

An extended empirical formula for inner-shell ionization of atoms

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Abstract

An extension of the analytical model of Campos *et al* (2007 *J. Phys. B: At. Mol. Opt. Phys.* **40** 3835) is proposed to evaluate electron impact single inner-shell ionization cross sections up to the *M*-shell. The new model includes ionic and relativistic factors in its structure and describes neatly the *K*-shell ionization cross section data up to 2 GeV, and *L*- and *M*-shell ionization data up to 300 MeV. Comparison is also made with other theoretical calculations.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The last few decades have produced both theoretical and experimental data for cross sections of inner-shell ionization [1, 2]. The knowledge of these cross sections not only has fundamental importance for understanding collision dynamics of electron–atom interactions, etc, but is also used extensively in many applied fields such as radiation science, astrophysics, plasma physics and elemental analysis using electron probe microanalysis (EPMA), Auger electron spectroscopy (AES), electron energy loss spectroscopy (EELS) and transmission electron microscopy (TEM) [1]. Quantum mechanical calculations and experiments generate cross sections at some specific energies and for selected target atoms suitable for calculations or experiments. The *ab initio* calculations [3–5], usually based on various approximations, are lengthy and hence time-consuming. The applied areas, as mentioned earlier, need enormous and continuous accurate data for cross sections for different targets over a wide energy range. This can be accomplished by the use of an analytical formula capable of producing rapid generation of cross sections with reasonable accuracy over a wide range of targets as well as projectile energies.

Analytical models with species-dependent parameters are available in the literature [1, 6]. However, these models cannot

be used for the absolute values of cross sections wherever theoretical calculations or experimental data are not available to fit the data for obtaining the optimal values of the parameters of the models and then applied to any desired incident energy. Thus, it underscores the need for the species-independent generalization of the parameters of an analytical model as far as possible while keeping the accuracy to a desired level.

In a pioneering work, Bethe [7, 8] developed a formula to compute inner-shell ionization cross sections (ISICS), based on the plane-wave Born approximation (PWBA) valid for high energies. Semiempirical modifications of PWBA have been proposed [9, 10] to describe data also at low energies. Other analytical models include classical and semi-classical formulations [11–13]. Finally, a large number of empirical and semiempirical models have been proposed to describe the electron impact *K*-shell ionization cross section as a function of the incident energies [10–12]. However, each of these formulae has a limited domain of applicability and no remarkable effort has been made for the extensive calculation of ISICS for the *L*- and *M*-shell ionization of atoms to the best of our knowledge.

Campos *et al* [14] proposed an analytical (henceforth referred to as CVTS) model to describe the *K*- and *L*-shell ionization of neutral atoms over a wide range of atomic numbers $4 \leq Z \leq 79$ at reduced energies $U \leq 10$ (where $U = E/I$ with E as the incident energy and I as the ionization potential). The CVTS model requires only two parameters

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which are monotonically decreasing functions of Z . These parameters are determined from fitting the absolute ISICS of the K - and L -shell, calculated by the distorted-wave Born approximation (DWBA). CVTS, thus, generates ISICS with the accuracy of DWBA and at the same time, being simple in its structure, amply reduces the computing time for obtaining the ISICS results. The success of the model provides impetus for a further extension of its applicability to a larger domain of Z and U by incorporating the appropriate ionic and relativistic correction factors. In the process, we infuse in the CVTS model a Gryzinski-type relativistic factor [11] and an ionic factor [15] to improve in accuracy as well as domain of applicability. The values of the parameters of the proposed model are determined by the best fits to the available K -, L - and M -shell experimental ionization cross section data. The proposed model is referred to as the XCVTS model.

In recent years, Haque *et al* have incorporated ionic and relativistic corrections in the empirical formula of Bell *et al* (BELL) [16], Kolbenstvedt (KLV) [17] and the Deutsch–Märk (DM) [18] model leading to the modified BELL (MBELL) model [15], the generalized Kolbenstvedt (GKLV) model [19] and a modified version of revised DM (MRDM) model [20], respectively. MBELL combines Bethe’s asymptotic form with the low-energy behaviour of collision through, respectively, the first and series terms in the cross section expression of the parent BELL model [15]. MBELL involves up to nine shell-dependent parameters, including an additional one in the ionic correction factor [15], for ionization up to the M -shell. GKLV, through its parent KLV, is based on quantum electrodynamics, comprises a close collision described by the Møller interaction and a distant encounter determined by the virtual exchange of photons, and involves two shell-dependent parameters. MRDM, on the other hand, has in its structure the quantum mechanical radial dependence, satisfies the Bethe asymptotic condition (although DM does not satisfy) and needs three free parameters for the K -shell ionization. Application of the MBELL and GKLV models to relativistic energies is made possible by incorporating appropriate relativistic correction factors and orbit-dependent generalization of the fitting parameters involved. Both MBELL and GKLV are found amply successful in accounting for the electron impact ionizing cross section (EIICS) data up to the M -shell. The prime objective of the present study is to examine the performance of the XCVTS model in describing the ISICS data up to the M -shell ionization and its computation speed compared to other models.

In the present work, the predictions from the proposed XCVTS model are compared with the available EIICS data for the inner K -, L - and M -shell ionization as well as the calculated cross sections employing the MRDM, MBELL and GKLV models. The results of our present calculations are compared with those of the parametrized plane-wave Born approximation (PWBA) of Khare and Wadehra [21], relativistic PWBA (RPWBA) of Scofield [22], distorted-wave Born approximation (DWBA) of Segui *et al* [3] and perturbation theory with exchange effects (PEX) of Luo and Joy [23].

The paper is organized as follows. The outline of the XCVTS model is given in section 2. Analyses and

discussions on the results obtained are provided in section 3 and conclusions are furnished in section 4.

2. Outline of the XCVTS model

In finding an analytical expression to describe the DWBA generated single absolute cross sections of the K - and L -shell ionization of atoms, Campos *et al* [14] chose Bethe’s asymptotic condition in a parametrized form to fit low-energy data. Their resultant expression, referred to as the CVTS model, is given by

$$\sigma_{\text{CVTS}}(U) = \frac{A_{\zeta}(Z)}{B_{\zeta}(Z) + U} \ln(U). \quad (1)$$

Here $A_{\zeta}(Z)$ and $B_{\zeta}(Z)$ represent the two Z -dependent parameters of the model and ζ denotes a particular sub-shell in which ionization takes place. The two parameters, $A_{\zeta}(Z)$ and $B_{\zeta}(Z)$, are obtained by fitting the calculated DWBA results. As mentioned earlier, equation (1) has been found to describe well the ISICS data for the reduced incident energies $U \leq 10$ but does not provide satisfactory results at high and ultra-relativistic energies. To take into account the relativistic effect manifested in the ionization cross sections, the present work proposes an extension by including in it a Gryzinski-type [11] relativistic factor $R(U)$ given by

$$R(U) = \left(\frac{1+2J}{U+2J} \right) \left(\frac{U+J}{1+J} \right)^{\delta_1} \times \left[\frac{(1+U)(U+2J)(1+J)^2}{J^2(1+2J) + U(U+2J)(1+J)^2} \right]^{1.5} \times (1.0 - \delta_2 U^{\delta_3} / J^2). \quad (2)$$

Here $J = mc^2/I$, where m is the mass of the electron and c is the speed of light in vacuum. The parameters δ_1 , δ_2 and δ_3 are to be determined from the K -shell ionization data as discussed below. The last factor on the right side is introduced, in line with Casnati *et al* [24] and Hombourger [25], to mitigate the divergence of ISICS at the ultra-relativistic region.

Now the electron approaching the inner-shell electrons feels the atom as an ion having an *effective charge* $q = Z - N_{\zeta}$, where N_{ζ} is the total number of electrons from the innermost $1s$ -orbit to the relevant ionizing orbit ζ of the target atom. This ionic effect dominates the threshold region and decreases with the increase of energy of the incident electron as the probability of finding the incident electron decreases with the incident energy. This leads to the consideration of an ionic factor of the type [15]

$$F_{\text{ion}}(U) = 1 + \xi \left(\frac{q}{U} \right)^{\eta}. \quad (3)$$

Here the parameters ξ and η are fitted for the experimental data. The ionic factor has been found to account for the ionic enhancement of the cross section [26]. The parameter $A_{\zeta}(Z)$ is redefined as

$$A_{\zeta}(Z) = C_{\zeta} Z^{\lambda_{\zeta}}, \quad (4)$$

in terms of shell-dependent but species-independent new parameters C_{ζ} and λ_{ζ} . The form of $A_{\zeta}(Z)$ with its two parameters in (4) leads to the redundancy of the parameter

$B_\zeta(Z)$ in (1). Combining equations (2)–(5), the XCVTS model is proposed as

$$\sigma_{\text{XCVTS}}(U) = R(U)F_{\text{ion}}(U)A_\zeta(Z)N_\zeta \frac{1}{U} \ln(U). \quad (5)$$

Here N_ζ is the number of electrons in each sub-shell contributing to total ionization. For the L - and M -shell ionization, the total ISICS is obtained by summing the contributions from the sub-shells composing the shell.

3. Analysis and results

The ionization potentials I of the sub-shells have been taken from the published results of Desclaux [27]. Total ISICS for an inner shell at a reduced energy U has been obtained by summing the individual σ_{XCVTS} contributions from each of the component sub-shells, calculated from the proposed formula in (4). The relativistic parameters δ_1 , δ_2 and δ_3 in equation (2); the ionic parameters ξ and η in (3), and the C_ζ and λ_ζ parameters in (5) have been optimized for best fits to the available experimental data over a range of incident energies and the targets considered herein. The quality of best fits is determined by minimizing the chi-square defined as

$$\chi^2 = \frac{1}{N_p} \sum_{i=1}^{N_p} \left[\frac{\sigma_{\text{cal}}(U_i) - \sigma_{\text{exp}}(U_i)}{\sigma_{\text{exp}}(U_i)} \right]^2. \quad (6)$$

Here N_p is the number of data points. $\sigma_{\text{cal}}(U_i)$ and $\sigma_{\text{exp}}(U_i)$ refer, respectively, to the calculated and experimental cross sections at the reduced energy point U_i for a particular ionizing shell. A nonlinear least-squares fitting code MINUIT [28] has been used to minimize χ^2 in obtaining the optimum values of the parameters. The optimization procedure, which is detailed below, has been repeated over a number of targets for the same ionizing shell until the parameter values converge in fitting the experimental data sets from various sources cited below. To derive the parameters of the XCVTS model, the data are chosen with the following criteria: (i) the systematic error associated with the experimental data collection is less than 20%, and (ii) in the case of multiple data sets for a given target, the data sets do not differ by more than 12% within error-bars.

In the first stage of the optimization procedure, the K -shell EIICS data of C, presumed to be insensitive to the relativistic parameters δ_1 , δ_2 and δ_3 due to low Z and not-too-much high incident energies, have been employed. Thus, setting $R(U) = 1.0$ and also assuming $F_{\text{ion}} \approx 1.0$, the parameters C_ζ and λ_ζ in (4) have been optimized to minimize the χ^2 for fits to the EIICS data. Then leaving the values for C_ζ and λ_ζ , thus obtained, unchanged and the relativistic factor fixed at $R(U) = 1.0$, the ionic parameters ξ and η in equation (3) have been searched upon to minimize the χ^2 for fits to the EIICS data of C and Ne as well as those of Si, Ar, Ni, Mo, Ag, Sn, Au, Bi and U around the threshold and peak regions as the ionic effect remains effective there. The derived η value has been very close to $\eta = 1.0$. In the subsequent parameter searches, $\eta = 1.0$ has been left unchanged. In the next step, keeping the ξ and $\eta = 1.0$ values, so derived, unchanged, C_ζ and λ_ζ have been searched upon the EIICS data of C and Ne

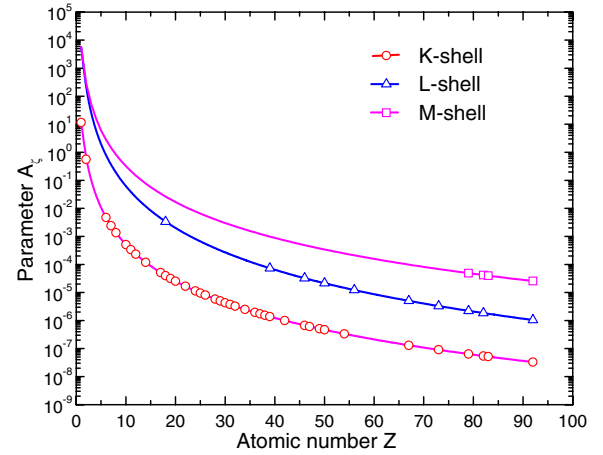


Figure 1. Variation of the parameter A_ζ in the cross section expression (5) of the present XCVTS model, with Z for the K -, L - and M -shell inner ionization. Symbols refer to the discrete values of A_ζ in (4) corresponding to the atomic targets used to evaluate the the species-independent C_ζ and λ_ζ parameters. Solid lines are the plots of A_ζ versus Z .

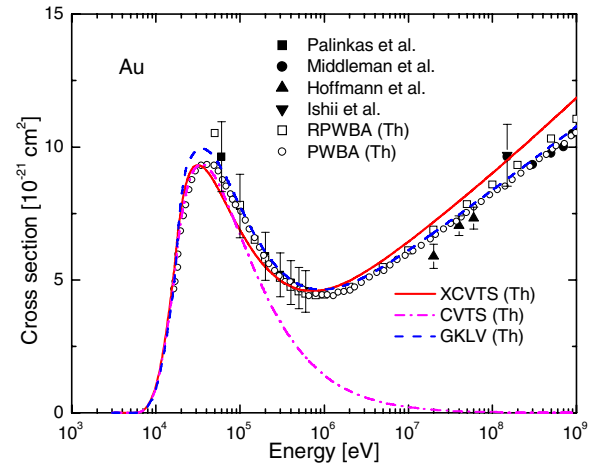


Figure 2. Experimental EIICS data (solid symbols) for the inner L -shell ionization are compared with the predicted results from the XCVTS (solid line) and GKLW [19] (broken line) models as well as the parametrized quantum mechanical PWBA [21] (open circles) and RPWBA [22] (open rectangles) calculations. Theoretical results from the CVTS model [14] are also shown by the dash-dotted line.

as well as those of Si, Ar, Ni, Mo, Ag, Sn, Au, Bi and U around the threshold and peak regions. In the next step, with the C_ζ and λ_ζ values just determined unchanged, the ξ value (with $\eta = 1.0$ fixed) has been finally optimized at $\xi = 0.01$ with again the same experimental data sets of C to U around the threshold and peak regions.

In the second stage, keeping fixed the values of ξ , η , C_ζ and λ_ζ derived in the first stage, and assigning $\delta_1 = 2.00$ (Gryzinski's value), the parameters δ_2 and δ_3 have been searched upon the K -shell ionization EIICS data of Si, Ar, Ni, Mo, Ag, Sn, Au, Bi and U for the incident electron energies from threshold up to 2 GeV. Having the parameters δ_2 and δ_3 , so derived, and $\delta_1 = 2$ as the starting values, all the three relativistic parameters have been reoptimized to obtain the final values $\delta_1 = 2.02$, $\delta_2 = 0.22$ and $\delta_3 = 0.27$. These values

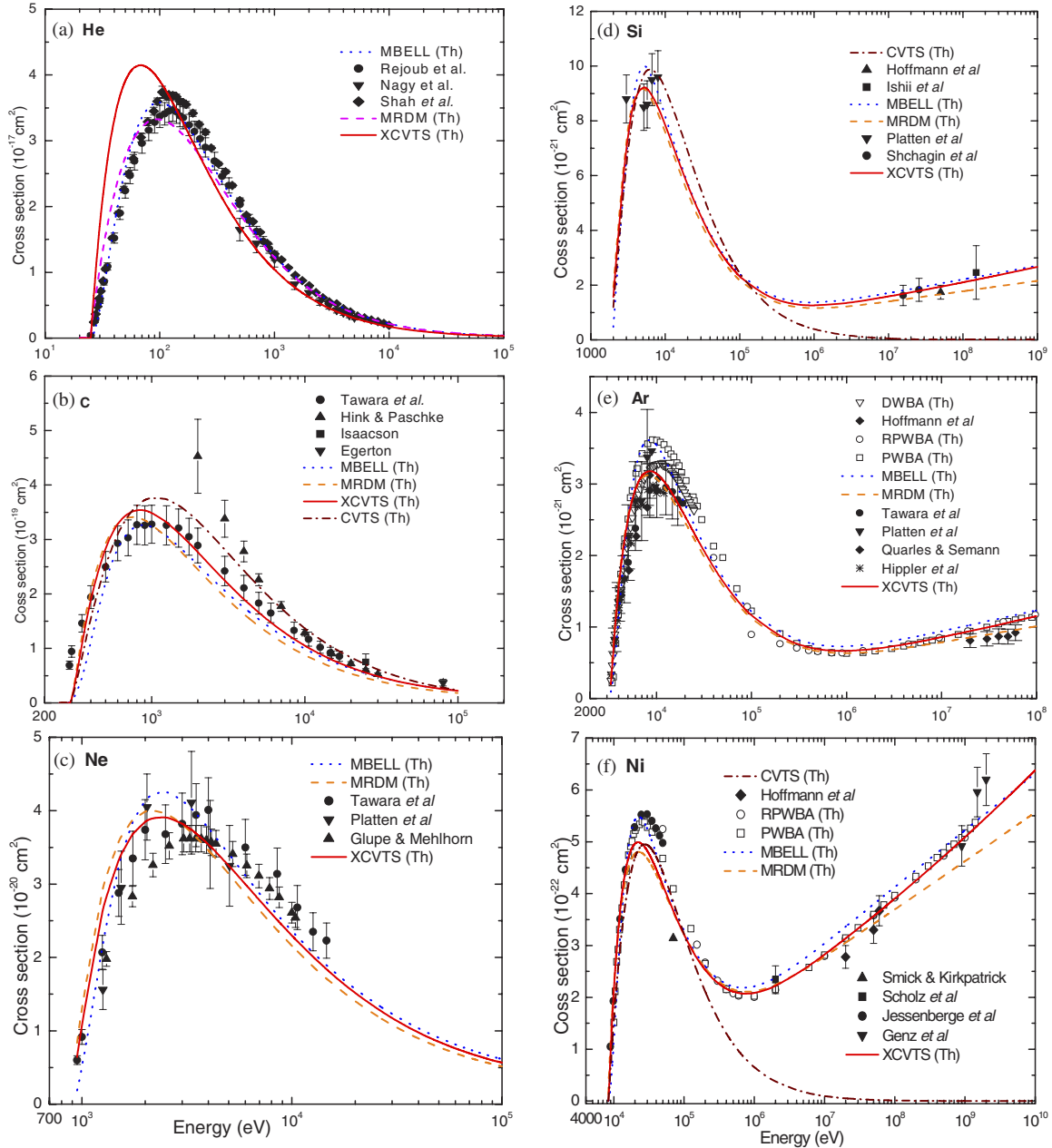


Figure 3. Same as in figure 2 for the inner K -shell ionization of (a) He, (b) C, (c) Ne, (d) Si, (e) Ar and (f) Ni. Here the MBELL [15] and MRDM [20] predictions are given, respectively, in dotted and broken lines. The quantum mechanical results including DWBA [3] are in open symbols. The CVTS predictions for Si and Ni are also shown by chain lines.

Table 1. The parameter $A_\zeta = C_\zeta Z^{\lambda_\zeta}$ in (3) as the function of the atomic number Z , the ionic parameters ξ and η , and the relativistic parameters δ_1 , δ_2 and δ_3 for K -, L -, and M -shell ionization

Shell	C_ζ	λ_ζ	A_ζ	ξ	η	δ_1	δ_2	δ_3
K	11.5	-4.35	$11.5 \times Z^{-4.35}$	0.01	1.00	2.02	0.22	0.27
L	5500	-4.95	$5500 \times Z^{-4.95}$	0.01	1.00	2.02	0.22	0.27
M	5700	-4.25	$5700 \times Z^{-4.25}$	0.01	1.00	2.02	0.22	0.27

are then kept fixed in the subsequent optimization of other parameters. Finally, all the experimental EIICS data for the K -shell ionization of He, C, Ne, Si, Ar, Ni, Mo, Ag, Sn, Au, Bi and U are fitted for optimizing the values of the C_ζ and λ_ζ parameters for the K -shell ionization. These parameter values

along with the ionic and relativistic parameters are given in table 1.

In the third stage, leaving the relativistic three parameters and ionic two parameters unchanged at the values shown in table 1, the C_ζ and λ_ζ parameters have been optimized using

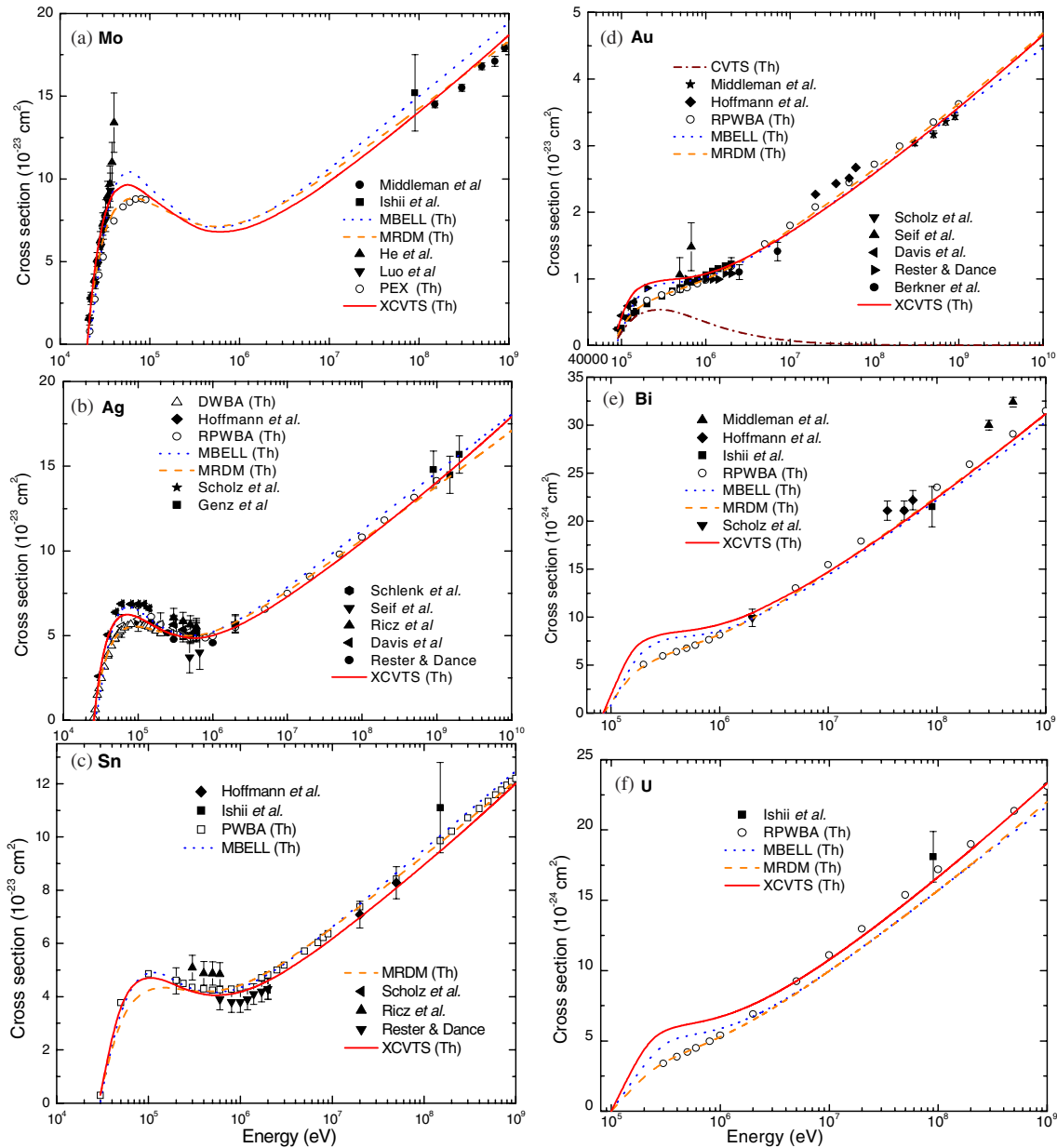


Figure 4. Same as in figure 3 for the inner *K*-shell ionization of (a) Mo, (b) Ag, (c) Sn, (d) Au, (e) Bi and (f) U. The quantum mechanical results including PEX [23] are in open symbols. The CVTS predictions for Au are shown by the dash-dotted lines.

the experimental EIICS data of Ag, Ba, Ho, Ta, Pb and U for the *L*-shell ionization up to 300 MeV, and those of Au, Bi, Pb and U for the *M*-shell ionization in the energy range of 10–300 MeV. The derived parameters are noted in table 1.

It is important to note that the values of the ionic parameters ξ and η are found independent of Z as well as the ionizing shell as expected. The values of A_ζ are plotted in figure 1 as a function of Z using the optimized values of the parameters C_ζ and λ_ζ in (4). From the figure, it is evident that $A_\zeta(Z)$ exhibits a monotonic decrease with Z for the *K*, *L* and *M* shells and it can take up a sub-shell-independent value within a particular shell.

A detailed comparison between the CVTS and XCVTS predictions of the *L*-shell EIICS for Au is shown in figure 2. To judge the relative performances of the two models, the

calculated EIICS are also compared with the experimental data of Palinkas *et al* [29], Middleman *et al* [30], Hoffmann *et al* [31] and Ishii *et al* [32] as well as the theoretical results from RPWBA [22], optimized PWBA [21] and GKL [19] calculations. It is evident from the figure that the CVTS model [14] fails to describe the data beyond 1 keV in conformity with the claim of Campos *et al* that their model works in the energy range with $U < 10$. The proposed XCVTS model, on the other hand, describes the EIICS data within 10% up to about 300 MeV and its overall performance is comparable to that of the GKL model.

Figures 3 and 4 show the comparison of the XCVTS predictions for the *K*-shell ISICS with the experimental data and other theoretical results from PWBA [21], RPWBA [22], DWBA [3] and PEX [23] and also those from our earlier

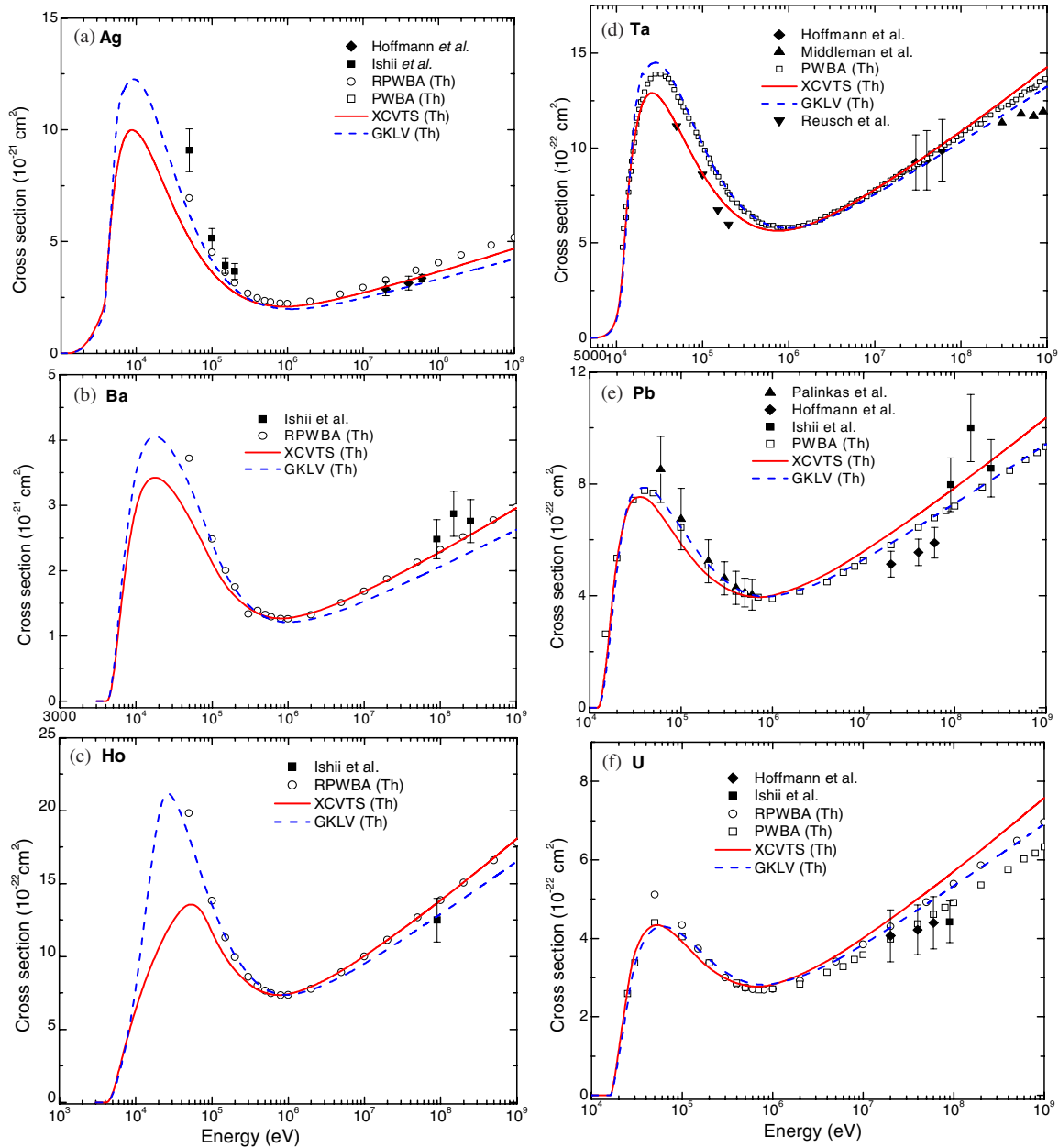


Figure 5. Same as in figure 2 for the inner L-shell ionization of (a) Ag, (b) Ba, (c) Ho, (d) Ta, (e) Pb and (f) U. The quantum mechanical results are shown by open symbols.

MBELL [15] and MRDM [20] models. The sources of experimental data are [33–35] for He, [32, 36, 37] for C, [36, 38, 39] for Ne, [31, 32, 38, 40] for Si, [31, 36, 38, 41, 42] for Ar, [31, 43–46] for Ni, [30, 32, 47, 48] for Mo, [31, 44, 46, 49–53] for Ag, [31, 32, 44, 51, 53] for Sn, [30, 31, 44, 50, 52–54] for Au, [30–32] for Bi and [32] for U.

In the overall picture, the XCVTS model provides a good agreement with the experimental data for all cases of the K-shell ionization excepting He near the threshold and peak regions where it overestimates the cross sections. For C, the description of the data is better with XCVTS than CVTS. For Au, the latter underestimates the experimental data even in the peak region and also at higher energies. The predicted EIICS of CVTS falls off rapidly for Si, Ni and Au at energies beyond

10–200 keV depending on the target, where the relativistic effect becomes important. Except the He target, the general performance of XCVTS is at par with that of the MRDM, MBELL and GKL models, and for Ni, the former performs better than MRDM at higher energies. Furthermore, the predictions from XCVTS agree with those of PWBA [21], RPWBA [22], DWBA [3] and PEX [23] except in the peak regions for the cases of Ar, Ni, Au, Bi and U.

Figure 5 shows the comparison of the predicted EIICS from XCVTS with the experimental data of Ag, Ba, Ho, Ta, Pb and U as well as the theoretical results from the GKL model [19], PWBA [21] and RPWBA [22]. The XCVTS model describes the EIICS data well up to about 300 MeV and its predictions agree with those of GKL, PWBA and RPWBA

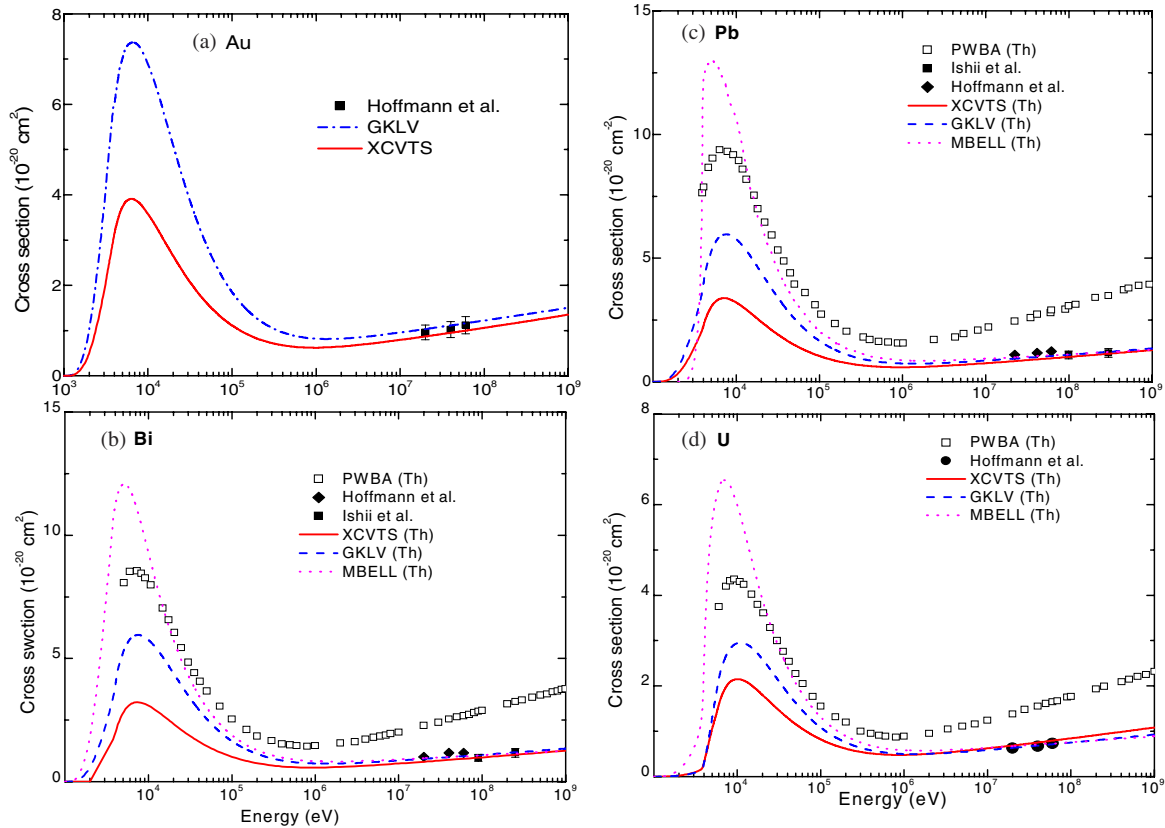


Figure 6. Same as in figure 2 for the M -shell inner ionization of (a) Au, (b) Bi, (c) Pb and (d) U. Open rectangles are parametrized PWBA [21] calculations. The predicted results from the GKL [19] and MBELL [15] models are shown by broken and dotted lines.

except at the peak regions for Ag, Ba, Ho and Ta. However, the XCVTS model does not work well to fit the data beyond 300 MeV for Au, as depicted in figure 2, and also Ta (see figure 5), where the GKL model performs better.

Figure 6 displays the XCVTS predictions for the M -shell ionization for Au, Pb, Bi and U with experimental data from [31] for Au, Pb, Bi and U and [32] for Pb and Bi. The predicted results reproduce the experimental EIICS data available in the energy range of 10–300 MeV and agree with those of the MBELL and GKL models. On the other hand, the calculations from PWBA [22] fail to reproduce the experimental data. The important feature with the calculations for the M -shell ionization is that the theoretical results, derived from XCVTS, MBELL, GKL and PWBA, are widely different in the peak regions for Pb, Bi and U. There are also discrepancies between the GKL and XCVTS results at the peak region. It would have been useful to have experimental data in the peak region to assess the best performer among the MBELL, GKL and XCVTS models.

From the above discussions, we note that the simplified XCVTS model provides better agreement with the experimental results over the entire energy and Z regimes. The attractive feature of the proposed model is that it provides reliable cross sections with just two shell-dependent fitting parameters like the GKL model. However, XCVTS is a rather simpler and faster model for generating reliable cross sections needed in the applied areas.

4. Conclusions

The present work reports the performance of the proposed XCVTS model, an extended version of CVTS which simulates the DWBA calculations. The XCVTS model accounts well for the K -shell ionization data up to 2 GeV, and L - and M -shell ionization data up to about 300 MeV. Furthermore, while the parametrized quantum mechanical PWBA calculations of Khare and Wadehra [21] fail to reproduce the data for the M -shell ionization, XCVTS works well to describe them for all the four targets considered herein. The overall performance of XCVTS is comparable to the GKL and MBELL models. However, while MBELL needs nine shell-dependent parameters to describe the M -shell ionization data, both XCVTS and GKL can do with only two parameters. Moreover, the underlying structure of the proposed XCVTS model is much simpler and is much faster in computation than the GKL model. To the best of our knowledge, XCVTS is the fastest model encompassing wide ranges of Z and U , available in the literature, and generates reliable results up to the M -shell ionization.

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