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Calculated electron impact cross sections for the K-shell ionization of Fe, Co, Mn, Ti, Zn, Nb, and Mo atoms using the DM formalism

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Abstract

We used the Deutsch-Märk (DM) formalism to calculate atomic K-shell electron impact ionization cross sections for the elements Fe, Co, Mn, Ti, Zn, Nb, and Mo. The calculated K-shell ionization cross sections are compared with recently measured K-shell ionization cross sections. Good to satisfactory agreement was found for all atoms with the exception of Ti. Moreover, when compared to other available K-shell ionization cross sections for these atoms, calculated using other theoretical methods and semiempirical formulae, the predictions of the DM formalism achieve a level of agreement with experimental data that is as good or better than the predictions from the other methods. (Int J Mass Spectrom 213 (2002) 5–8)
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1. Introduction

Cross sections for the removal of electrons from the innermost shell of atoms by electron impact are needed in many fields such as atomic physics, plasma physics, materials and surface science, and radiation chemistry [1]. Recently, new measurements of K-shell ionization cross sections were reported for the elements Sc and V [2] and Cr, Ni, and Cu [3]. All these metal atoms are of particular importance in fusion plasmas [4]. The authors of references [2] and [3] also compared the experimentally determined cross sections with a variety of predictions from various theoretical models and semiempirical formulae. An et al. [2] also mentioned the Deutsch-Märk (DM) formalism (see [4]) as a method to calculate K-shell ionization cross sections and said that the predictions based on the DM formalism are inferior to the results from many other methods. We would like to point out that this statement is erroneous. As shown recently and discussed in detail [4], the Deutsch-Märk (DM) formalism can be used to calculate K-shell ionization cross sections for these five atoms, and good to satisfactory agreement was found between the DM calculations and the measured K-shell ionization cross sections for these five atoms.

In this letter, we extend the calculations of K-shell

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ionization cross sections using the DM formalism to the atoms Fe, Co, Mn, Ti, Zn, Nb, and Mo, for which experimental data are also available [5–10]. The DM formalism expresses the K-shell ionization cross section σ_{1s} as

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

where $(r_{1s})^2$ is the radius of maximum radial density of the atomic 1s-shell taken from the tables of Desclaux [11]; ξ_{1s}, the number of electrons in the 1s-shell, is equal to 2; and g_{1s} is a weighting factor (see references [12–14] 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 [15] and has the form

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

where the parameters a, b, c, and d have the following values: $a = 1.06$, $b = 0.23$, $c = 1.00$, and $d = 1.1$. The function $F(U)$ is a relativistic correction factor, which is again similar (but not identical) to the one introduced by Gryzinski [15] and has the form, in our case, of

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

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

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

We used the DM formula of Eq. (1) to calculate the K-shell ionization cross sections for the atoms Fe, Co, Mn, Ti, Zn, Nb, and Mo, and we compare the calculation to recently measured experimental cross sections and to predictions from the empirical formula of Casnati et al. [16] and the theoretical calculations of Luo and Joy [17]. The advantage of the DM formalism lies in the simplicity of its use compared with other theoretical models. However, the DM formula is superior to purely empirical formulae as it contains quantum mechanically calculated information, and all parameters in Eq. (1) have a real physical meaning.

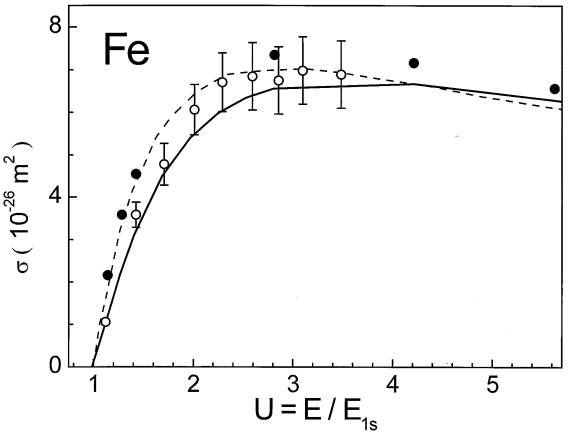

Fig. 1. K-shell ionization cross section σ for Fe as a function of the reduced impact energy $u = E/E_{ks}$. The experimental data are from Luo et al. [6]. The solid line represents the present DM calculation, the dashed line denotes the prediction of the empirical formula of Casnati et al. [16], and the filled circles are the calculated cross sections of Luo and Joy [17].

Fig. 1 shows the experimentally determined K-shell ionization cross section data for Fe of Luo et al. [6] in comparison with the calculated cross sections of Luo and Joy [17], Casnati et al. [16], and with the present result. It is apparent that all three calculated cross sections represent the experimental data quite well over the entire range of impact energies depicted in the figure. In the case of Co (Fig. 2), the DM calculation lies somewhat below the other two calculated cross section curves and the measured cross section [5] for energies from threshold to about twice the threshold energy but agrees with the experiment within the quoted margin of error of the measured data. For higher energies, the DM calculation is closer to the experiment than the other two calculations. The DM calculation provides the best description of the measured K-shell ionization cross section for Mn [6] over the entire range of impact energies (Fig. 3). Fig.

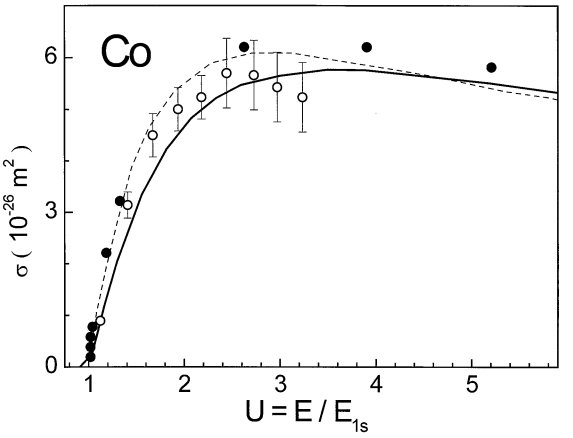

Fig. 2. Same as Fig. 1 for Co. The experimental data are from An et al. [5].

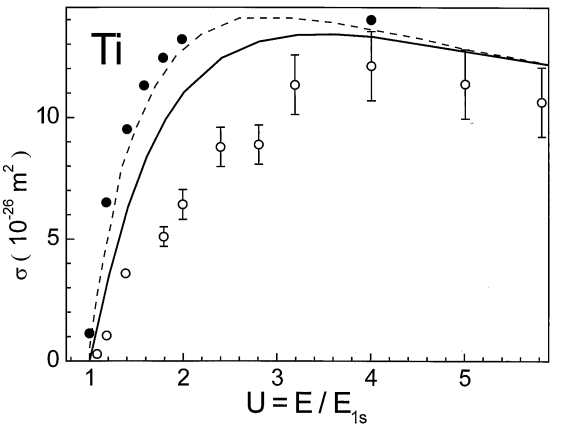

Fig. 4. Same as Fig. 1 for Ti. The experimental data are from He et al. [8].

4 shows the measured K-shell ionization cross section data of He et al. [8] for Ti; they lie systematically below the three calculated cross section curves, which, in turn, are in excellent agreement with each other. The discrepancy between experiment and calculation is most pronounced at low impact energies up to about three times the threshold energy. We have no simple explanation for this discrepancy. The case of Zn (Fig. 5) is very similar to the situation found in Mn (Fig. 3), with the DM calculation yielding excellent agreement with the measured data [10] whereas the other two calculations appear to overestimate the measured data systematically. In Nb (Fig. 6), where the energy range for which experimental data are available [9] is rather limited, the DM calculation and the calculation of Luo and Joy [17] reproduce the measured data very well, whereas the empirical formula of Casnati et al. [16] systematically overestimates the data. Mo (Fig. 7) is the only situation where the formula of Casnati et al. [16] provides the best description of the measured K-shell ionization cross section data [8], which are also limited to a narrow range of impact energies. The DM calculation and the

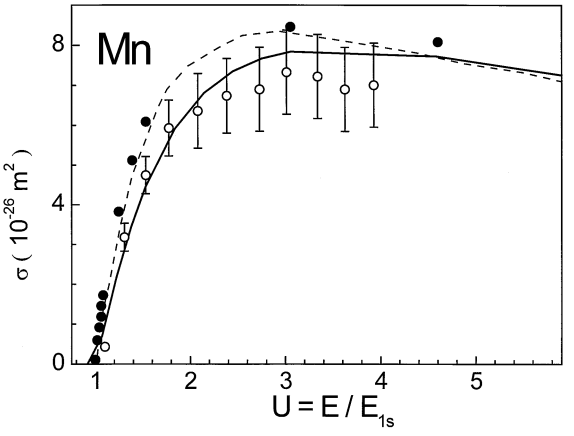

Fig. 3. Same as Fig. 1 for Mn. The experimental data are from Luo et al. [6].

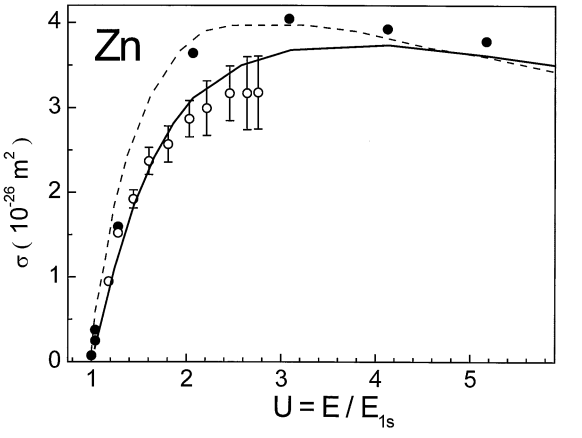

Fig. 5. Same as Fig. 1 for Zn. The experimental data are from Tang et al. [10].

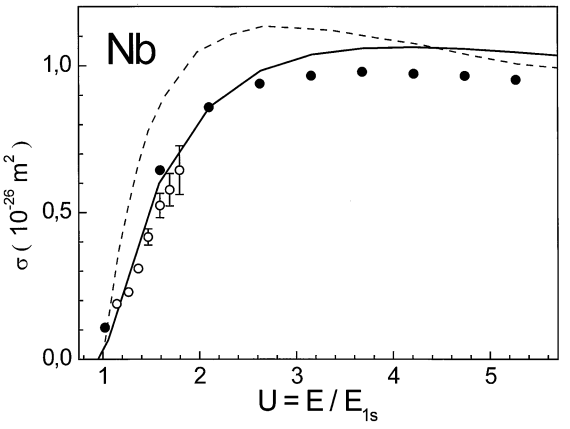

Fig. 6. Same as Fig. 1 for Nb. The experimental data are from Peng et al. [9].

calculation of Luo and Joy [17] are systematically below the measured data.

In summary, we have shown that the DM formalism allows the calculation of K-shell ionization cross sections for the seven elements Fe, Co, Mn, Ti, Zn, Nb, and Mo that show a level of agreement with existing measured data that is as good and often better than the predictions, based on other theoretical models and empirical formulae. The DM formula is comparatively easy to apply and contains information calculated by quantum mechanics. This renders the DM formalism an excellent choice for calculating K-shell and other ionization cross sections when compared with more rigorous methods, which are more difficult and time-consuming to apply, and with empirical formulae whose parameters have little, if any physical meaning.

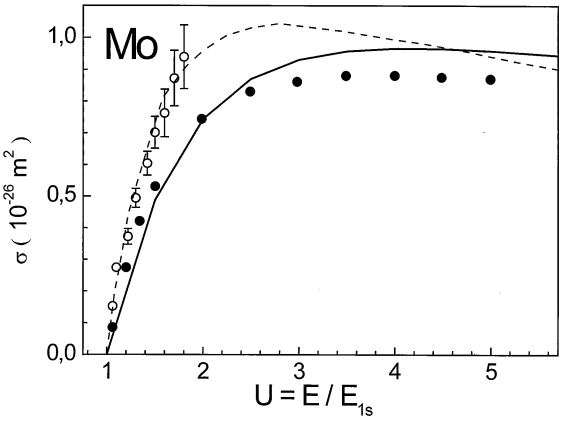

Fig. 7. Same as Fig. 1 for Mo. The experimental data are from He et al. [8].

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