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Calculated cross sections for the single ionization of atoms (N, Cu, As, Se, Sn, Sb, Te, I, Pb) by electron impact*

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By correcting some primary parameters in the semi-classical Deutsch–Märk (DM) formula, this paper calculates the absolute single electron-impact ionization cross sections of atoms N, Cu, As, Se, Sn, Sb, Te, I and Pb from threshold to 10000 eV. The calculated cross sections are compared with available experimental data and other theoretical results. An excellent agreement was achieved between the calculated and measured cross sections for these atoms over a wide range of impact energies.

Keywords: DM formula, ionization cross sections, electron-impact
PACC: 3480, 3480D

1. Introduction

The ionization of an atom by electron impact is one of the most important and fundamental collision interactions in atomic physics. The ionization process plays a very important role in many fields including discharges, plasma, planetary, atmosphere, spectrometry and chemical analysis. Although considerable advances s[1−3] in quantitative determination of ionization cross sections for light atomic targets have been made in the past decades, including the description of the simplest H-like and He-like atoms or ions in the periodic table by using the convergent close-coupling method,[4−6] and the calculation for the cross sections of atoms by using the plane wave Born approximation (BA) and so on,[7−9] rigorous quantum mechanical calculations of atomic ionization processes with high nuclear number Z are still very difficult. So the semi-classical and semi-empirical approaches have been used as the preferred methods for the calculation of the cross sections of many-electron atoms. The Born–Bethe formula provides an acceptable description of atomic impact ionization cross sections in the high energy region,[10] but fails in the low energy region. There are similar trends in the binary-encounter-dipole (BED) method introduced by Kim and Rudd.[11] The semi-classical Deulsch–Mařk (DM) formula was originally developed for using in plasma modelling applications and aiming at a description of atomic ionization cross sections in the energy range from threshold to 100 eV, that the energy dependence was described in terms of a Gryzinsky-type expression.[12] To improve the behaviour in the region of high impact energies, the modified DM formula was introduced, which is an easy-to-use formula to calculate atomic ionization cross sections for the entire range of impact energies from threshold to the high-energy region, and it is successful for many light elements such as F, P, Ar, Si and Na.[13−16] In the modified DM method, the fitting parameters are only from experimental data of light atoms H, He, C, Ne, Mg, Al, and Ag, correspondingly, the parameters for subshells 1s, 2s, 2p, 3s and 3p are more accurate. So the modified DM method can predict excellent cross sections for the atoms with nuclear number $Z < 18$. In the low-energy region for heavy elements, DM method is still excellent, but in high-energy region the deviation of DM method in comparison with experiment becomes larger. It is not a good prediction for those atoms with complex subshells, for example, when 4s, 4p, 4d, 4f, 5s, 5p and 6p are introduced. So it is necessary to correct some parameters for improving the

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results of the high Z atoms in the high-energy region of incident electrons. In this paper, on the basis of the reliable experimental data and with the consideration of quantum mechanics, we correct some parameters (Table 1) of subshells 2p, 4s, 4p, 5p and 6p in the modified DM formula by using the least square method, and apply the new parameters to the calculation of cross sections for atoms N, Cu, As, Se, Sn, Sb, Te, I and Pb, which have high Z numbers and complex electron structure except for N. Comparison between the present results and available experimental data was made, moreover, we also compared the present data with the result of modified DM formula using original parameters and BA.

2. Theory and background

The DM formula was proposed to incorporate the quantum mechanics into classical formulation of the cross sections $\sigma_{n,l}$,[13,17]

$$\sigma_{n,l} = \pi r_{n,l}^2 g_{n,l} N_{n,l} f(u), \tag{1}$$

where $r_{n,l}$ is the radius of maximum radial density of the atom in the nl-shell, $g_{n,l}$ is the weighting factors accounted for the different contributions from the various subshells[17,18] and $N_{n,l}$ is the number of electron in the nl-shell.[19,20] The energy dependence of the cross section is contained in the function$f(u)$ which is given by

$$f(u) = d\frac{1}{u}\left(\frac{u-1}{u+1}\right)^a \left\{b + c\left(1 - \frac{1}{2u}\right) \times \ln(2.7 + (u-1)^{1/2})\right\}, \tag{2}$$

where $u = E/E_{nl}$. Here E refers to the incident energy of the electrons and E_{nl} is the ionization energy in the (n,l) subshell. It is also found that different sub-shells with different $N_{n,l}$ have different $g_{n,l}$, but $g_{n,l}E_{n,l}$ is a constant. The constants a, b, c, d have different values for s, p, d and f electrons as one might expect on the basis of the different angular shapes of atomic s, p, d and f orbitals.[17] The sum extends over all atomic sub-shells labelled by n and l is

$$\sigma = \sum_{n,l} \sigma_{n,l}. \tag{3}$$

For extending the range of validity of DM formalism to high-energy, modified DM formula was introduced by replacing Gryzinsky-type energy dependence with 'scaled' energy dependence,[14]

$$\sigma(u) = \sum_{n,l} g_{n,l}\pi r_{n,l}^2 N_{n,l} b_{n,l}^q(u)[\ln(c_{nl}u)/u]. \tag{4}$$

The coefficient $b_{n,l}^q$ in the Bethe high-energy formula that depends on the energy has the explicit form

$$b_{n,l}^q(u) = \frac{a_1 - a_2}{[1 + (u/a_3)^p]} + a_2. \tag{5}$$

And coefficients a_1, a_2, a_3, p, c_{nl} were determined from the measured cross section for the various values of n and l, the superscript q refers to the number of electrons in the (n,l) sub-shell, so $b_{n,l}^q$ depends on the number of electrons in a given nl-shell.

After analysing and comparing the data of cross sections for different subshells from experiments with the result of DM method, we think that semi-empirical parameters in DM method are not accurate in some subshells for heavy elements.[21,22] We kept some parameters in DM method, which have been proved to be good by the previous calculations, especially, the parameters for light elements. Some parameters of subshells 2p, 4s, 4p, 5p and 6p are corrected by using the least square method, and the new parameters are summarized in Table 1.

Table 1. The atomic parameters of typical sub-shells; the parameters on the left are from the DM method and the present parameters are on the right in each column (the other parameters can be found in the literature).[13]

Shell	a_1		a_2		a_3		p		c		g_{nl}	
$2p^3$	–0.15	0.02	1.17	1.70							30.0	28.0
$4s^1$	0.31	1.20	0.87	1.80	2.32	3.50	1.95	5.20	1.00	1.02	7.40	10.0
$4p^3$	0.59	0.61	1.01	1.32	8.42	8.50	2.12	2.05			22.4	21.8
$4p^4$	0.59	0.60	1.01	1.10			2.12	2.05	0.95	0.82	22.4	24.5
$5p^2$	0.59	0.81	1.01	1.51								
$5p^3$	0.59	0.66	1.01	1.20								
$5p^4$	0.59	0.62	1.01	1.20								
$5p^5$	0.59	0.51	1.01	1.07	8.42	6.50						
$6p^2$	0.59	0.75	1.01	1.50	8.42	6.50						

3. Results and discussions

In order to obtain electron impact single ionization cross sections for atoms N, Cu, As, Se, Sn, Sb, Te, I and Pb, we have corrected some parameters of the modified DM formula to improve the results of the high nuclear number atoms in the high-energy region. Reliable experimental data have been reported,[23–26] and comparison between the present calculation, experiments and the BA method are given in the following figures. The total single ionization cross sections of atom N can be obtained from the experiment performed by Brook, and the data of cross sections for other atoms (Cu, As, Se, Sn, Sb, and Te) are obtained from Freund *et al.*[23–26] For atom N, there is distinct discrepancy between the experimental data and the results of DM or BA, but our results show a success for atom N, with almost all experimental dots covered on the solid line (the present results) within the whole energy region as shown in Fig.1.

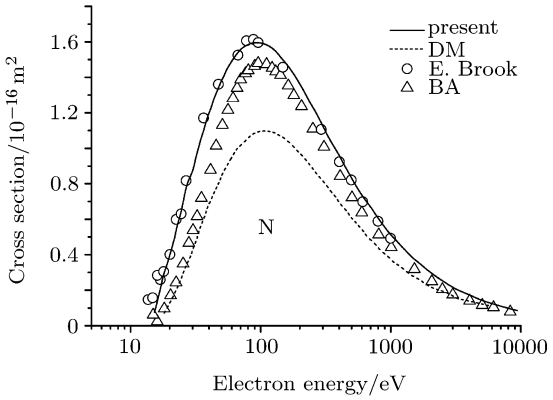


Fig.1. Calculated cross section as a function of electron energy for N impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represents the experimental data.

For Cu, in Fig.2 we can see that there is a large discrepancy between the DM with original parameters and experiment, and the result of BA calculation is lower in the low energy region and higher in the high-energy region than the experimental data. Yet the present calculation yields a better agreement with experimental result, especially in the electron energy from the threshold to 100 eV. Similarly, the present result yields a better agreement than the calculation of BA or DM with original parameters for the other atoms.[27,28]

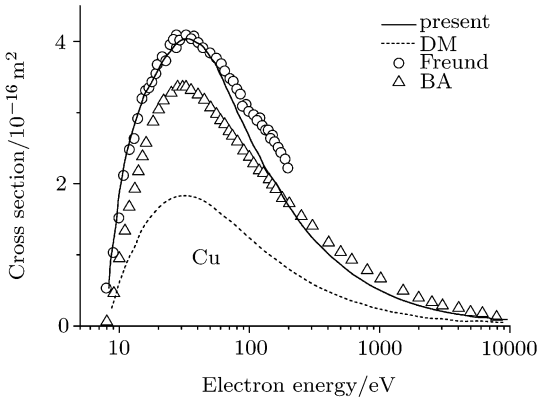


Fig.2. Calculated cross section as a function of electron energy for Cu impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represent the experimental data.

Figures 3 to 8 show the cross sections for As, Se, Sn, Sb, Te, and I respectively, in comparison with the available data including experimental data, DM and BA calculated data. All our present calculations are in agreement with the data of experiments. Although the shift between the calculated and measured cross sections in the low-energy range up to about 30 eV is exaggerated by the choice of logarithmic energy scale, the discrepancy is still slight. Under the 40 eV, the present calculation provides a precise description of the measured data at impact energies above 30 eV. On the contrary, other calculated results do not reproduce the experimental data. The cross sections of BA calculation are always higher than the experimental data in high energy region and lower in the low energy region except for I, whereas the result of DM method is remarkably good in the low energy region, but in

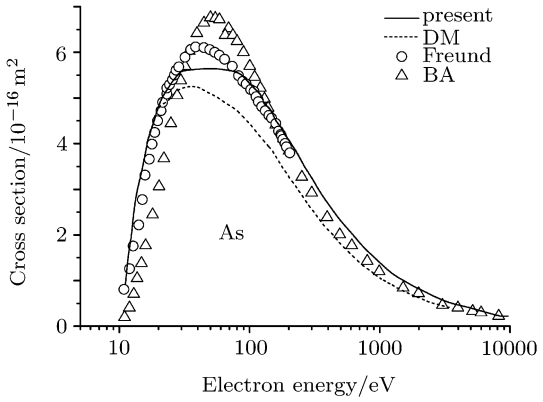


Fig.3. Calculated cross section as a function of electron energy for As impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represent the experimental data.

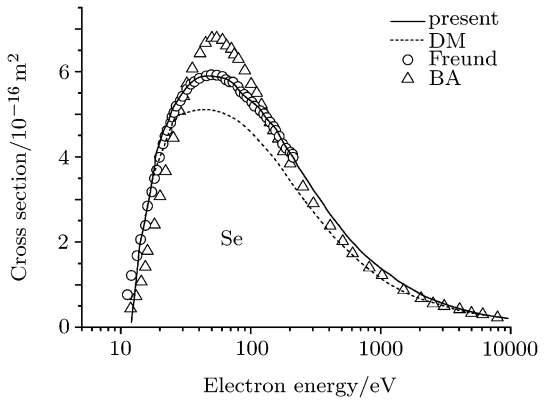


Fig.4. Calculated cross section as a function of electron energy for Se impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represent the experimental data.

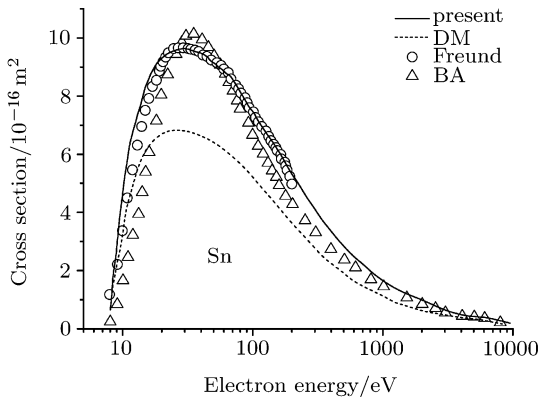


Fig.5. Calculated cross section as a function of electron energy for Sn impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represent the experimental data.

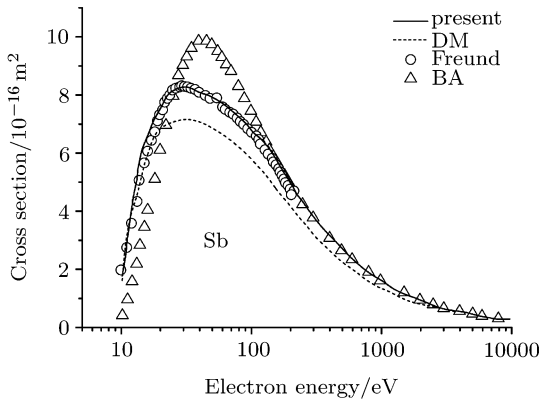


Fig.6. Calculated cross section as a function of electron energy for Sb impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represent the experimental data.

the high energy region some discrepancy appears. In the high energy region, our result is far more excellent than others, especially in reproducing the shape and peak of the experimental result.

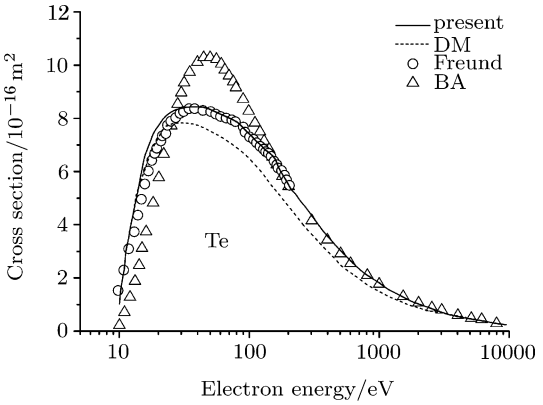


Fig.7. Calculated cross section as a function of electron energy for Te impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represent the experimental data.

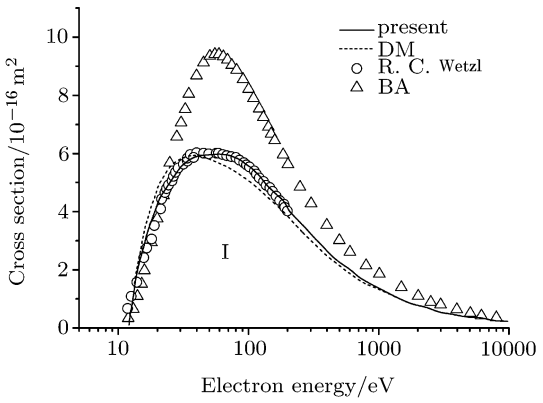


Fig.8. Calculated cross section as a function of electron energy for I impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represent the experimental data.

For Pb, to the best of our knowledge, there is no result for the BA method, so we only compare the results of the present calculation with the results of the DM calculation and experiment as shown in Fig.9. The results of the DM method show a large discrepancy with Freund's measurement, especially near the maximum; one of the reasons is the using of fitting parameters which are only based on some low Z atoms H, He, C, Mg, Al and Ag. However, after modifying or adding parameters, our results are in good agreement with experiment data except for a minor discrepancy in the region from 20–30 eV and 50–80 eV.

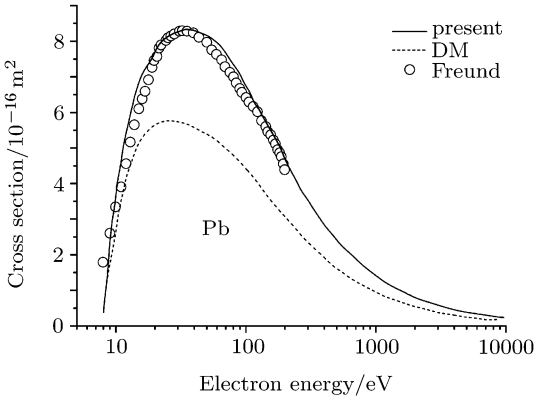


Fig.9. Calculated cross section as a function of electron energy for Pb impacted by electron. The solid line represents the present calculation, the dashed line represents the DM calculation, the open uptriangles represent BA and the open circles represent the experimental data.

4. Summary

Electron-impact ionizations are widely used in many areas of physics, such as astrophysics, atomic physics, plasma physics and laser fusion. The electron-impact ionization of atoms with high nuclear number and complex structures has been studied very intensively over many decades. The DM formula performs very well only in the low energy region, and the revised DM formula by Deutsch for improving the accuracy in the high energy region has still some problems for some sub-shells of atoms, especially when the number of atoms is large and the structures of atom become complex. In this paper, according to the original calculated results for atoms O, F, P, Ar, Kr, Na, K, Cs, Br, Cl, Si, S, and Ca, and experimental data of cross sections for different sub-shells, some parameters of sub-shells in DM formula were corrected and the cross sections of the following atoms N, Cu, As, Sn, Se, Sb, Te, I and Pb were calculated. A comparison of our calculations with available experimental data, and with the theoretical results of DM using the original DM parameters or BA shows that our results yield a better agreement with experimental data.

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