]*Sandia National Laboratories, Albuquerque, United States,* [3]*University of California, Davis, Davis, United States*

Quasi-isentropic compression enables one to study the solidification of metastable liquid states that are inaccessible through other experimental means. The onset of this non-equilibrium solidification is known to depend on the compression rate and material-specific factors, but this complex interdependence has not been well characterised. In this study, we use a combination of experiments, theory, and computational simulations to derive a general scaling law that quantifies this dependence. One of its applications is a novel means to elucidate melt temperatures at high pressures, utilizing time-dependent compression methods.



Carbon at Extremes: Discovery Science with Machine Learning, Exascale Computers and Experiment

Ivan Oleynik[1]
[1]*University of South Florida, Tampa, United States*

Outer Planets and Exoplanets 2, July 26, 2023, 16:30–18:30

Properties of carbon at extreme pressures and temperatures are of critical importance for constructing interior models of carbon-rich exoplanets. Among the questions that have long perplexed the scientific community are the existence and potential synthesis of high-pressure post-diamond carbon phases, and the inelastic response of diamond to strong shock compression. In particular, very recent ramp compression and X-Ray diffraction experiments at the National Ignition Facility (NIF) challenged theoretical prediction of the existence of a high-pressure BC8 post-diamond phase by compressing diamond to extreme pressures up to 20 Mbar. In this talk, I will describe recent advances in simulating atomic-scale dynamics of material's response at experimental time and length scales using quantum-accurate, billion-atom molecular dynamics simulations with machine-learning models of interatomic interactions and employing the most powerful computers in the world. Specifically, I will focus on atomic-scale mechanisms of solid-solid and solid-liquid phase transitions of carbon and nature of inelastic deformations in diamond. These transformative simulations guide our experimental campaigns at NIF, Omega, Z, and EuXFEL facilities towards observing predicted phenomena.

Hydrogen and deuterium at very high compressions

Eugene Gregoryanz[1,2,3], Xiao-Di Liu[2], Ross Howie[1,3]
[1]University of Edinburgh, Edinburgh, United Kingdom, [2]Institute of Solid-State Physics, Hefei, China, [3]HPStar, Shanghai, China

Hydrogen, July 25, 2023, 10:15–12:30

The rich and fascinating physics, which governs the behaviour of dense hydrogens, is very interesting and it can provide some unexpected and unusual results. The recent discoveries of phases IV and V of H2(D2) has reignited the interest in the studies of the dense hydrogen and its isotopes. As a result of these discoveries, the phase diagrams of hydrogen and deuterium above 180 GPa at room temperature have been extensively studied both experimentally and theoretically. The former studies radically expanded both phase diagrams by pushing the achievable P-T conditions to new limits. Despite the remarkable progress in our understanding of the behaviour of both isotopes at high pressures and ambient temperature, the picture at low temperatures is much less clear with several conflicting reports and claims about the behaviour of H2 at low temperatures and at medium to high compressions. The behaviour of hydrogen and deuterium at these conditions is important to understand the evolution of the system during its transformation from the weak intermolecular state with strong intra-molecular forces (e.g., phases I, II, and III) to the layered phases (e.g., phases IV and V) with weaker intra-molecular bonding and stronger intermolecular interactions.

We will revisit P-T phase diagrams of hydrogen and deuterium and present our resent measurements on both hydrogen and deuterium in a wide pressure and temperature range.

Tailored Software and Hardware development for emerging synchrotron high pressure research at HPCAT

Dr Maddury Somayazulu[1], Curtis Kenny-Benson[1], Arunkumar Bommannavar[1], Richard Ferry[1], Eric Rod[1], Changyong Park[1], Rostoslav Hrubiak[1], Jesse Smith[1], Dmitry Popov[1], Evgenii Vasilev[1], Nenad Velisavljevic[2]

[1]Argonne National Laboratory, Lemont, United States, [2]Lawrence Livermore National Laboratory, Livermore, United States

Next Gen Synchrotrons, July 25, 2023, 14:00–16:00

With four simultaneously running synchrotron based high pressure beamlines, there is a considerable need for ancillary capabilities from sample loading to characterization. In addition, many of the experimental techniques benefit enormously not only from optimised data acquisition strategies but also simultaneous evaluation of the data to allow for rapid redesign of the on-going experiment. Recently, with the uptick in high-profile experiments that require several simultaneous, concurrent probes, there is also a need to integrate several experimental probes and platforms.

The discovery of superconductivity in LaH10-x required the simultaneous confirmation of superconductivity as well as characterization of stoichiometry based on a precise determination of unit cell volume. This was achieved with the integration of transport measurements with in-situ laser heating. Similarly, the characterization of ramp compression effects on materials such as Zr needed an in-situ pressure determination achieved by developing an in-line ruby fluorescence system and diffraction mapping of the final phase mixture. The determination of high P-T elastic behaviour in the PEC required the integration of sound velocity measurements, radiography, and diffraction as well as a precise determination of P-T variation across bulk samples. Understanding grain growth in Zr across the a-w transition needed integration of rapid multi-grain, white beam Laue diffraction. These examples highlight the integration of software and hardware development in HPCAT that enables world-class user science and will be presented. In addition, efforts to collaborate with user groups in establishing new data acquisition and analysis strategies that include AI/ML methods that will become necessary for handling higher data volumes post-upgrade, will be discussed.

Understanding quantum materials by X-ray techniques under high pressure

Ricardo Dos Reis[1]
[1]*Brazilian Synchrotron Light Laboratory, Campinas, Brazil*

Magnetic Materials 2, July 26, 2023, 14:00–16:00

The research exploring the limits of thermodynamic parameters, such as pressure, temperature, and magnetic field, is a rapidly growing and fascinating discipline of science and technology that uncovers many truths and facts about nature that are not possible to observe in ambient conditions. In this talk, we will discuss how we can use synchrotron techniques, including X-ray absorption, diffraction, and scattering, together with external pressure (hydrostatic and uniaxial), low temperature, and high magnetic fields to continuously and cleanly tune quantum correlations, and drive materials through the critical region where the state of matter changes, and inherently quantum effects dominate. We will focus on materials that are on the verge of a phase instability with distinct crystalline structures and electronic behaviour that display nontrivial topology. We will also present the first results of the Extreme Condition Methods of Analysis beamline (EMA) at the Brazilian light source, which was specifically designed to overcome the challenges of obtaining high-quality experimental data under extreme thermodynamic conditions. The EMA provides both ~0.5x1 μm^2 and ~100x100 nm^2 focused beam sizes with well-defined Gaussian beam shape, enabling us to carry out X-ray absorption (XAS), X-ray diffraction (XRD), coherent diffraction imaging (CDI), and X-ray Raman experiments at extreme pressures with good spatial selectivity and to avoid pressure gradients. The talk will highlight the findings of our current research using several synchrotron techniques to investigate quantum materials.

Equation of state for molybdenum at high pressures and temperatures in shock waves

Konstantin V. Khishchenko[1,2,3,4]
[1]Joint Institute for High Temperatures RAS, Moscow, Russia, [2]Moscow Institute of Physics and Technology, Dolgoprudny, Russia, [3]South Ural State University, Chelyabinsk, Russia, [4]Federal Research Centre of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia

Equation of State 2, July 27, 2023, 14:00–16:00

A semi-empirical equation of state for molybdenum is developed taking into account the effects of melting and evaporation. The results of calculations of the thermodynamic characteristics of the solid, liquid and gas phases of this metal in a wide range of pressures and temperatures are presented. The calculation results are compared with the available experimental data for molybdenum under the action of shock waves. The resulting multiphase equation of state of the material can be effectively used in the numerical simulation of various processes at high pressures and temperatures. The work is supported by the Russian Science Foundation (grant No. 19-19-00713).