Synthesis of boron-nitride nanostructures in plasma volume

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Synopsis We report a channel for direct nanosynthesis of boron-nitride (BN) nanostructures from a mixture of BN diatomic molecules in arc plasma at high pressure. Using the quantum-classical molecular dynamics, we were able to synthetize BN fullerenes, nanocages, nanococoons and nanotubes of various size. No catalyst is needed for this synthesis, however the conditions for the synthesis of each of the nanostructures, such as temperature and flux of the BN precursors, were identified.

Boron-Nitride (BN) Nanostructures (BNS) can be synthetized in various forms like fullerenes, nanocages, nanococoons, nanoflakes and nanotubes, similarly to the carbon nanostructures. Synthesis of BN nanotubes (BNNTs) is carried out experimentally by a number of methods, with ultimate goals to reach high-rate production of impurity and defect free nanostructures. However, complete understanding of the BNNT nanosynthesis process at the atomic level has been missing so far.

Most of the models invoke self-assembly processes through interaction of atomic nitrogen with the boron nanodroplets, similarly to modeling of the root-growth synthesis of carbon-nanotubes from catalysts. In this work we present quantum-classical molecular dynamics (QCMD) simulations based on DFTB which show that all BNS can be built by self-organization from a mixture of BN diatomic molecules (Fig. 1a) at high temperatures (~ 2000K) and concentrations, consistent with the conditions in the volume of an electric arc plasma.

Most interestingly, we have succeeded to grow a BNNT from a short BNNT template (Fig. 1b). Growth of BNNT is completed by self-organization of a BN side chains, which migrated and accumulated at the top end of the tube. We observe several similarities between SWBNNT formation and SWCNT simulations, In agreement with SWCNT formation simulations, the feedstock supply times are crucial: The slower feedstock is added, the higher the chances for defect healing and the growth of ordered structures.

Irradiation of boron cluster with hydrogen rich compounds (e.g. ammonia molecules, NH_3) leads to synthesis of nanoflakes (Fig. 1c). Hydrogens prevent the structure closing.

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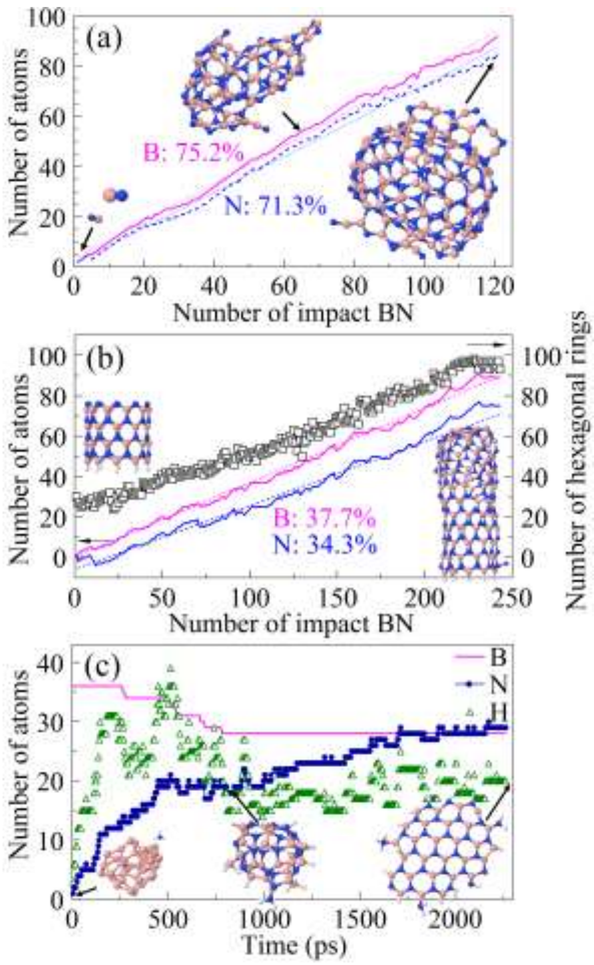

Figure 1. Predicted evolution of BN nanostructures: (a) nanocage formation, (b) SWBNNT growth from BN molecules, and (c) nanoflake formation from a boron cluster and NH_3 molecules.

The simulation results could serve as guideline for the future efficient arc and laser plasma-based synthesis of BN nanostructures, accomplished by the self-organization of feedstock of BN molecules at high density and temperature.

References

[1] L. Han and P. Krstic, Nanotechnology 28 (7), 07LT01 (2017)