Molecular effects in M-shell ionization by slow light ions

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Synopsis The studies of M-shell ionization, or M-X-ray emission, by slow light ions indicate rather strong, up to a factor of 3-5, underestimation of the measured cross sections by the available theoretical calculations describing direct Coulomb ionization by charged particle impact. Guided by our earlier systematic measurements of M-shell ionization cross sections by ^{1,2}H and ^{3,4}He ions we demonstrate here that for the low energy ions, i.e. in the adiabatic regime, the electron binding energy does not saturates at the united atoms (UA) limit, commonly used in the calculations, but instead it has a smaller value corresponding to a transient molecule (MO) formed in collision. This effect, when described in the one-electron molecule approximation, can explain the observed discrepancies between the measured and calculated M-shell ionization cross sections.

Inner-shell ionization by charged particles is a process of both fundamental interest and in applications, namely, for the particle induced X-ray emission (PIXE) technique which needs accurate knowledge of the M-X-ray production cross sections by light ions. Based on our earlier systematic measurements of the X-ray production cross sections for dominating M-X-ray lines and the M-shell ionization cross sections for heavy atoms bombarded by hydrogen ^{1,2}H and helium ^{3,4}He ions in the energy range 0.1-1.0 MeV/amu [1,2], as well as the recent results reported by other authors [3-5], here we discuss the observed underestimation of the measured M-shell ionization cross sections by available calculations for the lowest energies. The existing theories treating the direct Coulomb ionization process, expected to dominate for asymmetric collisions, are based on the plane wave Born approximation (PWBA), semiclassical approximation (SCA) and the binary encounter approximation (BEA). The PWBA approach was further developed to include the higher-order effects and is known as the ECPSSR [6] or ECUSAR [7] theories. In the ECPSSR theory the electron binding effects is treated within the perturbed stationary state approximation (PSS), while in the ECUSAR the saturation of the binding effect at the united atom limit (UA) was introduced for the lowest ion energies.

Generally, the measured M-subshell X-ray production cross sections were found [1-5] to be systematically up to a factor of 3-5 higher than the predictions of the ECPSSR and ECUSAR theories at low energies. For this reason the present data on the M-subshell ionization by light ions were compared with the predictions of the SCA [8] and BEA [9] calculations in order to investigate a role of the electronic wave function and the electron binding effects. In particular, to calculate the M-subshell ionization cross sections different electronic wave functions, from nonrelativistic hydrogenic to relativistic Dirac-Fock types, were used within the SCA while in the BEA both the nonrelativistic and relativistic hydrogenic and the Hartree-Fock-Roothan wave functions (see Ref. [9]) were used.

The electron binding effect was taken into account within the extreme separated-atom (SA) and united-atom (UA) limits as well as the proposed molecular (MO) model describing the variation of the electron binding energy with respect of separation between the projectile and target atom in the adiabatic regime. We found that within the molecular picture the united atom limit cannot be reached, but instead slightly smaller molecular electron binding energy has to be used to calculate the electron binding effect. Consequently, the experimental results for the M-shell ionization by light ions can be interpreted in terms MO effects using the SCA calculations [8] in order to explain the observed discrepancies, in particular, for the lowest impact energies.

References

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