§15. Electron-Impact Single Ionization of Medium-Z Ions from the Ground and Excited States

Shevelko, V.P. (P.N. Lebedev Physics Institute, 117924 Moscow, Russia)
Tawara, H.

On the basis of CBE calculations (Coulomb-Born approximation with exchange) of direct single ionization cross sections, the fitting parameters were evaluated for the cross sections σ and Maxwellian rate coefficients $\langle v\sigma \rangle$ of the target states $1s \le nl \le 6h$ and for the *l*-averaged values of σ and $\langle v\sigma \rangle$, where *n* and *l* are the principal and orbital quantum numbers of the target atom or ion. The data obtained made it possible to extrapolate the fitting parameters to the arbitrary n-states with $n \ge 7$.

A new classical formula has been deduced from the general Stabler formula for the energy transfer of the incident electron to the target. The result has the form:

$$\sigma = N\left(\frac{Ry}{I}\right)^2 \Phi(u)[\pi a_0^2], \quad u = E/I - 1,$$

$$\Phi(u) = \frac{4}{3}(u+1)^3 \begin{cases} u(5u+3), & u \le 1, \\ 4u^2+5u-1, & u > 1 \end{cases} \quad (1)$$

where *I* is the binding energy of the target electron shell (for highly excited n states $I = z^2/2n^2$), *N* is the number of equivalent electrons in the shell and *u* is the reduced incident electron energy.

The function F(u) is continuous, but its derivative experiences a jump at u = 1. However, Eq.(1) seems to be the most accurate formula for ionization cross section in the classical impulse approximation.

At high incident electron energies E >> I the asymptotic of the cross section can be presented as a sum of the classical and dipole terms (Bethe logarithm):

$$\sigma = \sigma^{cl} + \sigma^{dip} \approx (Ry/I)^2 \frac{\pi a_0^2}{u}\left(A + \frac{B}{n}\ln(4u)\right)$$

$$B = n\frac{1}{\pi\alpha}\left[\sigma_{nl}^{ph}(\omega)/\pi a_0^2\right](I/\hbar\omega)d\hbar\omega \quad (2)$$

Here α is the fine striucture constant, $\sigma(\omega)$ is the corresponding photoionization cross section. According to (1) the classical constant A=16/3. The use of the *l*-averaged Kramers cross section in (2) gives for all *n* states a single value for B: $B = 64/9\sqrt{3}\pi \approx 1.31$. In this work the constant *B* was also obtained for different *nl* states from 1s up to 4f. The logarithmic term in (2) is important if the reduced electron energy *u* satisfies the inequality :

$$u > e^{4n}/4, \quad (3)$$

where *n* is the principal quantum number. For example, if n = 1 the dipole term prevails at energies u > 10; if u < 10 the logarithmic term has to be taken into account for the states with n = 1, 2 and 3. This can be seen from Fig.1 where ionization cross sections from the states n = 1, 2 and 4 of hydrogen ions calculated in the Coulomb-Born approximation with exchange (CBE) by the ATOM code are shown.

Calculations carried out in this work showed that the CBE ionization cross sections coincide with the Born cross sections when u > 50. The long-dash curve in the Fig. 1 corresponds to the classical formula (1), shot-dash one to the Lotz formula. It is seen that in a given energy range u < 10 the contribution of the dipole ionization cross section is the largest for the state n = 1: $\sigma^{Born}/\sigma^{cl} \approx 2.6$, i.e., $\sigma^{dip}/\sigma^{cl} \approx 1.6$ at u = 10 . At u > 50 the Born ionization cross sections from the states with n > 4 in the scale of the Figure practically coincide with the classical ionization cross section (1).