
Empirical Model for the Electron Impact *K*-Shell Ionization Cross Section of Atoms

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ABSTRACT: A new semiempirical model comprising few important features of the DM model of Deutsch et al. (*Int J Mass Spectrom* 1998, 177, 47) and the widely used empirical model of Bell et al. (*J Phys Chem Ref Data* 1983, 12, 891) has been proposed. The proposed model has been examined to evaluate the electron impact *K*-shell ionization cross sections of 30 atomic targets ranging from H to U ($Z = 1-92$) and found to describe with considerable success the experimental results over a wide range of incident energies up to 2 GeV using a single set of species independent parameters. © 2008 Wiley Periodicals, Inc. *Int J Quantum Chem* 109: 897–906, 2009

Key words: cross-sections; electron-impact *K*-shell ionization; relativistic effects; atomic targets

Introduction

Cross sections for electron impact *K*-shell ionization (KSI) of atoms are not only important in basic theories for atomic and molecular collisions but also needed in many scientific and industrial applications. The latter encompass modeling of ra-

diation effects in materials, biomedical researches, understanding of fusion plasmas, quantitative elemental analyses, semiconductor etching, and so on.

KSI cross sections have been object of experimental and theoretical studies since 1940s [1]. A comprehensive review of the experimental KSI data has been provided by Long et al. [2]. In the last decade, the demand for the cross-section data has increased. Various areas of applications require cross-section data for an arbitrary combination of incident energy T and atomic number Z of the atomic

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targets over a wide domain of interest. Experiments, however, provide cross sections at discrete values of T and include only a few of the elements.

Existing quantum mechanical methods generate individual cross-section values through complex numerical computations. Moreover, to ease rigorousness of the exact formalism, all these ab initio methods are based on some approximations thus restricting their validity to certain domains of T and Z . The gap between the high demand and scarcity of data can be best filled up by sufficiently accurate analytical models that provide a fast generation of cross-section values over wide domains. This fact triggered attempts for development of empirical and semiempirical models for generation of reliable cross sections. A comprehensive review of these models has been provided by [3, 4]. Among the widely used models are the empirical model of Lotz [5], model of Deutsch et al. (DM) [6, 7], binary-encounter Bethe (BEB) and its relativistic version (RBEB) models of Kim and Rudd [8], and empirical model of Casnati et al. [9].

Haque et al. [10] incorporated ionic and relativistic corrections in the empirical model of (BELL) [11]. to account for well the experimental data of the electron impact ionization cross sections (EIICS) of atomic targets in the range $Z = 1-92$ up to $T \approx 1,000$ MeV. The resulting model of [10] is referred to as MBELL. The BELL model and its modified version MBELL satisfy the Bethe asymptotic condition [12] through a dipole interaction term.

Recently, a generalization of the Kolbenstvedt model [13], noted henceforth as GKLV [14], has been found to be amply successful in describing the experimental EIICS data of the K , L , and M -shell ionization. In the GKLV model, only two parameters can adequately account for the KSI over a wide range of incident energies up to 2 GeV.

The relativistic DM model [6, 7] has been found to generate reasonable EIICS for some atoms within the interval of $Z = 18-79$ up to $T \approx 1,000$ MeV. The DM model does not fulfill the asymptotic Bethe behavior, supported by experimental data. The DM model depends explicitly on the radii of the atomic shells. It may be of interest to combine the radius feature of DM with the Bethe asymptotic form.

The BELL model uses the polynomial expansion $\sum_i B_i (1 - 1/U_K)^i$ with the reduced energy $U_K = T/I_K$, I_K being the binding energy of an electron in the K -shell. As pointed out by Godunov and Ivanov [12] that a better fit to experimental KSICS data may be achieved through using a nonlinear term like $\exp[\sum_i (1 - i/U_K)^i]$ instead of the aforementioned

polynomial expansion for the cross section [11]. We propose a semiempirical model by incorporating in its structure the radius of the ionized K -shell (from the DM model), the dipole interaction term (from the BELL model), and the aforementioned feature of nonlinear exponential term. The model, so framed, is referred to as the DMEMP model.

We examine the DMEMP model on the KSI of 30 atomic targets in the range of $Z = 1-92$ over a wide range of incident energies up to $T \approx 2$ GeV. We then compare our findings of DMEMP with our calculated results from the DM, MBELL, and GKLV models. In Outline of the DMEMP Model Section, we present a brief description of the proposed DMEMP model. Discussions on the results are furnished in Results and Discussions Section and a brief summary of the conclusions is given in last section.

Outline of the DMEMP Model

The DM model [6, 7] expresses the KSI cross-section σ_{DM} as

$$\sigma_{DM}(T) = \pi r_K^2 N_K g_K f(U_K) F(U_K). \quad (1)$$

Here, r_K is the root-mean-square radius of the K -shell. N_K is the number of electrons in this shell and g_K is the weighting factor. The energy dependence of the KSI cross sections (KSICS) is given by the product of the two functions $f(U_K)$ and $F(U_K)$. $U_K = T/I_K$ refers to the reduced impact energy with I_K as the binding energy of the K -shell electrons. The energy dependent term $f(U_K)$ is given by

$$f(U_K) = \frac{1}{U_K} \left[\frac{U_K - 1}{U_K + 1} \right]^a \times \left[b + c \left(1 - \frac{1}{2U_K} \right) \ln \{ 2.7 + (U_K - 1)^{1/2} \} \right]. \quad (2)$$

Here, a , b , and c are adjustable parameters. The function $F(U_K)$ is a relativistic factor defined by

$$F(U_K) = R(U_K) \left[1 + \frac{2(U_K)^{0.25}}{(J_K)^2} \right], \quad (3)$$

with $J_K = m_e c^2 / I_K$ and m_e the electron rest mass. $R(U_K)$ is Gryzinski's relativistic factor [15, 16] given by

$$R(U_K) = \frac{1 + 2J_K [U_K + J_K]^2}{U_K + 2J_K [1 + J_K]} \times \left[\frac{(1 + U_K)(U_K + 2J_K)(1 + J_K)^2}{J_K^2(1 + 2J_K) + U_K(U_K + 2J_K)(1 + J_K)^2} \right]^{3/2} \quad (4)$$

In the Bell model, the expression for KSICS is given by

$$\sigma_{\text{BELL}}(T) = \frac{1}{I_K T} \left[A \ln \left(\frac{T}{I_K} \right) + \sum_{i=1}^2 B_i \left(1 - \frac{I_K}{T} \right)^i \right] \quad (5)$$

Here, the dipole interaction term is represented by $\ln(T/I_K)$, which explains the behavior of cross section at high energies. The B_i terms account for cross sections at the threshold and medium energy regions.

Combining the features of the DM and BELL models as expressed in (1) and (5), the KSI cross-section σ_{DMEMP} in the proposed DMEMP model is then written as

$$\sigma_{\text{DMEMP}}(T) = \pi r_K^2 N_K g_K F_{\text{ion}} G_R(U_K) / (Z^\lambda U_K) \times \left[A \ln \left(\frac{T}{I_K} \right) + \exp \left\{ \sum_{i=1}^2 B_i \left(1 - \frac{I_K}{T} \right)^i \right\} \right] \quad (6)$$

In line with the argument of Ref. 12 in favor of using a nonlinear fitting formula, which usually require less parameters, we have chosen to replace the polynomial expansion in $B_i (1 - 1/U_K)^i$ of (5) by an exponential function of the corresponding term in Eq. (6). F_{ion} is the ionic correction factor defined by

$$F_{\text{ion}} = 1 + m \left(\frac{q}{Z U_K} \right)^n \quad (7)$$

Here, $q = Z - N_K$ is the effective charge of the target atom as seen by the incident electron approaching the K -shell electrons. This factor is introduced to account for the ionic enhancement of cross section [8]. This ionic effect decreases with increase of the incident energy as the probability of finding the incident electron decreases with increase of the incident speed. The weighting factor g_K in (6) is defined by

$$g_K = \frac{D_K}{I_K} (1 + \beta q / Z), \quad (8)$$

where D_K and β are parameters. The relativistic factor G_R in (6) replaces that $F(U_K)$ in (1) with a slight change in the form:

$$G_R = R(U_K) [1 + (U_K)^{0.25} / (J_K)^2], \quad (9)$$

where $R(U_K)$ is again given by [4].

Results and Discussions

The KSICS values are calculated from the DM model using (1) and the proposed DMEMP model using (6). We used the binding energies I_K and root-mean-square radii r_K given by Desclaux [17]. The values of the parameters a , b , and c in (1) are taken from [6]. The parameters of the DMEMP model, occurring in (6), are obtained by optimization through comparison of the calculated KSICS with the available experimental data. The criterion of the best fit parameters has been taken as those producing the minimum χ^2 defined by

$$\chi^2 = \frac{1}{N_p} \sum_{j=1}^{j=N_p} \left(\frac{\sigma_{\text{Th}}^j - \sigma_{\text{Ex}}^j}{\sigma_{\text{Ex}}^j} \right)^2 \quad (10)$$

Here, N_p is the number of data points. σ_{Th}^j and σ_{Ex}^j are, respectively, the predicted and experimental values of the cross sections. A nonlinear least-squares fitting code MINUIT [18] has been used to minimize χ^2 in the goal of obtaining the optimum values of the parameters A , B_1 , B_2 , and λ in (6); m and n in (7); and D_K and β in (8) involved in the DMEMP model. In the optimization process, overall fits to all the 30 atomic targets from H to U are considered.

The experimental data are taken from Shah et al. [19] for H; Rejoub et al. [20], Schram et al. [21], Shah et al. [22], and Nagy et al. [23] for He; Tawara et al. [24] for C, N, Ne, and Ar; Egerton [25] and Isaacson et al. [26] and for C; Gulpe and Mehlhorn [27] for N and Ne; Platten et al. [28] for Ne, Si, and Ar; McDonald and Spicer [29] for Al; Hoffmann et al. [30] for Al, Si, Ar, Cr, Ni, Cu, Y, Mn, Ag, Sn, Au, Pb, and Bi; Hink and Ziegler [31] for Al; Kamiya et al. [32] for Al; Ishii et al. [33] for Al, Si, Zn, Se, Y, Mo, Pd, In, Sn, Ba, Au, Pb, Bi, and U; Quarles and Semaan [34] for Ar; Scholz et al. [35] for V, Cr, Co, Ni, Cu, Zn, Se, Rb, Sr, In, Sn, Ba, Au, Pb, and Bi; An et al. [36] for V and Co; Luo et al. [37] for Cr and Mo; He et al. [38] for Cr; Jessenberger and Hink [39], and Pockman et al. [40] for Ni; Genz et al. [41] for Ni,

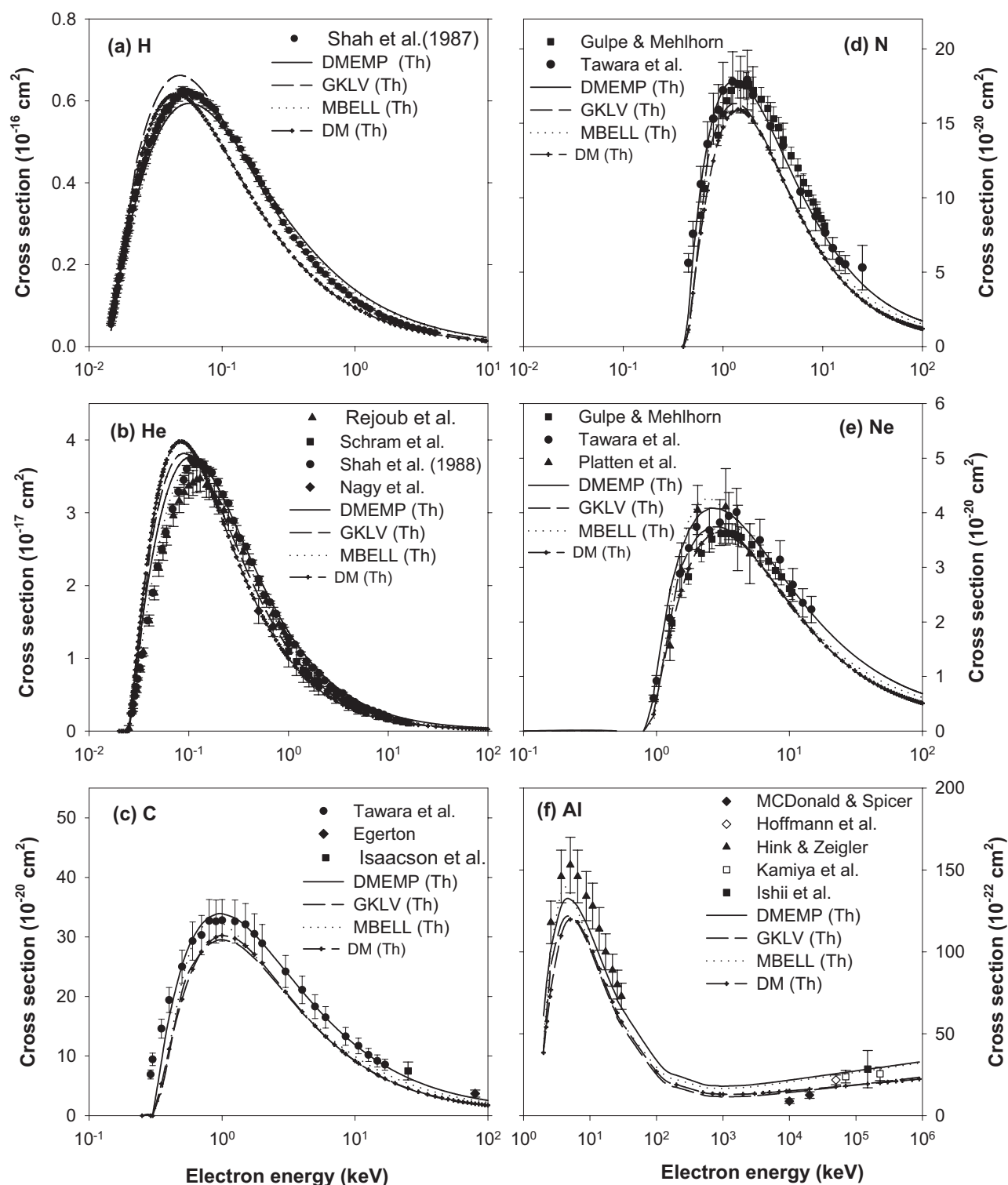


FIGURE 1. Electron impact K-shell ionization cross sections for (a) H, (b) He, (c) C, (d) N, (e) Ne, and (f) Al. Experimental data are in solid dots. The sources of data are given in the text. The predicted results from the proposed DMEMP, GKLv, MBELL, and DM models are in solid, dashed, dotted lines, and dashed lines with pluses.

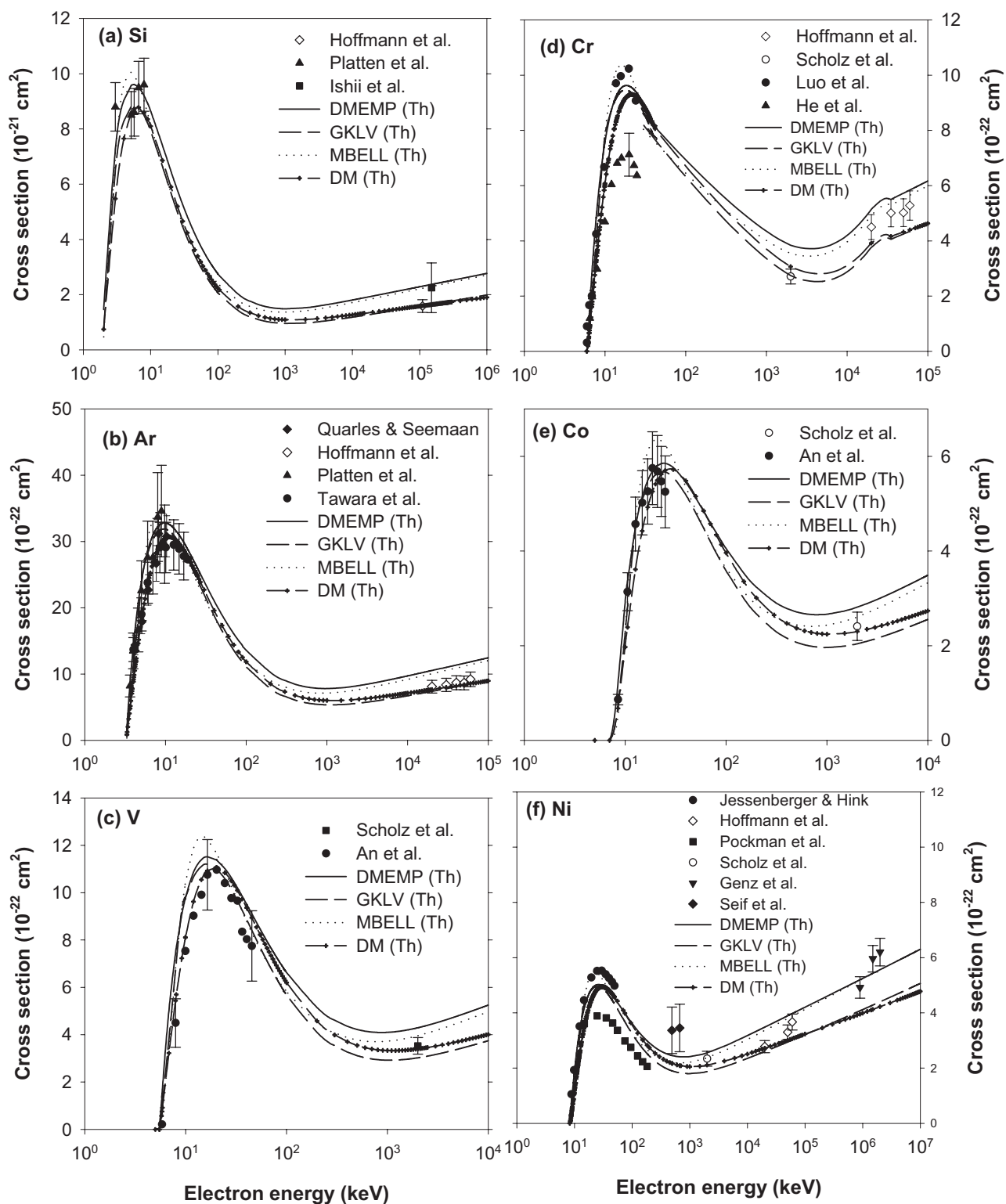


FIGURE 2. Same as in Figure 1 for (a) Si, (b) Ar, (c) V, (d) Cr, (e) Co, and (f) Ni.

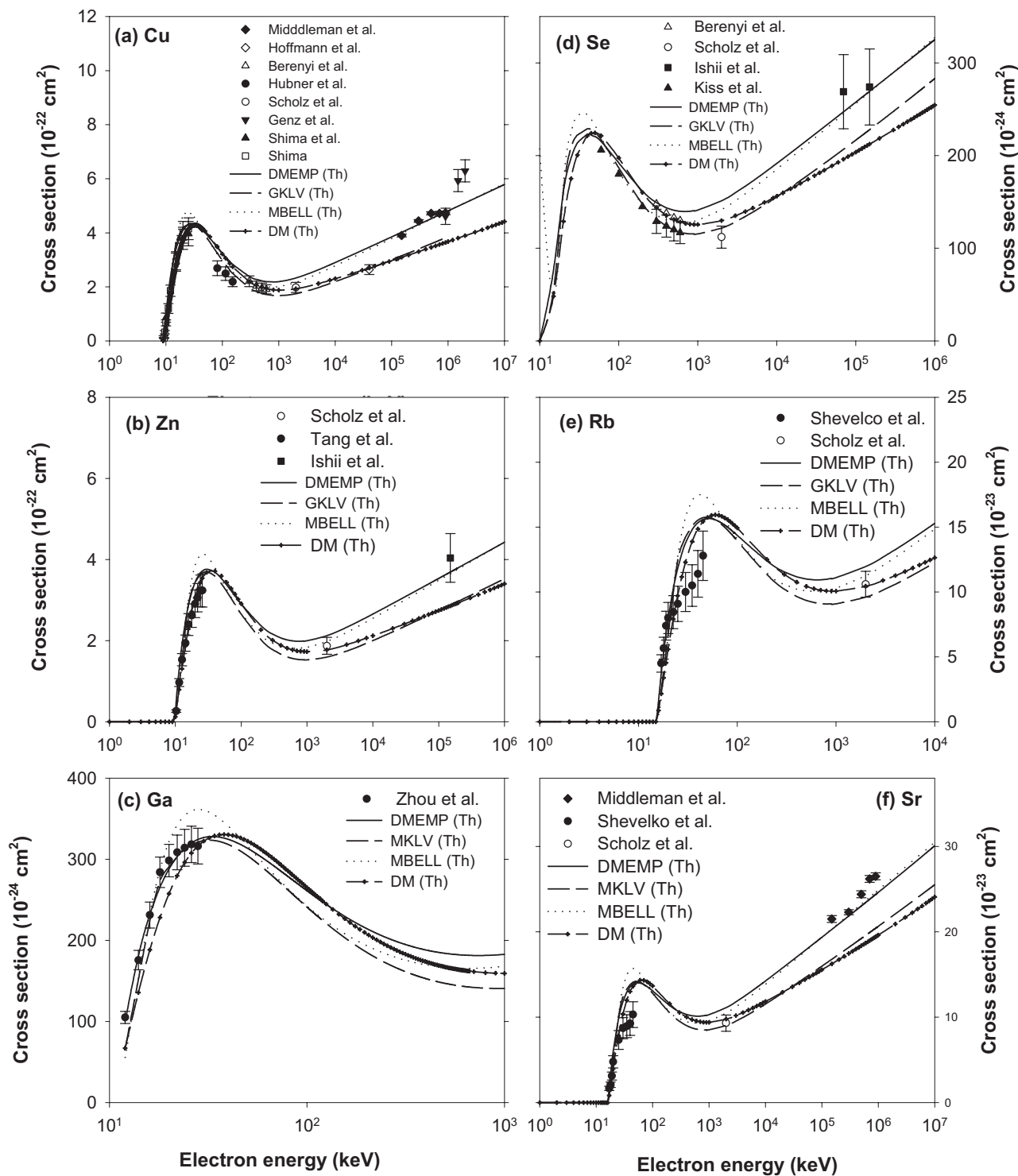


FIGURE 3. Same as in Figure 1 for (a) Cu, (b) Zn, (c) Ga, (d) Se, (e) Rb, and (f) Sr.

Cu, and Ag; Seif el Naser et al. [42] for Ni, Y, Ta and Pb; Middleman et al. [43] for Cu, Sr, Mo, In, Ta, Au, and Bi; Berenyi et al. [44] for Cu and Se; Hubner et

al. [45], Shima et al. [46], and Shima [47] for Cu; Tang et al. [48] for Zn; Zhou et al. [49] for Ga; Kiss et al. [50] for Se and Ag; Shevelco et al. [51] for Sb

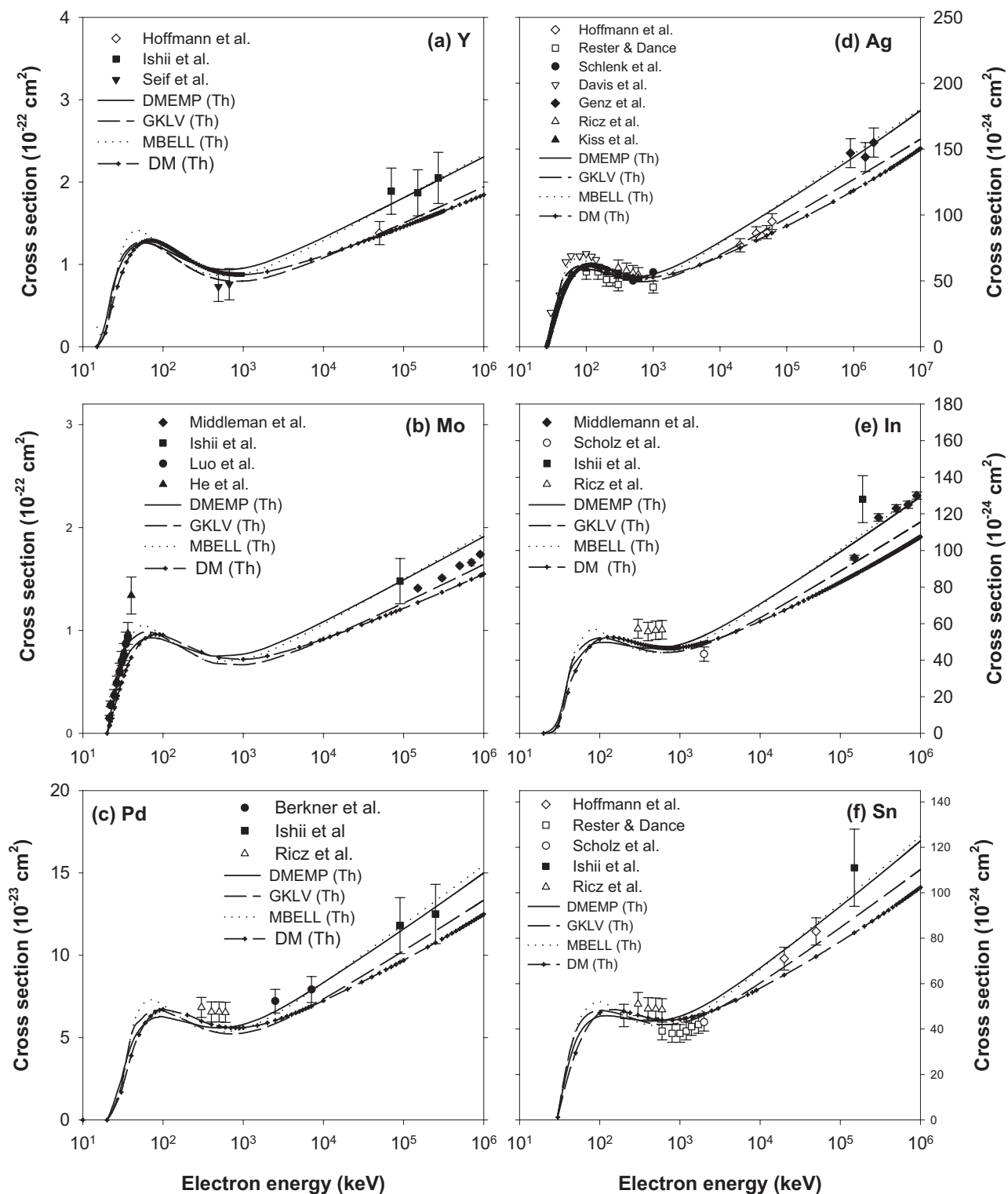


FIGURE 4. Same as in Figure 1 for (a) Y, (b) Mo, (c) Pd, (d) Ag, (e) In, and (f) Sn.

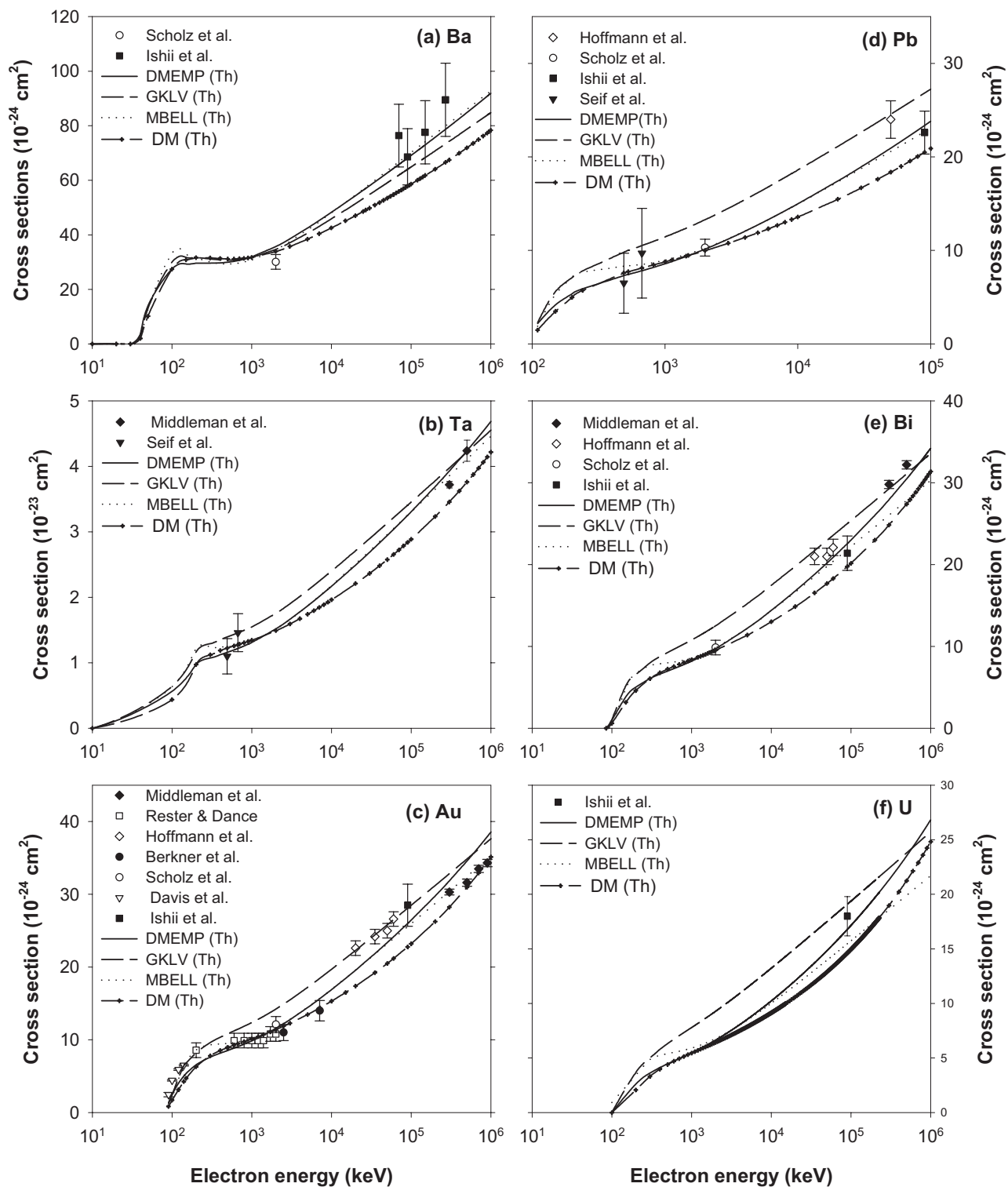


FIGURE 5. Same as in Figure 1 for (a) Ba, (b) Ta, (c) Au, (d) Pb, (e) Bi, and (f) U.

and Sr; He et al. [52] for Mo; Berkner et al. [53] for Pd and Au; Ricz et al. [54] for Pd, Ag, In, and Sn; Rester and Dance [55] for Ag, Sn, and Au; Schlenk et al. [56] for Ag; and Davis et al. [57] for Ag and Au. The optimum values of the parameters in the DMEMP model are $A = 2.00$, $B_1 = B_2 = 0.50$, $D_K = 5.2$, $\lambda = 0.16$, $m = 1.6$, $n = 1.1$, and $\beta = 0.4$.

In Figures 1–5, the predicted cross sections using the DMEMP model are compared with the experimental data and our calculated values from the MBELL, GKL V, and DM models. The following general observations can be noted from the comparisons, presented in the figures:

- a. The DMEMP and MBELL results agree except in the peak region.
- b. The DM and GKL V predictions are, in general, close but for Ga and targets heavier than Ag differences arise. Although the DM fits to the data are not satisfactory near the peak region for He, both of them underestimate the cross-section data beyond about 100 MeV for heavier atoms.
- c. Apart from the case of Mo [Fig. 4(b)] and the overestimation of the experimental data for Ar beyond 20 MeV [Fig. 2(b)], for V [Fig. 2(c)] and Se [Fig. 3(d)] around 2 MeV, and for Cu around 40 MeV [Fig. 3(a)]; the DMEMP model accounts for well all the experimental data.
- d For Ag, In and Sn (see Fig. 4), and Au [Fig. 5(c)], the DMEMP predictions satisfy the average trend of experimental data at different energy ranges. Even for the case of Ni [Fig. 2(f)], where the data from different sources disagree, the DMEMP results follow the average course. (e) It is really amazing to note the excellent quality of fits to the data of Ni [Fig. 2(f)], and Pd, Ag, In, and Sn (see Fig. 4), where the data extend up to energies of 1–2 GeV.

Conclusions

The present work demonstrates the performance of the proposed DMEMP model on the KSI of thirty atomic targets with $Z = 1$ –92 over a wide energy range from the threshold energy to 2 GeV. With a single set of species independent parameters, DMEMP is found profoundly successful in reproducing the experimental data of a wide range of targets up to ultra relativistic energies. For the wide range of target species including the heavier atoms

with atomic numbers up to $Z = 92$, it is found that the DMEMP model turns out to be best performer among other successful models like DM [6, 7], GKL V [14], and MBELL [10] propounded so far. With the simplicity in the structure of DMEMP and its predictive power, this semiempirical model may become a very useful tool for a fast generation of accurate KSICS data for future applications.

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