Computation of electron-impact *K*-shell ionization cross sections of atoms

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The total cross sections of electron impact single *K*-shell ionization of atomic targets, with a wide range of atomic numbers from $Z=6-50$, are evaluated in the energy range up to about 10 MeV employing the recently proposed modified version of the improved binary-encounter dipole (RQIBED) model [Uddin *et al.*, Phys. Rev. A **70**, 032706 (2004)], which incorporates the ionic and relativistic effects. The experimental cross sections for all targets are reproduced satisfactorily even in the relativistic energies using fixed generic values of the two parameters in the RQIBED model. The relativistic effect is found to be significant in all targets except for C, being profound in Ag and Sn.

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I. INTRODUCTION

The knowledge of cross sections of *K*-shell ionization by electron impact are needed in many fields, such as atomic physics, plasma physics, materials and surface science, and radiation chemistry [1]. The *K*-shell ionization cross sections are also useful for electron microscopy and are essential for the elemental analysis, through the intensity estimation of the characteristic x rays, in conjunction with the electron distribution function [2].

The total ionization cross sections, measured prior to 1990, have been compiled by Long *et al.* [3]. Since then additional measurements have been reported [4–9]. An inspection on these data reveals that the currently available experimental data are inadequate for many atoms. Moreover, significant discrepancies between data from different sources exist, which reflects the considerable difficulties associated with the cross-section measurements of the *K*-shell ionization. The dearth in the adequate data of the *K*-shell ionization cross sections underscores the need for the theoretical determination of the cross sections. Unfortunately, a systematic method for calculating the electron impact ionization (EII) cross sections for atoms from first principles has not yet reached the desired goal. Although the distorted-wave-Born approximation (DWBA) calculations of inner-shell ionization cross sections for neutral atoms are feasible, it has its validity for the limited energy and energy-loss ranges [10]. Moreover, the quantal methods, based on various approximations, are difficult to implement and time consuming in application to the modeling codes requiring quick calculations over a wide range of species and energies. For these reasons, it is preferable to develop a method that is simple to use in generating cross sections within an accuracy of 30%. Owing to this situation, many simple approaches have been implemented for the practical use [1,11–15]. Huo [16] proposed an improved version of binary-encounter dipole (iBED) and the simplied iBED (siBED) models by replacing the Bethe part of the BED model [17] with a two-parameter Born term.

Recently, Uddin *et al.* [18] introduced two modifications in the siBED model: (i) ionic correction leading to the QIBED model and (ii) ionic and relativistic corrections giving rise to the RQIBED model. The QIBED and RQIBED models, using constant generic values of the two parameters in them, have been applied to the atomic targets in the He [18] isoelectronic sequences with a remarkable success. However, the relativistic effect in RQIBED could not be properly tested due to lack of high-energy experimental data, apart from its examination in Ref. [18] with just one stray experimental point for U^{90+}. In this paper, we present a thorough investigation of the RQIBED model in reproducing the experimental EII cross sections, where the relativistic effect is dominant, and report the results of the application of the RQIBED model, with again constant values of two parameters in its structure, to the *K*-shell ionization of atoms with the atomic numbers, $Z=6-50$, for the incident energy up to about 10 MeV. The results are compared with the available experimental data and predictions from other theoretical methods including the quantal theories like plane-wave Born approximation (PWBA) due to Khare and Prakash [19] and Hippler *et al.* [20]; relativistic DWBA due to Segui *et al.* [10]; and the perturbation theory with exchange effect due to Luo and Joy [21].

The paper is organized as follows. The RQIBED model is sketched in Sec. II. In Sec. III, we discuss the results in comparison with the available experimental cross sections and other theoretical findings. Section IV is devoted to the discussion of the results and the conclusions arrived at.

II. OUTLINE OF THE RQIBED MODEL

The cross section in the RQIBED model, as proposed in Ref. [18], is given by

$$\sigma_{\mathrm{RQIBED}} = \sigma^{R}_{\mathrm{Mott}} + \sigma^{R}_{\mathrm{Born}}, \tag{1}$$

where

$$\sigma^{R}_{\mathrm{Mott}} = S^{R} H, \tag{2}$$

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$$\sigma_{\mathrm{Born}}^{R} = F^{R} G, \tag{3}$$

$$S^{R} = \frac{4\pi N_0 \alpha^2}{\beta_t^2 + (\beta_b^2 + \beta_a^2)/(q+1)}, \tag{4}$$

$$H = \left[\frac{k_0^2 - \alpha_0^2}{k_0^2 \alpha_0^2} - \frac{\ln(k_0^2/\alpha_0^2)}{k_0^2 + \alpha_0^2} \right], \tag{5}$$

$$F^{R} = \frac{64\beta_a^3 N_0}{\alpha \beta_t^2}, \tag{6}$$

$$G = \int_0^{(k_0^2-\alpha_0^2)/2} k_p (k_p^2 + \alpha_0^2)^2 dE_p \times \int_{K_{\min}}^{K_{\max}} \frac{1 + d_1 t + d_2 t^2}{K[(K+k_p)^2 + \alpha_0^2]^3[(K-k_p)^2 + \alpha_0^2]^3} dK, \tag{7}$$

with

$$t = \frac{K^4}{[(K+k_p)^2 + \alpha_0^2][(K-k_p)^2 + \alpha_0^2]}. \tag{8}$$

In the above equations, $k_0^2/2$ is the energy of the incident electron; $k_b^2/2$ is the kinetic energy of the bound electron; $E_p = k_p^2/2$ is the energy of the ejected electron; and $\alpha_0^2/2$ is the binding energy of the target electron with the quantities expressed in the atomic units. N_0 is the number of electrons in the orbit considered, q is the charge of the ionic target, and α is the fine-structure constant. For the K-shell ionization, the target atom can be regarded to have $q = Z - 2$. The Born cross section in Eq. (3) involves the parameters d_1 and d_2 of the model through the expression for G in Eq. (7). Using c as the velocity of light in the free space, the quantities (in the atomic units) β_t, β_b, and β_a in Eqs. (4) and (6) are defined in terms of $t' = k_0^2/(2c^2)$, $b' = k_b^2/(2c^2)$, and $a' = \alpha_0^2/(2c^2)$, respectively, as

$$\beta_t^2 = 1 - \frac{1}{(1+t')^2}, \tag{9}$$

$$\beta_b^2 = 1 - \frac{1}{(1+b')^2}, \tag{10}$$

and

$$\beta_a^2 = 1 - \frac{1}{(1+a')^2}. \tag{11}$$

The momentum transfer $\mathbf{K}$ in Eqs. (7) and (8) is given by $\mathbf{K} = \mathbf{k_0} - \mathbf{k_1}$ with $\mathbf{k_1}$ representing the momentum of the incident electron after a collision. The limits of integration in Eq. (7), $K_{\max}$ and $K_{\min}$, are taken from Eq. (2.16) of Ref. [22], which in the atomic units can be expressed as

$$K_{\pm}^2 = \frac{k_0^2}{R}\left[1 - \frac{(k_p^2 + \alpha_0^2)}{2k_0^2} \pm \left(1 - \frac{(k_p^2 + \alpha_0^2)}{k_0^2} \right)^{1/2} \right], \tag{12}$$

where K_+ and K_- refer, respectively, to $K_{\max}$ and $K_{\min}$, and R is the Rydberg energy.

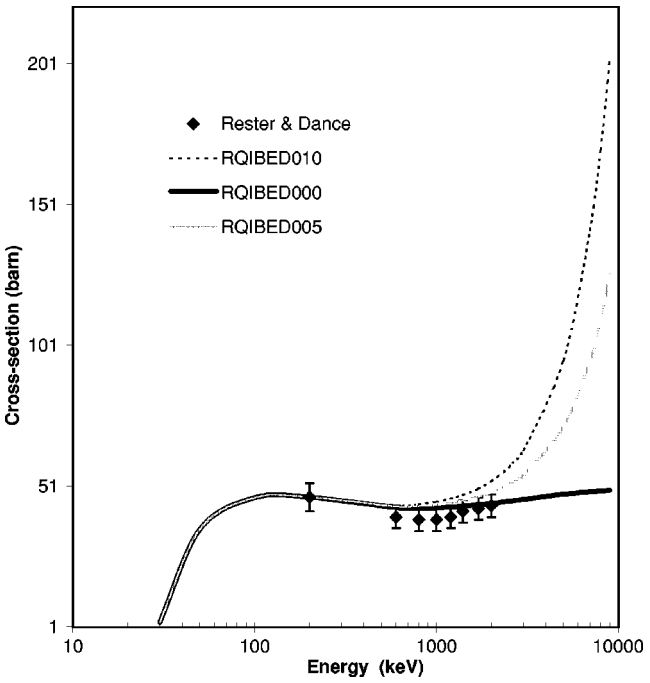

FIG. 1. Electron impact cross sections for Sn for different values of the parameter d_2.

III. RESULTS AND DISCUSSIONS

In the present calculations of the EII cross sections in the Deutsch-Märk (DM) model [13,14], the ionization potentials of the K-shell of atoms and radii of maximum charge density are taken from Desclaux [23]. The same ionization potentials have been used for the other model calculations. The kinetic energies are obtained using the Dirac-Hartree-Fock code [24]. The two-demensional integrations in the siBED, QIBED, and RQIBED models are carried out numerically using the 64-point Gauss-Legendre rule [25]. Out of the two parameters d_1 and d_2, the value of $d_1 = 0.0$, which determines the cross-section peak, is taken from Huo [16] and is found appropriate to generate the peak cross sections for the atoms, considered herein. The parameter d_2 is varied to optimize the fit to the data at the higher incident energies. The same set of values $d_1 = d_2 = 0.0$ gives the required convergence and produces the best overall description of the experimental data for all targets. In Fig. 1, we show the sensitivity of the parameter d_2 in the context of the calculated cross sections of Sn. The solid (RQIBED000), shaded (RQIBED005), and dashed (RQIBED010) curves are the results using $d_2 = 0.0$, 0.05, and 0.10, respectively. Clearly $d_2 = 0.0$ gives the convergence beyond 3000 keV and at the same time reproduces the experimental cross sections of Rester and Dance [26].

In Figs. 2–8, we compare the predicted EII cross sections from the RQIBED model with the available experimental cross sections and other calculations, including the siBED [16], QIBED [18], DM [13], and relativistic binary-encounter Bethe (RBEB) [15] models, and the quantal theories like PWBA of Refs. [19,20], DWBA of Ref. [10], and perturbation with the exchange effect of Ref. [21]. All the cross sections from the siBED, QIBED, RQIBED, DM, and RBEB models are calculated in the present work.

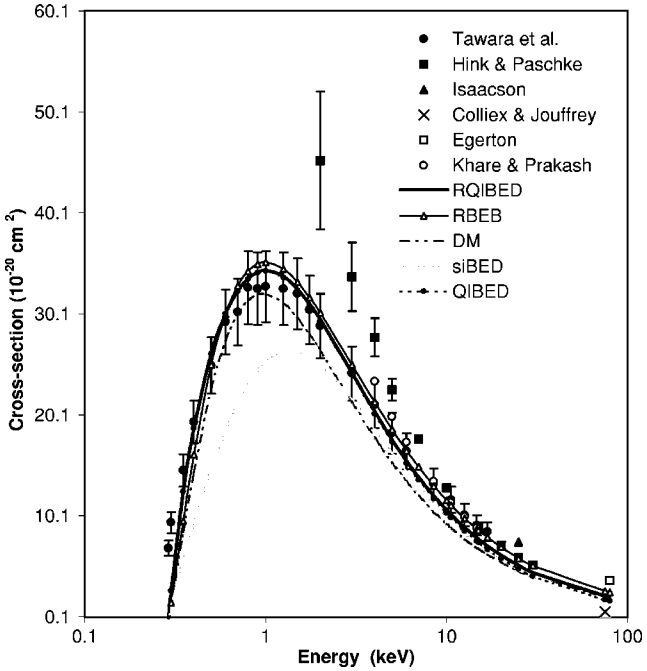

FIG. 2. Electron impact ionization of C.

A. Ionization of C

Figure 2 shows the experimental cross sections [27–31] for C in comparison with the PWBA predictions of Khare and Prakash [19], and the present calculations using the siBED [16], QIBED [18], RQIBED, DM [13], and RBEB [15] models. Except for the data of Hink and Paschke [28] and the siBED calculations, all the experimental and theoretical results agree with one another. The QIBED and RQIBED results, while remaining indistinguishable, produce the best level of agreement with the experimental data of Refs. [27,29]. The lower values of siBED justify the ionic correction in QIBED or RQIBED. The relativistic effect does not come into play due to the nonrelativistic environment created by the binding and kinetic energies of the *K* shell even at the high incident energies of several tens of keV.

The features of the RQIBED, QIBED, RBEB, DM, and PWBA results for N and O (not displayed in figures) are also found almost identical in relation to their experimental EII data, respectively, of Refs. [27,29,32] and Refs. [27,29,32,33].

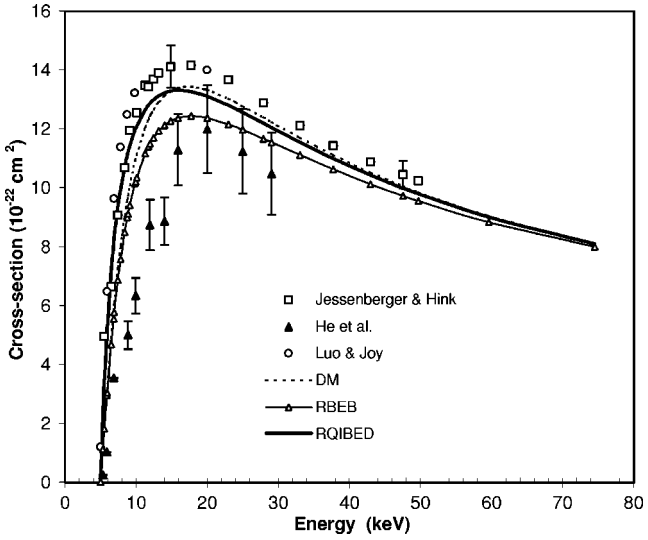

FIG. 4. Ell cross sections for Ti.

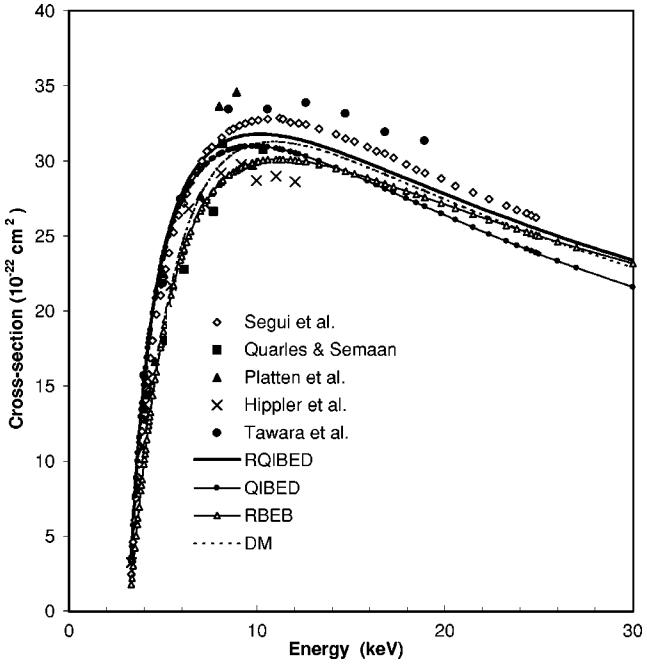

FIG. 3. Same as Fig. 2 for Ar.

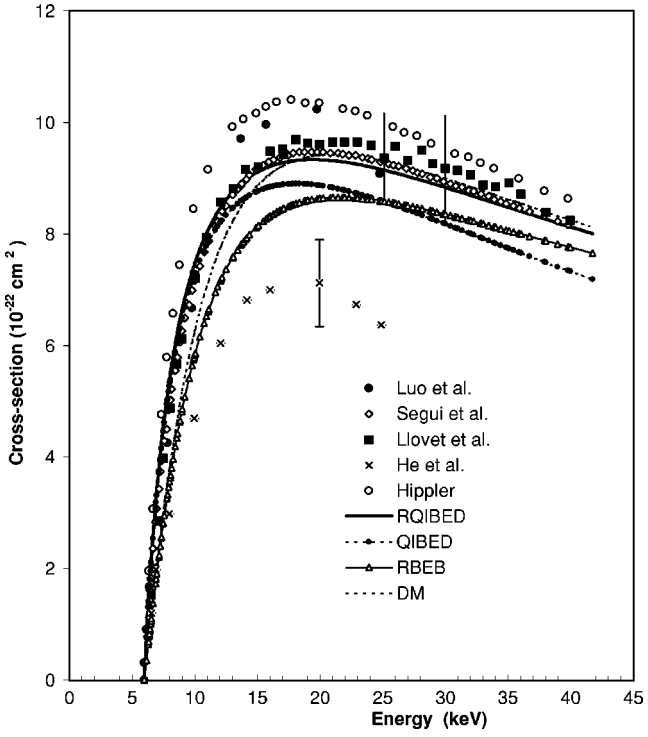

FIG. 5. Same as Fig. 2 for Cr.

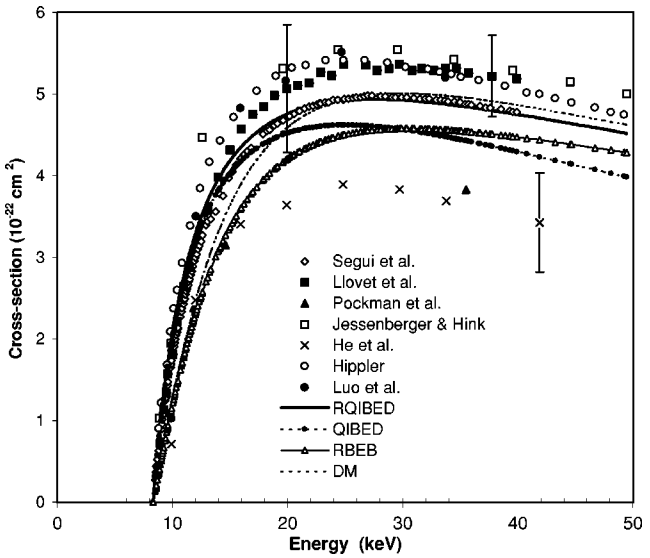

FIG. 6. Same as Fig. 5 for Ni.

B. Ionization of Ar

The experimental data of Refs. [27,33–35] for Ar are compared, in Fig. 3, with the predictions from the QIBED, RQIBED, DM, and RBEB models and the DWBA results of Segui *et al.* [10]. The DM and RBEB results agree reasonably with each other. While the experimental data from the four sources have large discrepancies amongst them, the RQIBED calculations follow the mean position of the data sets and agree well with the DWBA results of Ref. [10]. The difference between the QIBED and RQIBED calculations reflect the relativistic effect.

C. Ionization of Ti

In Fig. 4, the experimental EII cross sections of He *et al.* [6] and Jessenberger and Hink [36] for Ti are compared with the predicted results from the RQIBED, DM, and RBEB models and the perturbation theory of Luo and Joy [21]. The measured cross sections of [6] are systematically lower than all the predicted values and the experimental data of Ref. [36] are all higher in magnitudes. The RQIBED findings are favorably close to the predictions of Luo and Joy, and DM; and the experimental data of Ref. [36]. The RBEB curve follows the mean path of the two data sets of Refs. [6,36], with both measurements lying within 10% of the RQIBED cross sections.

The predicted cross sections for Sc and V (not shown in figures) from the RQIBED, RBEB, and DM models and the perturbation theory are also found to maintain similar differences with one another and the experimental data of Ref. [37] as for Ti.

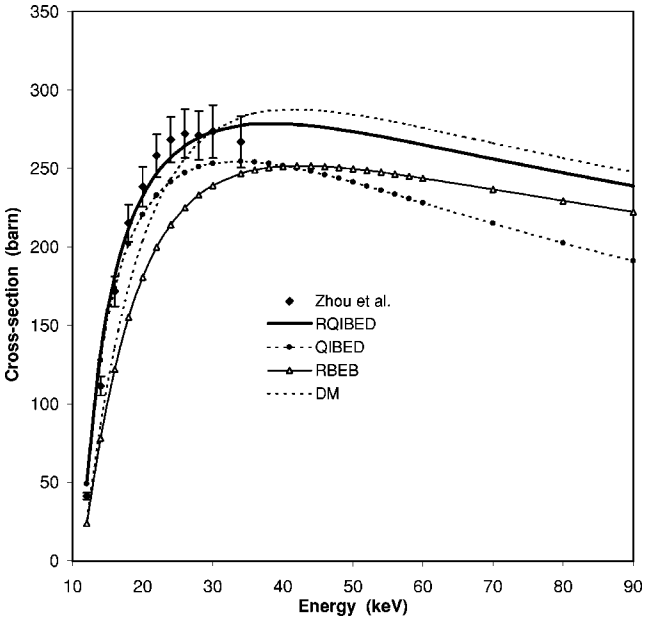

FIG. 7. Ell cross sections for Ge.

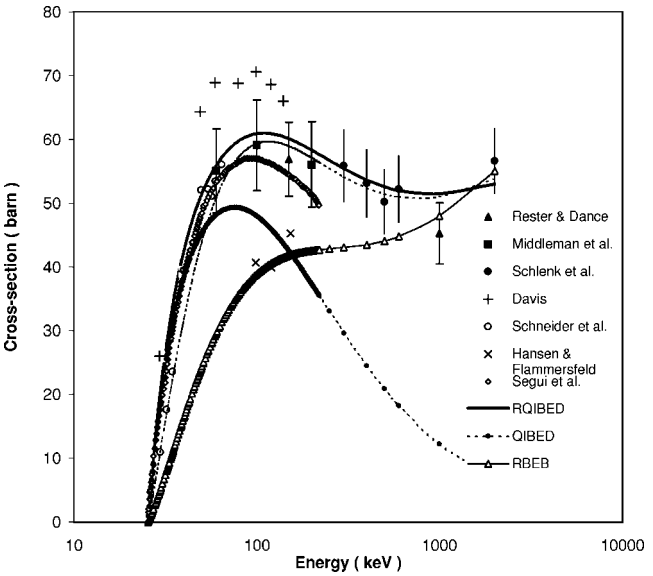

FIG. 8. Same as Fig. 5 for Ag.

D. Ionization of Cr

In Fig. 5, we compare the Cr results from RQIBED with those of the experiments [5,6,8]; the predictions of the QIBED, DM, and RBEB models; and the quantal calculations of Segui *et al.* [10] and Hippler [20]. The RQIBED predictions agree closely with the data of Llovet *et al.* [8] and the DWBA calculations of Ref. [10] over the entire domain and with the DM results beyond the peak region. RBEB underestimates the data of Ref. [8] over the whole energy range. The cross sections of He *et al.* [6] are much lower than the other measurements. The discrepancy between the results of QIBED and RQIBED is due to the relativistic effect becoming significantly large beyond 10 keV and justifies the relativistic correction implemented in RQIBED. In the overall judgement on the level of performance, the relativistic DWBA calculations of Ref. [10] come first and RQIBED next. It is surprising that RQIBED, with its simple structure, demonstrates almost the same level of performance thereby giving an edge over the quantal method of Ref. [10] in applications to the plasma modeling, where a quick generation of cross sections is sought.

It is also found that for Fe (not shown in figure), the experimental data of Refs. [5,6,8] compare with the RQIBED, QIBED, DM, RBEB, and DWBA results in a similar manner as for Cr; the RQIBED predictions being within 20% of all the data when the measurements of Refs. [5,6] for Cr differ by about 40%.

E. Ionization of Ni

It is evident from Fig. 6 that the predictions from the QIBED, RQIBED, DM, and RBEB models and the DWBA calculations of Ref. [10] for Ni show almost the same patterns and levels of agreement, as in the case of Cr (Fig. 5), in relation to the experimental cross sections of Llovet *et al.* [8] and He *et al.* [6]. The PWBA calculations of Hippler [35] produce the best agreement with the data of Refs. [8,36]. The experimental cross sections of Refs. [6,38] are mostly much lower than the other measurements and predictions. The RQIBED and DWBA curves follow the course in between the different data sets, albeit closer to those due to Refs. [8,36], showing an excellent agreement with each other.

For the Mn and Cu targets (not shown in figures), the available experimental EII cross sections, respectively, from Refs. [5,8,39] and Refs. [6,8,37,39–41] are also found to compare well within 15% with the RQIBED and DWBA predictions, the latter two results being very close to each other as in the case of Ni.

F. Ionization of Ge

Figure 7 compares the predicted cross sections of Ge from the RQIBED, QIBED, DM, and RBEB models with the experimental data of Zhou *et al.* [42]. The RQIBED model produces the best level of agreement with the data. The DM model underestimates the data in the threshold region. The discrepancy in the results from the QIBED and RQIBED models, beyond the threshold region, is the manifestation of the substantial relativistic effect.

For Ga and MO, the respective experimental data from Refs. [42,5] compare (not shown in figure) in a similar way with the RQIBED and DWBA predictions as for Ge.

G. Ionization of Ag

The RQIBED, QIBED, DM, RBEB, and RQIBED predictions for Ag are depicted, in Fig. 8, along with the experimental cross sections of Schneider *et al.* [4], Davis [41], Rester and Dance [26], Hansen *et al.* [43], Middleman *et al.* [44], and Schlenk *et al.* [45]; and the DWBA calculations of Segui *et al.* [10]. The RQIBED, DM, and DWBA results produce excellent agreement with the data of Refs. [4,26,44] and their curves pass between the data of Refs. [41,43]. RBEB not only underestimates most of the experimental data, but also differs in pattern from other calculations and the data in the 100–1000-keV region. The relativistic effect becomes more prominent as is evidenced by the large discrepancy between the QIBED and RQIBED predictions.

H. Ionization of Sn

The predicted cross sections for Sn from the QIBED, RQIBED, DM, and RBEB models are compared, in Fig. 9, with the experimental data of Rester and Dance [26]. RQIBED and DM both produce excellent fits to the data, with the former having an edge in the level of performance. The large discrepancy in the QIBED and RQIBED results is a signature of the significant contribution from the relativistic effect, incorporated in the latter. Although the RBEB model greatly underestimates the cross sections at around 100 keV, its curve passes through the error bars of the data points beyond 500 keV, albeit with a pattern different from the data.

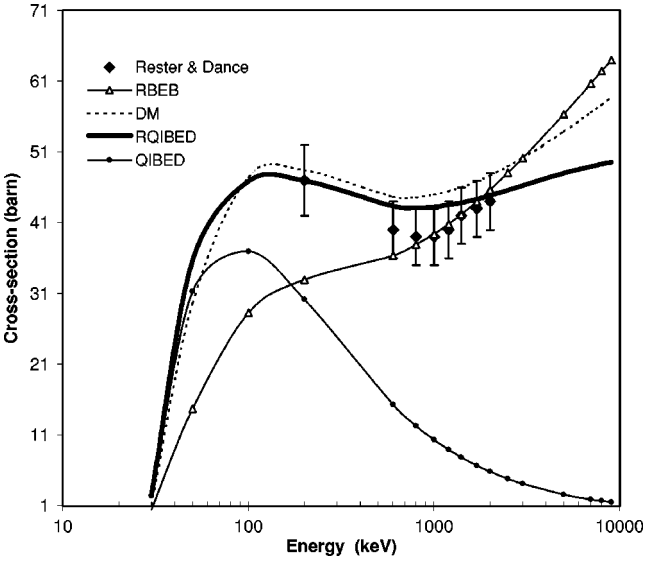

FIG. 9. Same as Fig. 7 for Sn.

IV. CONCLUSIONS

The present work reports the efficacy of the RQIBED model along with the sensitivity of its two parameters, d_1 and d_2, on the *K*-shell ionization of atoms. While the former predominantly determines the peak cross section, the latter controls the high-energy behavior. A generic set of values, which has been applied to atomic targets in the range $Z=6-50$ up to about $E=10$ MeV, has been obtained as $d_1=0.0$ and $d_2=0.0$. This result, in conjunction with the findings on the He [18] isoelectronic targets, demonstrates the existence of the constant generic values of the two parameters, linked to the electronic configuration of the target atom in confirmation with the earlier observation [16] in application of the parent siBED model to the neutral molecules. However, the exact nature of dependence of these two parameters on the electronic structure is yet to be understood.

The present study examines the relativistic effect in the RQIBED model using the experimental data and provides testimony to its success in describing the EII cross-section data of all the targets. The relativistic effect is found to be significant in all but C, being profound in Ag (Fig. 8) and Sn (Fig. 9). In the latter two cases the QIBED model, with only the ionic correction in it, fails to account for the data.

The RQIBED model, with a constant set of values $d_1=d_2=0.0$ for the two parameters in it, yields an encouraging description of the EII cross sections on the wide range of

atomic targets, considered herein. The RQIBED results agree with the entire sets of the experimental cross sections of all the targets mostly within 25%, where the measurements from different sources on a specific target differ by about 40% (e.g., the experimental data of Refs. [5,6] for Cr in Fig. 5 may be noted). As is evidenced in Figs. 3, 5, 6, and 8 for the cases of Ar, Cr, Ni, and Ag, the performance of RQIBED is almost similar to the sophisticated relativistic DWBA method of Segui *et al.* [10] in describing the experimental data. However, the RQIBED model with its simple structure and faster speed of calculations can serve as a lucrative tool for easy generation of data.

In common with the EII feature on the atomic targets in the He [18] isoelectronic sequences, the present *K*-shell ionization process occurs from a filled electronic orbit, thus offering similarity in electron configuration. This leads to the existence of the constant generic values for the two parameters in the RQIBED model. Thus the model with its powerful predictive power is particularly useful for exotic atomic targets with the same electronic configuration for the ionizing orbit for which the parameter values are known. One may hope therefore that by treading this path of looking for the generic values of the two parameters of the RQIBED model, the long cherished goal of a model that can routinely generate the EII cross sections for a wide range of energies and species may reach its fruition.

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