N-shell ionization cross sections by proton impact in the binary-encounter approximation

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Synopsis The N-shell ionization cross sections of heavy elements by proton impact have been calculated in the binary encounter approximation with different electron momentum distributions. The calculated results are compared with the experimental data and other theoretical calculations.

The ionization processes during ion-atom collisions have been extensively investigated for K-, L- and M-shell electrons of various atoms both theoretically and experimentally. On the other hand, studies on N-shell ionization cross sections are scarce. In the present work, the N-shell ionization cross sections of heavy elements have been calculated in the binary-encounter approximation (BEA).

When \( v_1 \) and \( v_2 \) are the velocities of the projectile and the target electron in atomic units, respectively, and \( u = v_0^2 \) is the ionization potential of the bound electron in rydberg, the ionization cross section in the BEA in \( \pi a_0^2 \) is given by [1]:

\[
Q(s) = N_e \int_0^\infty f(t)Q(s, t)u^{1/2} \, dt, \tag{1}
\]

where \( a_0 \) is the first Bohr radius of hydrogen, \( N_e \) is the number of electrons in the \( N \) subshell, \( s = v_1/v_0, t = v_2/v_0, Q(s, t) \) is the ionization cross section and \( f(t) \) is the momentum distribution of the target electron.

The BEA calculations were made with different choice of \( f(t) \). We used the momentum distributions corresponding to the nonrelativistic (BEA) and relativistic (RBEA) hydrogenic, the Hartree-Fock-Roothaan (HFR) and relativistic HFR (RHFR) wave functions.

In Fig. 1, the \( N_{4,5} \)-subshell ionization cross sections of W by protons are shown. The BEA calculations for the BEA, RBEA, HFR and RHFR are compared with the experimental results [2] (solid circles) and the same data with different choice of the fluorescence yield [3] (solid squares). For comparison, other theoretical calculations, i.e. the plane-wave Born approximation with Dirac-Hartree-Slater wave functions (RPWBA) [3], the RPWBA with binding and Coulomb corrections (RPWBA-BC) [3], the RPWBA with screened hydrogenic wave functions (RPWBA-SH) [3] and the semiclassical approximation (SCA) [2], are also plotted.

It is interesting to note that the wave-function effect is important in the \( N \)-shell ionization. On the other hand, the electronic relativistic effect plays a minor role. The BEA cross sections underpredict the experimental values in low-energy region, but overestimate them at high energies. This trend is similar to the RPWBA-BC cross sections.

References

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