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Improved low-energy dependence of calculated cross sections for the K-shell ionization of atoms using the Deutsch-Märk formalism

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Abstract

We present an improved formula to describe the energy dependence in the low-energy regime of calculated atomic K-shell ionization cross sections using the semiclassical Deutsch-Märk formalism. The modified energy dependence was obtained from a fitting procedure using recent K-shell ionization cross section data for atomic sulfur. A comparison of calculated K-shell ionization cross sections using this modified energy dependence with (1) critically evaluated experimental data for 11 other atoms and (2) cross section shapes derived from other predictive formulae revealed good agreement, not only in the low-energy regime, but also at relativistic impact energies. (Int J Mass Spectrom 177 (1998) 47–50) © 1998 Elsevier Science B.V.

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1. Introduction

Cross sections for the removal of the inner shell electrons of atoms by electron impact are needed in many fields, such as atomic physics, plasma physics, materials and surface science, and radiation chemistry [1]. A comprehensive analysis of measured and calculated cross sections for atomic inner shell ionization, in particular for K-shell ionization, including a comparison with cross sections derived from various predictive formulae, is currently underway by Powell [2] who has so far reviewed K-shell ionization cross sections for 11 elements (C, N, O, Ne, Al, Ar, Fe, Ni, Cu, Mo, and Ag). It was pointed out [2] that there is a systematic underestimation of the cross sections predicted from the Deutsch-Märk (DM) formalism [3] in the regime of low impact energies up to about five times the ionization threshold. This provided the motivation for us to revisit the application of the DM formalism to the calculation of K-shell ionization cross sections. It is also noteworthy in this context that the application of the DM formalism to the calculation of total single ionization cross sections of atoms [4] showed poor agreement in the low-energy regime of the calculated cross sections for the alkali atoms. The ionization of the alkali atoms is dominated by the removal of a single s-electron, a process similar to K-shell ionization where one of the two 1s-electrons is removed.

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In this paper, we report a modified formula for the energy dependence of the K-shell ionization cross sections in the low-energy regime calculated in the framework of the DM formalism. The modified energy dependence was derived from the analysis of recent K-shell ionization cross section data for sulfur [5] obtained from two targets, SO_2 and SF_6. These recent K-shell ionization cross section data for sulfur are in good agreement with earlier data of Quarles and Eskp [6]. We subsequently applied this new energy dependence to all available K-shell ionization data for the 11 elements listed above and it was found that this improved energy dependence derived from the sulfur data resulted in a significantly improved agreement of the predicted DM cross sections in the low-energy regime with the experimental data and with cross section shapes from other predictive formulae.

2. DM formalism applied to K-shell ionization

The DM formalism, which was originally developed for the calculation of total single ionization cross sections of atoms [4], can be extended to atomic K-shell ionization as shown by Deutsch et al. [3]. The DM formalism expresses the K-shell ionization cross section σ_{1s} as

$$\sigma_{1s} = g_{1s}\pi(r_{1s})^2\xi_{1s}f(U)F(U) \quad (1)$$

where $(r_{1s})^2$ is the mean square radius of the atomic 1s-shell, ξ_{1s}, the number of electrons in the 1s shell, is equal to 2, and g_{1s} is a weighting factor (see Deutsch et al. [3] and Margreiter et al. [4] for further details). The energy dependence of the K-shell ionization cross section is given by the product of the two functions $f(U)$ and $F(U)$. Here U refers to the reduced impact energy, $U = E/E_{1s}$, where E is the energy of the incident electron and E_{1s} refers to the binding energy of 1s-electrons. The function $f(U)$ is similar (but not identical) to the energy dependence first given by Gryzinski [7] and has the form

$$f(U) = (1/U)[(U\text{-}1)/(U + 1)]^a \times\{b + c[1 - (2U)^{-1}] \times\ln[2.7 + (U - 1)^{1/2}]\} \quad (2)$$

According to Deutsch et al. [4], the parameters a, b, c have the values $a = 1.75$, $b = 1$, and $c = 1$ for s electrons. The function $F(U)$ is a relativistic correction factor that is again similar (but not identical) to the one introduced by Gryzinski [7] and has the form in our case

$$F(U) = R(U)[1 + 2(U)^{1/4}/(J)^2]$$

with $J = (m_ec^2)/E_{1s}$ and m_e being the electron mass. The function $R(U)$ is given by

$$R(U) = (1 + 2J)/(U + 2J)[(U + J)/(1 + J)]^2 \times\{[(1 + U)(U + 2J)(1 + J)^2]/[J^2(1 + 2J) + U(U + 2J)(1 + J)^2]\}^{3/2} \quad (3)$$

The above energy dependence results in cross section shapes that systematically rise more slowly in the energy region from threshold to about five times the threshold than the experimental K-shell ionization cross section data and the cross section shapes derived from other predictive formulae [8,9]. In an effort to improve the low-energy behavior of our DM K-shell ionization cross sections we used recent low-energy K-shell ionization data for sulfur [5] (which were in good agreement with earlier data [6]) to modify our energy dependence in that region. This resulted in a modified energy dependence of the form

$$f(U) = d(1/U)[(U - 1)/(U + 1)]^a \times\{b + c[1 - (2U)^{-1}] \times\ln[2.7 + (U - 1)^{1/2}]\} \quad (4)$$

where the parameters a, b, and c now have the values $a = 1.06$, $b = 0.23$, and $c = 1.00$ and the additional parameter d has the value $d = 1.1$. No changes were made in the relativistic correction factor $F(U)$. However, because the overall energy dependence is given by the product of $F(U)$ and $f(U)$, the modified functional dependence of $f(U)$ leads to a modified energy dependence at all impact energies.

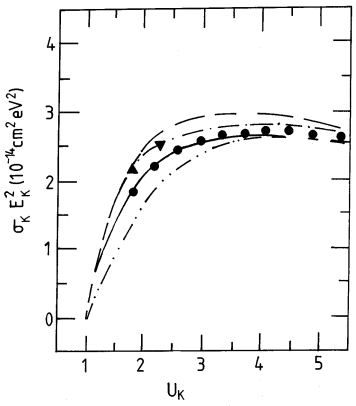

Fig. 1. Scaled K-shell ionization cross section σE^2 for oxygen as a function of the reduced impact energy $U = E/E_{1s}$ in the low-energy regime. The various curves refer to the present calculation (dash-dot-dash line), the previous DM calculation (dash-dot-dot-dash line), the prediction of the formula of Jakoby et al. [9] (solid line) and the prediction of the formula of Casnati et al. [8] (dash-dash line). The experimental data are from Glupe and Mehlhorn [10] (filled circle), Tawara et al. [11] (filled triangle), and Platte et al. [12] (filled inverted triangle).

3. Results and discussion

We used the modified energy dependence of Eq. (4) in combination with Eq. (1) in a series of revised calculations of the K-shell ionization cross sections for the 11 atoms listed above for which critically evaluated K-shell ionization data are available [2]. Figs. 1–3 show three typical examples of the results. We show the enlarged low-energy regions from the ionization threshold to five times the threshold energy for the elements O, Ne, and Cu. In addition to the

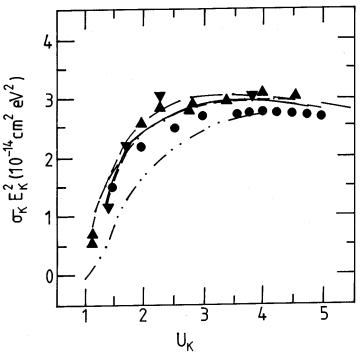

Fig. 2. Same as Fig. 1 for neon.

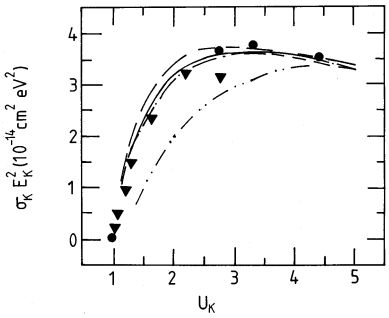

Fig. 3. Same as Fig. 1 for copper. The experimental data are from Davis et al. [13] (filled circle) and Shima et al. [14] (filled inverted triangle).

experimental data indicated by the various symbols, we show the cross section shapes derived from our modified DM calculation, as well as cross section shapes from the predictive equations of Casnati et al. [8] and Jakoby et al. [9]. For reasons of comparison, we also included the cross section shapes from the earlier version of the DM formalism according to Eq. (2) and Eq. (1). It is apparent that the modified energy dependence of Eq. (4) results in cross section shapes of the DM cross sections that are in much better agreement with the shapes predicted by the other two predictive formulae [8,9] and with the experimental data. Situations similar to those depicted in Figs. 1–3 were found for all 11 elements listed above. In all cases, the modified low-energy dependence led to a marked improvement of the DM cross section shape in the near-threshold energy regime.

As discussed before, the modified low-energy part of the DM cross section shape, $f(U)$, leads to a modified overall energy dependence, because the energy dependence is given by the product of $f(U)$ and the relativistic factor $F(U)$ [see Eq. (1)]. Fig. 4 shows K-shell ionization cross section data for Ar (as an example) over a wide energy range from threshold to 10^6 keV. The theoretical cross section data of Scofield [15] and the experimental data compiled by Long et al. [16] are shown in comparison with the prediction of the DM formalism (dash-dot line) and the data (solid line) and Born-Bethe calculations (dashed line) of Khare and Wadehra [17]. It is apparent that the DM formalism predicts a cross

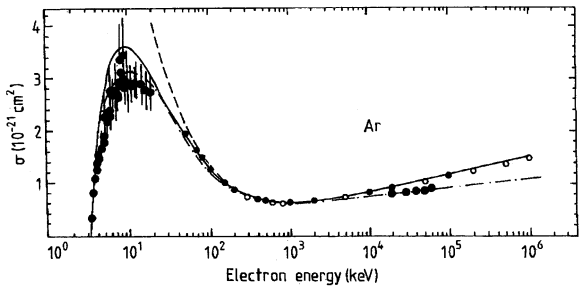

Fig. 4. K-shell ionization cross section for Ar as a function of impact energy. The various symbols refer to the present DM calculation (dash-dot-dash), the theoretical data of Scofield [15] (open circle), the experimental data compiled by Long et al. [16] (filled circle), and the data (solid line) and Born-Bethe calculations (dash line) of Khare and Wadehra [17].

section shape that agrees with the available data over the entire energy range. Again, similar situations are found for other atoms for which critically evaluated data and calculations are available over a wide energy range [15].

4. Conclusions

We derived a modified formula to describe the energy dependence in the low-energy regime of atomic K-shell ionization cross sections calculated in the framework of the DM formalism. The modified energy dependence was obtained from a fitting procedure using recent K-shell ionization cross section data for atomic sulfur. A comparison of the calculated K-shell ionization cross sections using this modified energy dependence with critically evaluated experimental data for 11 other atoms and cross section shapes derived from other predictive formulae revealed good agreement in the low-energy regime as well as at relativistic impact energies.

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