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Empirical model for electron impact ionization cross sections of neutral atoms

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Abstract. A simple empirical formula is proposed for the rapid calculation of electron impact total ionization cross sections both for the open- and closed-shell neutral atoms considered in the range $1 \leq Z \leq 92$ and the incident electron energies from threshold to about 10^4 eV. The results of the present analysis are compared with the available experimental and theoretical data. The proposed model provides a fast method for calculating fairly accurate electron impact total ionization cross sections of atoms. This model may be a prudent choice, for the practitioners in the field of applied sciences e.g. in plasma modeling, due to its simple inherent structure.

PACS. 34.80.Dp Atomic excitation and ionization by electron impact

1 Introduction

Electron impact ionization has fundamental importance in understanding collision dynamics and structure of matter. Besides, electron impact total single ionization (EITSI) cross section data are needed in such applied fields [1] as plasma physics, radiation science, mass spectroscopy, lasers and semiconductor physics, and so on. Several quantum mechanical methods have been proposed [2–6] to calculate EITSI cross sections during the last decades for different neutral atoms. These methods are, developed by solving the Schrödinger equations, and capable of deducing differential ionization cross sections as well as total ionization cross sections. Quantum methods such as R-matrix method, distorted wave Born approximation and convergent close coupling method have, used a variety of numerical methods, been employed to calculate cross sections. Experiments and quantum methods calculate cross sections for discrete energies and selected species. Besides, these theoretical methods require not only large computational resources but also computational time. Moreover, quantum mechanical procedures do not usually lead to analytic or semi-analytic models. Consequently, these methods are not user-friendly for the practitioners in the field of applied sciences. The requirement can be best fulfilled by analytic models, which can calculate reliable data over wide domains of validity. Hence, there is an acute need for simple, and reliable theoretical methods to calculate EITSI cross sections for the large number of neutral atoms and ions that may be used in the wide range of scientific and industrial applications.

Reviews on various empirical, semi-empirical and semi-classical models are provided by Younger and Mark [6]. Lotz formula [7], Deutsch-Mark (DM) formula [8] and binary-encounter-dipole (BED) model of Kim and Rudd [9] have been widely used for calculation and representation of cross sections. The latter two models [8,9] have been largely used for calculating EITSI cross sections for molecular species, and for selected atoms and ions. Bernshtam et al. [10] proposed a simple-to-use empirical model valid for selected ionic targets only with charge $q > 1$. Gryzinski [11] has formulated a semi-classical model, valid for atoms as well as ions but the model does not calculate accurate cross sections in most cases. Godunov and Ivanov [12] proposed a number of models for the calculation of EITSI cross sections but without generalization of parameters of the models.

There have been very little theoretical works using classical, quantal, or empirical method with a wide range of validity for the calculation of EITSI cross sections of neutral atoms. EITSI cross sections are difficult to evaluate quantum mechanically since it requires model accounting for all the relevant mechanisms and reaction channels. Kim and Desclaux [13] proposed an empirical model for the calculation of EITSI cross sections. On the other hand, Kim and Rudd [9] proposed a model, taking into account binary encounter Bethe (BEB) model for direct electron impact ionization and scaled Born cross sections for dominant inner-shell excitation-autoionization, only for C, N, and O neutral targets. Their model calculates EITSI cross

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sections from threshold to several keV in the incident electron energy. A simple-to-use model capable of calculating sufficiently accurate cross section data for wide ranges of species and energies may contribute to fill up, to some extent, the gap between the available data and the demand level. With this motivation, we propose a simple empirical model for the fast calculation of EITSI cross sections of neutral atoms, covering not only the wide variety of targets from $Z = 1-92$ but also the wide range of incident electron energies.

The predicted results of the model are compared with the available experimental data and other theoretical calculations. This paper is organized as follows. Section 2 provides the outline of the proposed model. Section 3 deals with the presentation of results of analysis. Conclusions are drawn in Section 4.

2 Outline of the model

Bell et al. [14] proposed a semi-empirical formula, known as the BELI form [12], for fitting the EITSI cross sections of atoms and ions. The formula is of the form

$$\sigma(E) = \frac{1}{EI}\left\{ A\ln(E/I) + \sum_{k=1}^{5} B_k(1 - I/E)^k \right\}. \quad (1)$$

Here, E is the kinetic energy of the incident electron, I is the ionization potential, and A and B_k are the fitting coefficients.

To improve the efficiency and to reduce the number of fitting coefficients of the BELI model for the description of EITSI cross sections to cover the wide range of neutral targets from $Z = 1-92$, we suggest, in line with the empirical model of Kim and Rudd [9], the following model. The EITSI cross section is given by

$$\sigma(E) = \sum_{nl} \frac{N_{nl} I_{nl}}{E} \left\{ A_{nl} \ln(E/I_{nl}) + B_{nl}(1 - I_{nl}/E) \right\}, \quad (2)$$

where A_{nl} and B_{nl} are the fitting parameters expressed as the function of normalized potential U_R. I_{nl} is the ionization potential of the ionizing nl orbit. E and I_{nl} both are expressed in eV. N_{nl} is the number of electrons in the ionizing nl orbit. The parameter A_{nl} is the Bethe coefficient and determines the high energy behavior of the cross section. Here the summation is over the orbit nl of the target atoms. Equation (2) contains two orbital dependent parameters A_{nl} and B_{nl}. This formula also ensures the correct behavior of the cross sections at both low and high impact energies. The coefficients A_{nl} and B_{nl} in equation (2) are determined from the overall best fits of our predicted cross sections to experimental data of 36 atomic targets in the range of atomic numbers $Z = 1-92$, considered here in. The quality of best fit is obtained by minimizing the chi-square defined by

$$\chi^2 = \sum_i \left[\frac{\sigma(E_i) - \sigma_{\exp}(E_i)}{\sigma(E_i)} \right]^2,$$

where $\sigma(E_i)$ and $\sigma_{\exp}(E_i)$ refer, respectively, to the predicted and experimental cross sections at the energy point E_i. A_{nl} and B_{nl}, are then generalized by making them dependent on I_{nl}. The parameters A_{nl} and B_{nl} are expressed as

(a) for s-orbit, as the outermost one

$$A_{nl} = \frac{9.14 \times 10^{-11} U_R}{(1 + 68.32U_R)^3}, \quad (3a)$$

$$B_{nl} = \frac{3.83 \times 10^{-11} U_R}{(1 + 60.95U_R)^3}, \quad (3b)$$

(b) for p- and d-orbits, as the outermost one

$$A_{nl} = \frac{1.22 \times 10^{-6} U_R}{(1 + 566.46U_R)^{3.5}}, \quad (3c)$$

$$B_{nl} = -\frac{4.39 \times 10^{-9} U_R}{(1 + 102.87U_R)^{3.7}}, \quad (3d)$$

(c) for s-orbit, as the innermost one

$$A_{nl} = \frac{3.97 \times 10^{-11} U_R}{(1 + 20.74U_R)^{3.6}}, \quad (3e)$$

$$B_{nl} = \frac{2.29 \times 10^{-10} U_R}{(1 + 39.9U_R)^{3.6}}, \quad (3f)$$

(d) for p- and d-orbits, as the innermost one

$$A_{nl} = \frac{3.88 \times 10^{-14} U_R}{(1 + 6.96U_R)^3}, \quad (3g)$$

$$B_{nl} = \frac{4.36 \times 10^{-16} U_R}{(1 + 0.33U_R)^8}. \quad (3h)$$

Ionization potential is normalized by $U_R = I_{nl}/R$, where R is the Rydberg energy. The units of A_{nl} and B_{nl} are expressed in cm^2.

3 Results and discussions

The ionization potentials I_{nl} are taken from Desclaux [15]. Using the proposed model we have calculated EITSI cross sections, using equation (2) along with equations (3), for H, He, Li, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, Fe, Cu, Ga, Ge, As, Se, Br, Kr, Ag, In, Sn, Sb, Te, I, Xe, Ba, Hg, Pb, Bi, and U targets, as shown in Figures 1–6, over a wide incident electron energies from threshold to 10^4 eV. The calculations proposed by Kim and Desclaux [13], and Godunov and Ivanov [12] are also included for comparison with the proposed model. We have presented here only those targets whose experimental data are available. Most recent experimental as well as theoretical results are taken into account to compare the results obtained by the proposed model. Experimental and theoretical data are collected from, Shah et al. [16] for H; Rejoub et al. [17], Schram et al. [18], Nagy et al. [19], Shah et al. [20] Montague et al. [21], Stephan et al. [22], and Wetzel et al. [23] for He; Zapesochnyi

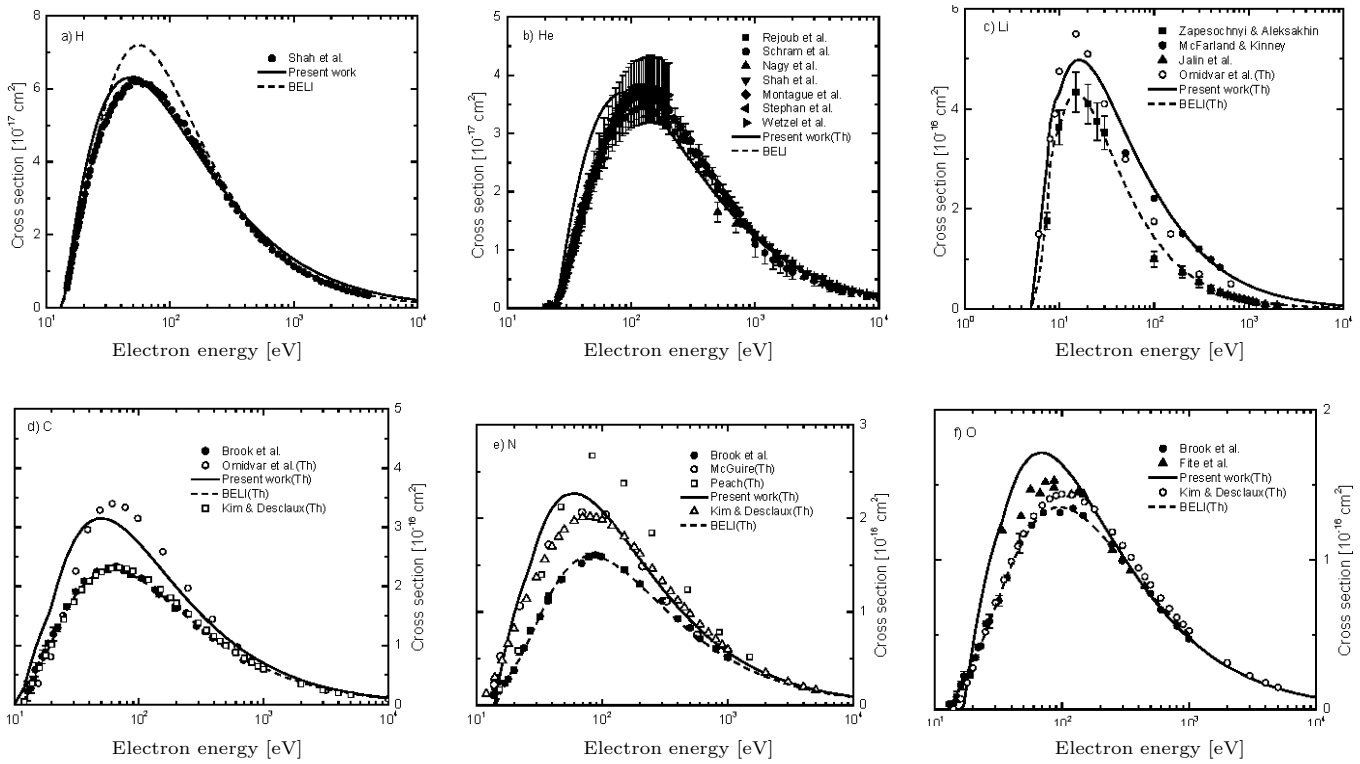

Fig. 1. Electron impact total single ionization across sections as function of incident electron energy. (a) H, (b) He, (c) Li, (d) C, (e) N, and (f) O.

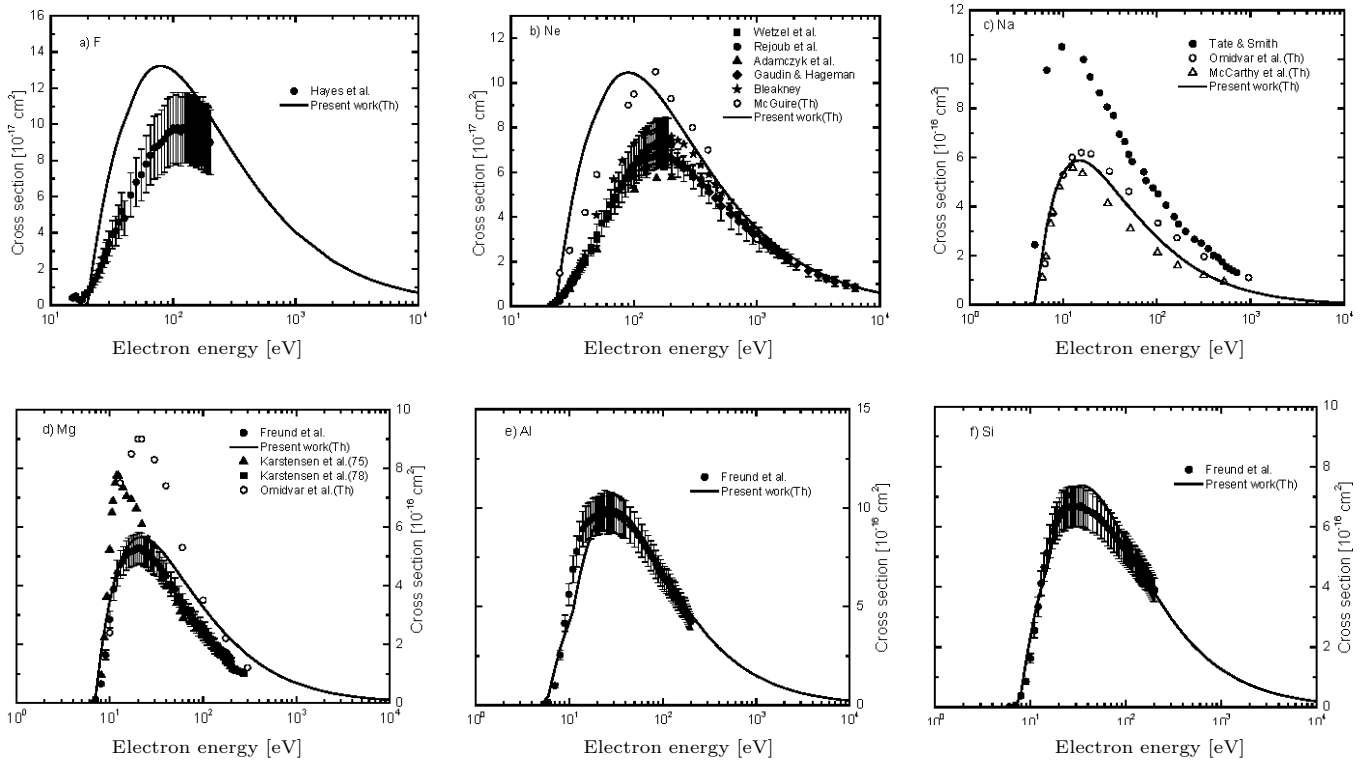

Fig. 2. Same as in Figure 1: (a) F, (b) Ne, (c) Na, (d) Mg, (e) Al, and (f) Si.

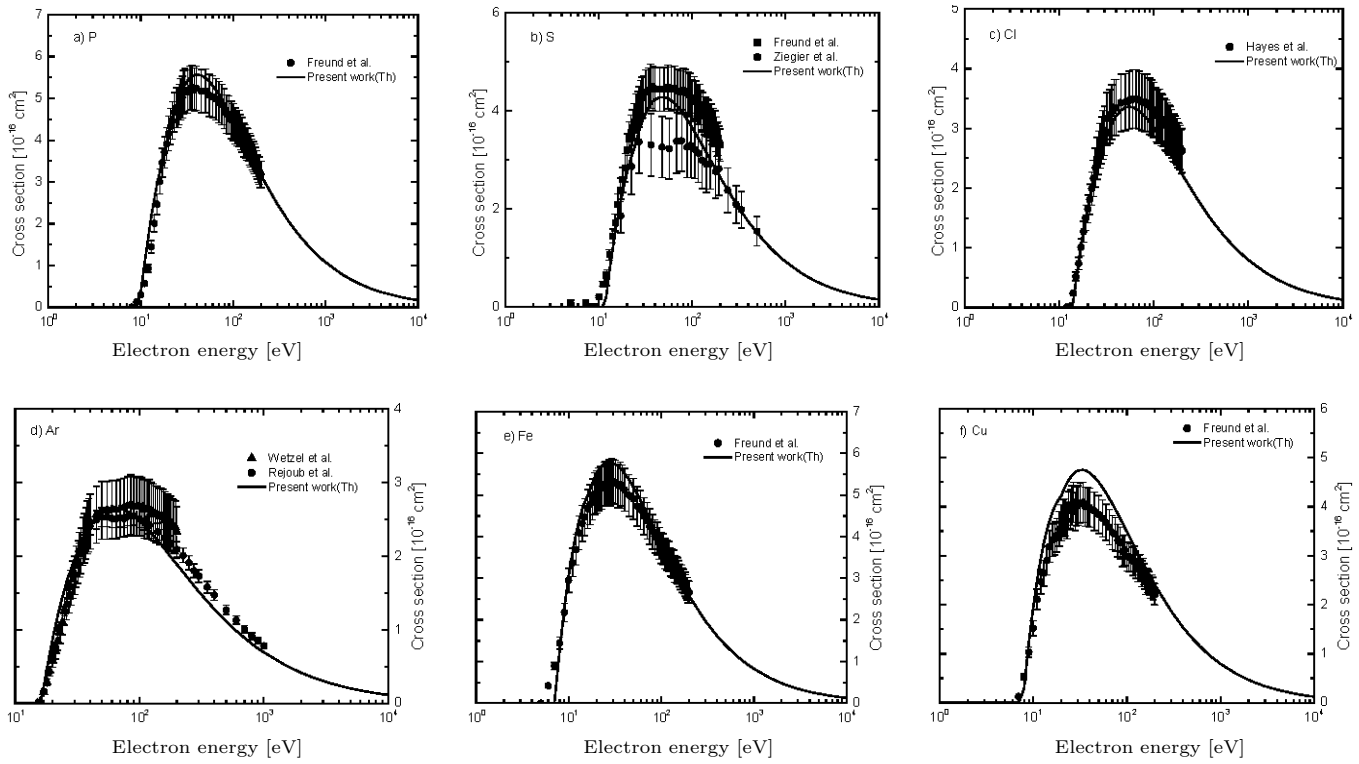

Fig. 3. Same as in Figure 1: (a) P, (b) S, (c) Cl, (d) Ar, (e) Fe, and (f) Cu.

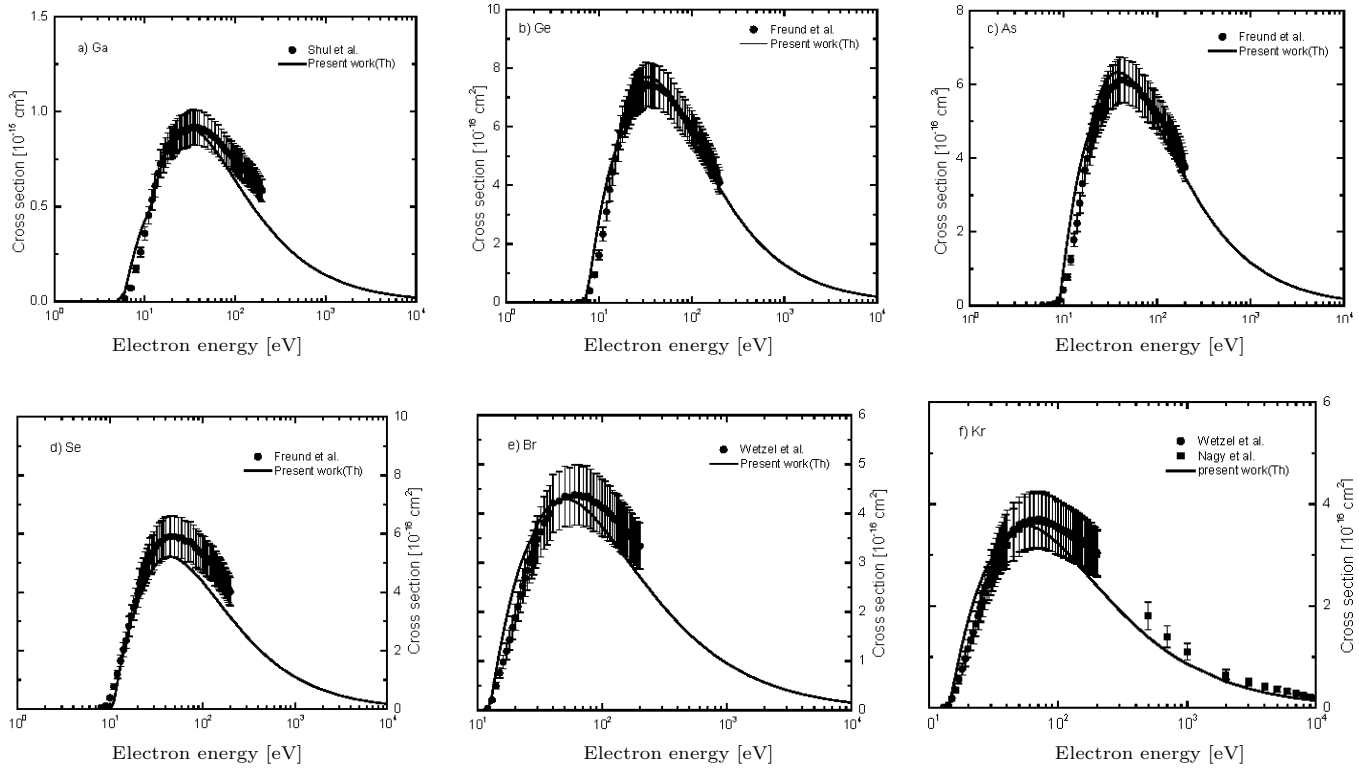

Fig. 4. Same as in Figure 1: (a) Ga, (b) Ge, (c) As, (d) Se, (e) Br, and (f) Kr.

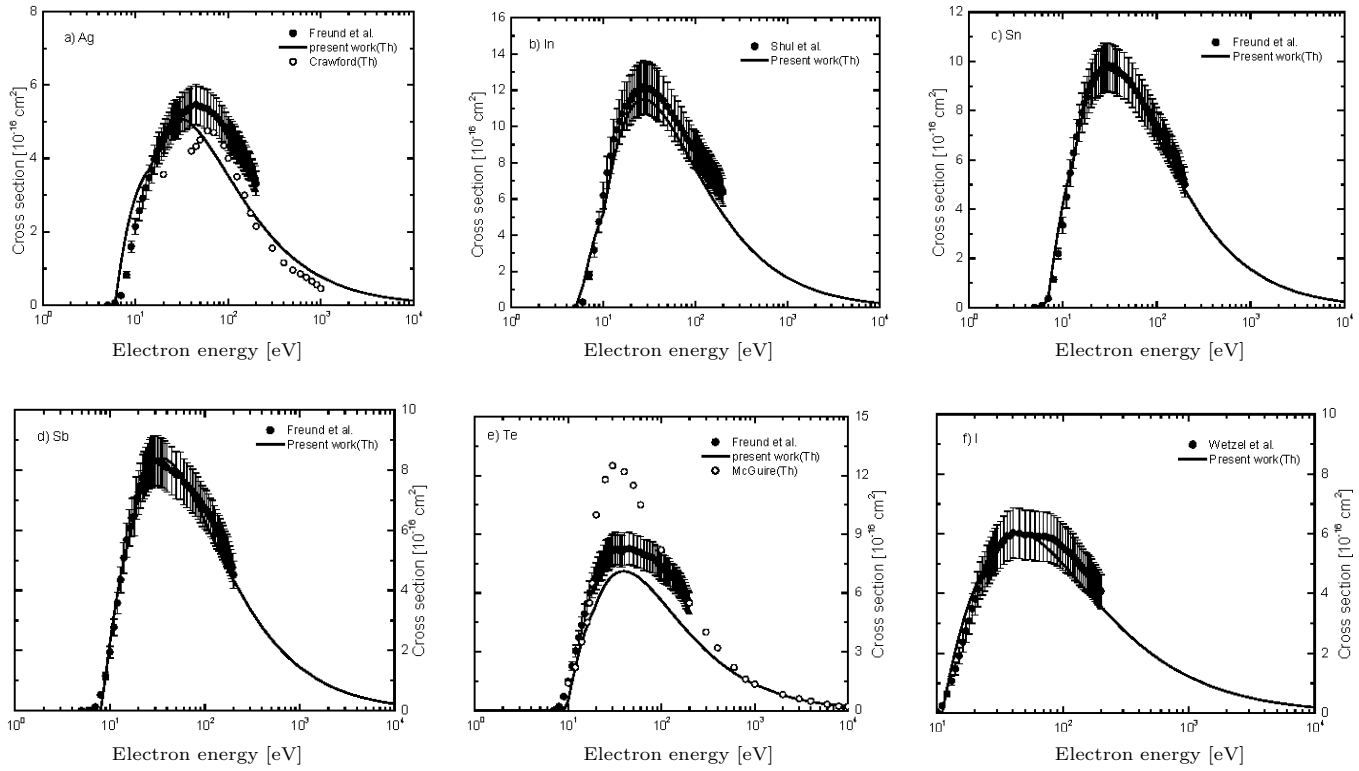

Fig. 5. Same as in Figure 1: (a) Ag, (b) In, (c) Sn, (d) Sb, (e) Te, and (f) I.

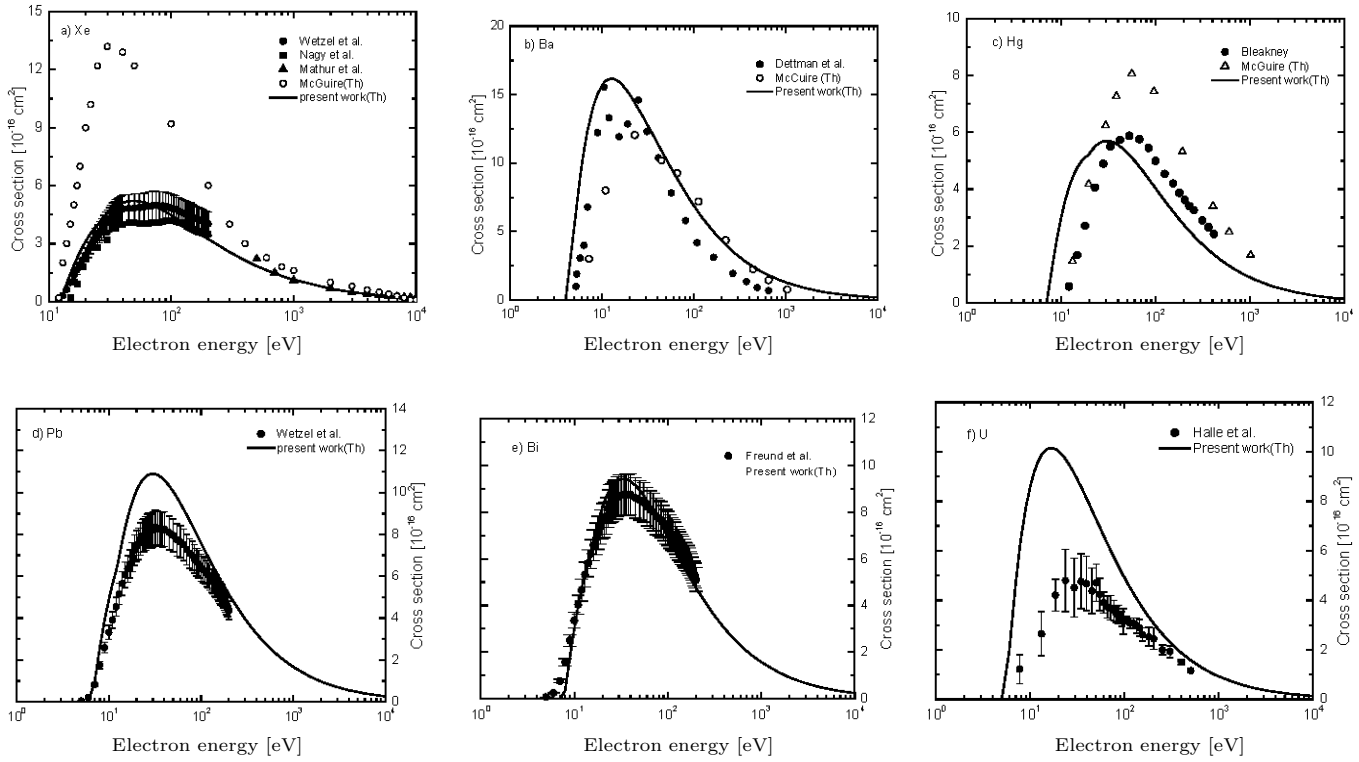

Fig. 6. Same as in Figure 1: (a) Xe, (b) Ba, (c) Hg, (d) Pb, (e) Bi, and (f) U.

and Aleksakhin [24], McFarland and Kinney [25], Jalin et al. [26], Omidvar et al. [27] for Li; Brook et al. [28], Omidvar et al. [27], and Kim and Desclaux [13] for C; Brook et al. [28], McGuire [29], Peach [30] and Kim and Desclaux [13] for N; Brook et al. [28], Fite et al. [31] and Kim and Desclaux [13] for O; Hayes et al. [32] for F; Wetzel et al. [23], Rejoub et al. [17], Adamczyk et al. [33], Gaudin and Hageman [34], Bleakney [35], and McGuire [29] for Ne; Tate and Smith [36], Omidvar et al. [27], McCarthy et al. [37] for Na, Freund et al. [38], Karstensen et al. [39],Karstensen et al. [40], Omidvar et al. [27] for Mg; Freund et al. [38] for Al, Si, and P; Freund et al. [38], Ziegler et al. [41] for S; Hayes et al. [32] for Cl; Wetzel et al. [23], and Rejoub et al. [17] for Ar; Freund et al. [38] for Fe and Cu; Shul et al. [42] for Ga; Freund et al. [38] for Ge, As and Se; Wetzel et al. [23] for Br; Wetzel et al. [23] and Nagy et al. [19] for Kr; Freund et al. [38] and Crawford [43] for Ag; Shul et al. [42] for In; Freund et al. [38] for Sn and Sb; Freund et al. [38] and McGuire [44] for Te; Wetzel et al. [23] for I; Wetzel et al. [23], Nagy et al. [19], Mathur et al. [45] and McGuire [44] for Xe; Dettman et al. [46] and McGuire [47] for Ba; Bleakney [35] and McGuire [46] for Hg; Wetzel et al. [23] for Pb; Freund et al. [38] for Bi; and Halle et al. [48] for U, respectively. In all the figures, open- and filled symbols represent the theoretical and experimental data, respectively. As seen in Figure 1, thick continuous line represents the prediction by the proposed model while the dashed line is the prediction by BELI formula, the EITSI cross sections predicted by BELI model greatly underestimates the experimental data points of, Shah et al. [16] for H, McFarland and Kinney [25] for Li, and theoretical calculations of, Omidvar et al. [27] for Li and C, McGuire [29] and Peach [30] for N, Kim and Desclaux [14] for O, in the peak region. But BELI model predicts excellent EITSI cross sections for He only. On the contrary, theoretical calculations predicted by Kim and Desclaux [14] overestimates the experimental data of Brook et al. [28] for N and O while it underestimates for C. However, the present model for EITSI cross sections predicts experimental as well as theoretical data either excellently or fairly good from H to U neutral targets over the wide incident energy range. But it overestimates the data of Hayes et al. [32] for F below 200 eV, for Ne below 200 eV, for Te from 20 eV to 200 eV, for Pb from 10 eV to 200 eV and of Halle et al. [48] for U from 10 eV to 200 eV. It is clearly evident from these figures that the present model describes all the experimental or theoretical data either excellently or satisfactorily (within 10–15%) except for F, Ne, Te, Pb and U only in the study of thirty-six neutral atoms.

4 Conclusions

The present model calculates reasonably accurate EITSI cross sections for neutral targets with $1 \leq Z \leq 92$ and for incident energies ranging from the threshold to about 10^4 eV. In the description of the available experimental data with respect to domain of species and incident energies, the level of performance of the present model seems to be the best or as good as the other theoretical methods considered herein for the comparison. With the inherent simplicity of its structure, this model may be a prudent choice in the plasma modeling calculations which require a rapid calculation of the EITSI cross sections.

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