CALCULATION OF ABSOLUTE IONISATION CROSS SECTIONS OF He, He*, He^+, Ne, Ne*, Ne^+, Ar, Ar*, Hg and Hg*

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Recently Gryzinski developed a theory [1,2] of atomic collisions by which it is possible to calculate in good approximation absolute cross sections for ionisation of atoms by electrons. The principal idea of this theory is that ionisation of an atom can be approximated as a two-particle collision, in which the ionizing electron "hits" one atomic electron. The atom is ionised when the energy transfer to the atomic electron is greater than its binding energy. This is valid for each atomic electron separately; thus the theory can also be applied to inner-shell ionisation. For the calculation of an absolute cross section use is made of the experimentally known ionisation energy U and the number of electrons in the shell. In this theory no free parameter is introduced. Some approximation that are of no fundamental importance are made. We remark that the agreement between theory and experiment becomes better because of these approximations.

In contradiction to Gryzinski's first paper [1] he now [2] chooses an energy distribution of the atomic electron:

$$f(E_2)\,\mathrm{d}E_2 = \frac{E}{2E_2^2}\exp - \left(\frac{E}{E_2}\right)^{\frac{1}{2}}\mathrm{d}E_2\,, \qquad (1)$$

where E_2 is the kinetic energy of the atomic electron, and where he takes E equal to the average kinetic energy of that electron. This gives the following expression for the cross section for detachment of one electron from the atom:

$$Q_i = \frac{\sigma_0 E}{U^2 E_1}\left(\frac{E_1}{E+E_1}\right)^{\frac{3}{2}}\left[\frac{U}{E}+\frac{2}{3}\left(1-\frac{U}{2E_1}\right)\ln\left(2.7+\sqrt{\frac{E_1-U}{E}}\right)\right]\left(1-\frac{U}{E_1}\right)^{\frac{2E+U}{E+U}}, \qquad (2)$$

where E_1 is the kinetic energy of the impinging electron and $\sigma_0 = 6.56\times10^{-14}$ cm^2 eV^2. In first approximation Gryzinski takes E equal to U which is exactly true for the hydrogen atom. Then eq. (2) simplifies to:

$$Q_i = \frac{\sigma_0}{U_2}\,g(x)\,, \quad \text{with } x = E_1/U \text{ and}$$
$$g(x) = \frac{1}{x}\left(\frac{x-1}{x+1}\right)^{\frac{3}{2}}\left[1+\frac{2}{3}\left(1-\frac{1}{2x}\right)\ln\left(2.7+\sqrt{x-1}\right)\right]. \qquad (3)$$

When the number of electrons in the shell k is N_k, corresponding to a binding energy U_k, the cross section becomes $N_k\,Q_{ik}$. In order to get the total cross section for ionisation of an atom we have to sum only over the different shells:

$$Q_{i\,tot} = \sum_k N_k Q_{ik}\,. \qquad (4)$$

With eq. (4) we calculated [3] ionisation functions for He, He*, He^+, Ne, Ne*, Ne^+, Ar, Ar*, Hg and Hg*. We indicated the metastable states by an asterisk. Our results are given in figs. 1 to 7. We compare our results with experimentally measured absolute cross sections, except for ionisation from the metastable states, as for this process the ionisation functions have not yet been measured. The reason why we calculated these ionisation functions for metastable atoms is twofold: first because they are important for gaseous discharges and secondly because we are building apparatus to measure them.

We see that in most cases the agreement between theory and experiment is very good, especially for ionisation of Ar and He^+.

An exception we must make for ionisation of Ne. Interesting is that the theory can be applied very well to ionisation of ions; from this we conclude that the extra Coulomb attraction in these cases has no great resulting effect on the ionisation cross sections.

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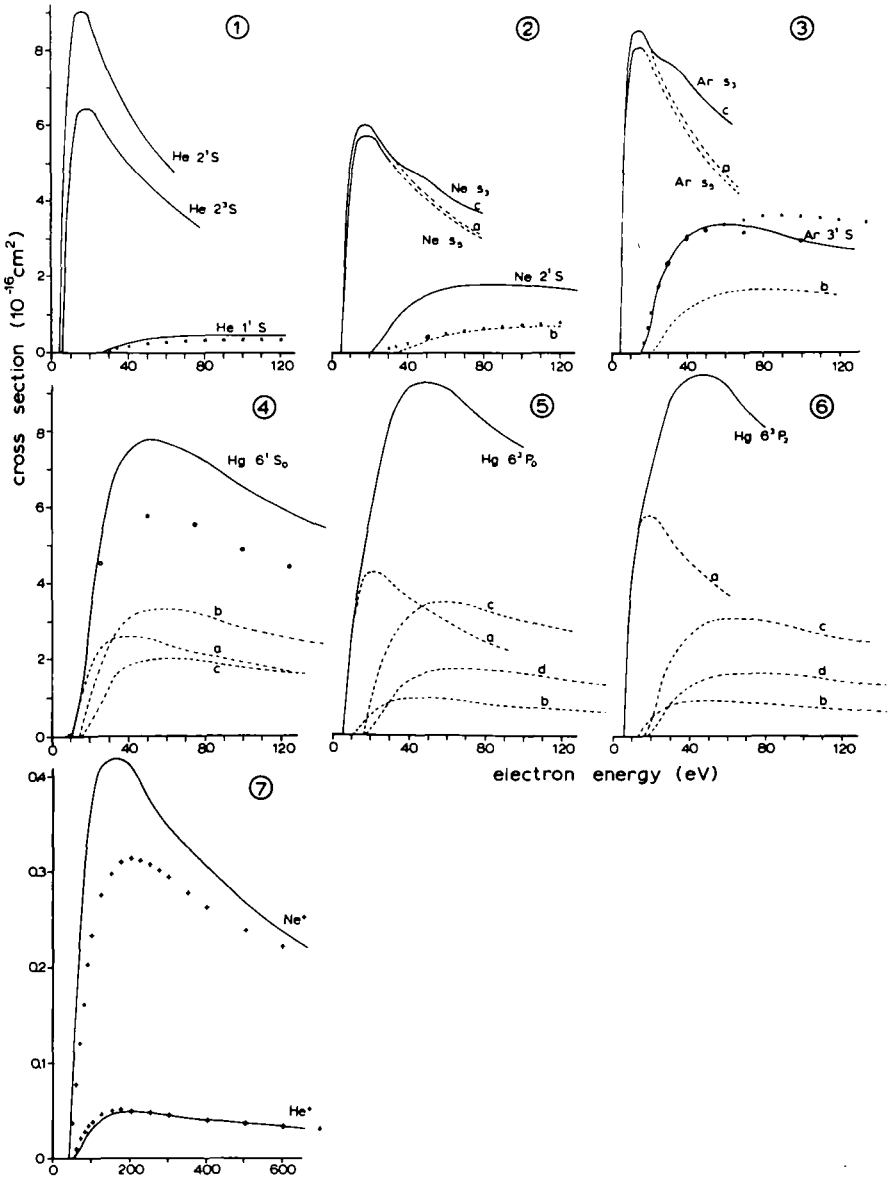

Figs. 1-7. The calculated ionisation functions are given by solid curves, the contributions of the different shells by dashed curves. In fig. 2a and b correspond to the 3s respectively 2p shell of Ne s_3 ($c=a+b$). In fig. 3a and b correspond to the 4s and 3p shell of Ar s_3 ($c=a+b$). In fig. 4 we denote by a, b and c the 6s, $5d_{2\frac{1}{2}}$ and $5d_{1\frac{1}{2}}$ shell. In figs. 5 and 6 we denote by a, b, c and d the 6p, 6s, $5d_{2\frac{1}{2}}$ and $5d_{1\frac{1}{2}}$ shell. The measured functions are from Smith [4] (xxx), Bleakney [5,6] (ooo) and Dolder et al. [7,8] (+++).

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