

Article

Elastic Electron Scattering from Be, Mg, and Ca

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Abstract: We present a comprehensive set of theoretical results for differential, integrated, and momentum transfer cross sections for the elastic scattering of electrons by beryllium, magnesium, and calcium at energies below 1 keV. In addition, we provide Sherman function values for elastic electron scattering from calcium in the same energy range. This study extends the application of our method of calculations, already employed for barium and strontium, to all stable alkaline-earth-metal atoms. Our semi-empirical approach to treating target polarization has produced in our earlier work a satisfactory agreement with experimental values and precise theoretical results such as convergent close-coupling calculations for barium. The present data are expected to be of similar high accuracy, based on our previous success in similar calculations for barium and all inert gases.

Keywords: elastic electron scattering; beryllium; magnesium; calcium

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1. Introduction

In our previous paper [1], we extended our relativistic approach to treat elastic electron collisions with inert gases [2] to two heavy alkaline-earth-metal atoms, barium and strontium. Our results compared well with the few available experimental and the convergent close-coupling (CCC) calculations data for barium, and hence we presented our set of values of cross sections for strontium. The present work intends to expand the data to all stable alkaline-earth-metal atoms. Similar to strontium, there is a small amount of experimental data available for elastic electron scattering from beryllium, magnesium and calcium. In fact, the elastic electron scattering from neutral beryllium, to the best of our knowledge, has attracted no experimental attention at all. Therefore, all available data come from theoretical calculations. The introduction of beryllium as a surface material in the JET project [3] created a need for atomic data in the early and mid-1990s. This motivated some precise calculations in *R*-matrix and CCC formulations [4–8]. However, those calculations did not provide much information on elastic scattering. The theoretical data on elastic electron scattering from beryllium were, for a long time (up until 2016), limited to some older calculations. Those included the relativistic calculations of Fink and Ingram [9] for 100, 250, 500, 1000, and 1500 eV, the close-coupling calculations of Fabrikant [10] for energies below 8.16 eV, the nonrelativistic partial-wave calculations of Kaushik et al. [11] for a few energies in the 5–30 eV range, and the low-energy integrated cross section (ICS) calculations of Yuan and Zhang [12] for energies below 1 eV. The work of Fink and Ingram [9] also gives the only data on the spin polarization of electrons scattered from the beryllium atom. Recent B-spline and CCC calculations of Zatsarinny et al. [13] for energies up to 100 eV and relativistic complex optical potential (ROP) calculations of McEachran et al. [14] for energies up to 5000 eV provided theoretical data with more precision and range to the field.

The interest in elastic electron scattering from magnesium and calcium is mostly driven by the importance of such data in the modeling of an array of studies ranging from evolution of galaxies and interstellar clouds to laboratory plasma to biophysical investigations of metabolic processes [15–21].

For magnesium, there have been a few experimental works on elastic scattering, most of which date back to the 1970s and early 1980s. Burrow and Comer [22] and Burrow et al. [23] performed experiments to identify the low-energy resonant scattering using the electron transmission method. Kazakof and Khristoforov [24] studied this ^2P resonance by measuring the differential cross section (DCS) at angle 90° . Nevertheless, the only experimental DCS and ICS data for magnesium are those provided by Williams and Trajmar [25] for 10, 20, and 40 eV and, more recently, Predojević et al. [26] for energies up to 100 eV. On the theoretical side, there are three old close-coupling calculations for magnesium. Van Blerkom [27] reported a few low-energy ICSs and Fabrikant provided low-energy cross sections in Refs. [10,28] and ICS and DCS values for 10 and 20 eV in Ref. [29]. Comparison between the ICSs of Van Blerkom [27] and Fabrikant [28] yielded a total disagreement. Other theoretical investigations for magnesium are the relativistic treatment of Gregory and Fink [30] for 100, 250, 500, 1000, and 1500 eV impact energies, nonrelativistic partial-wave calculations of Khare et al. [31] for some intermediate energies, the low-energy DCS and ICS results of Yuan and Zhang [12,32], coupled-channels approximation calculations of Mitroy and McCarthy [33], nonrelativistic partial-wave calculations of Pandya and Baluja [34], B-spline calculations of Zatsarinny et al. [35] and ROP calculations of McEachran et al. [36] for energies up to 5000 eV. In the absence of experimental data, the work of Gregory and Fink [30] is the only available study on the spin polarization of scattered electrons from magnesium, which provides Sherman functions at the aforementioned energies.

In the case of calcium, for long the only experimental work was that of Romanyuk et al. [37], which provided low-energy ICS values and was refined some years later [38]. The measurement of differential and integrated cross section values for energies up to 100 eV by Milisavljević et al. [39] is the only other experimental work for elastic scattering of electrons off the calcium atom. The theoretical calculations for calcium include the close-coupling calculations of Fabrikant [10] for energies below 5.44 eV, a relativistic study on some intermediate energies by Khare et al. [40], data by Gregory and Fink [30] at the same abovementioned energies, the low-energy studies of Yuan and Zhang [12,32], Cribakin et al. [41], Yuan [42], Yuan and Fritsche [43] and Yuan and Lin [44], partial wave oriented calculations of Raj and Kumar [45], B-spline and R-matrix studies of Zatsarinny et al. [46] for energies up to 4 eV and later up to 100 eV [47], and optical potential calculations of Wei et al. [48]. On the subject of spin polarization of scattered electrons from calcium, there are three works in the literature, all from the theoretical sector. Gregory and Fink [30] and Khare et al. [40] provide Sherman functions for some intermediate and high energies, whereas the Sherman function values of Yuan [42] are limited to a few low-impact energies.

As noted, there has been very little experimental attention toward these three atoms. The present work aims to furnish a consistent set of elastic DCS, ICS, and momentum transfer cross section (MTCS) data in a wide energy range and for all these three atoms, which could be useful to future experimental works.

2. Results

We present our results and comparisons with those of other works for each atom separately.

2.1. Beryllium

Our DCS values for beryllium are shown in Figures 1 and 2. As we already know, there are no experimental data available to compare with. Our results, however, are in good agreement with the DCS values of Fink and Ingram [9] at 100, 500, and 1000 eV, except for

the forward direction. There is a marked discrepancy between our DCSs and those of Fink and Ingram [9] at small scattering angles, as seen in Figure 1. This is understood, knowing that the calculations of Fink and Ingram [9] did not account for the effect of polarization of the atomic target and, less importantly, the effect of exchange in the scattering process. This difference is limited to the very forward direction angles at high energies, as can be seen in the magnified portions of 500 and 1000 eV graphs but expands to larger angles at lower energies, e.g., 100 eV. This behavior is expected (and even verified by calculating DCSs with no polarization and exchange) since the polarization of the atomic target contributes to a wider scattering angle range in the forward direction when interacting with slower incident electrons. The comparisons in Figure 2 show a behavioral agreement between our DCSs and those of Kaushik et al. [11]. At 30 and 40 eV, our DCS is visibly lower than those of Kaushik et al. [11], and at 10 and 5 eV, disagreements on the position of the DCS's minimum form. To visualize the behavior of differential cross section as a function of impact energy and scattering angle, in Figure 3, we present a three-dimensional (3D) graph of the logarithm ($\log_{10}$) of beryllium's DCS versus the logarithm of the energy and the scattering angle. The simplicity of the atomic structure of the beryllium atom is even more obvious if one compares Figure 3 with the 3D graphs presented in Refs. [1,2] for heavier atoms. Our elastic ICS and MTCS values for beryllium and comparisons with four other theoretical results are shown in Figure 4.

Our ICS values are in agreement with the results of CCC106 calculations by Fursa and Bray [5,6] over the energy range 5–1000 eV. The same agreement exists with B-spline and CCC values of Zatsarinny et al. [13] and ROP values of McEachran et al. [14] down to around 0.5 eV. However, our ICS values attain a different maximum than those of other theoretical results at low energies. The placement of the maximum of our ICS values is at a higher energy than those of Yuan and Zhang [12] and Fabrikant [10] by about 0.1 eV while being at lower energy than those by Refs. [13,14] by about the same 0.1 eV. From this maximum point down to 0.01 eV, the disagreement between theoretical results is rather profound. In the absence of experimental ICS data, no solid conclusion can be drawn in this region. However, the agreement with other theoretical calculations is a credible test for our ICS values at energies above 0.5 eV. Unfortunately, the momentum transfer cross section has not attracted the same theoretical attention. There is only one MTCS theoretical data available [14] with which our values agree fragmentarily over the wide energy range of 0.5–1000 eV. Our MTCS values display the same disagreement with those of Ref. [14] at very low energies as our ICS values did at the same energies.

2.2. Magnesium

We present our DCS results for magnesium in Figures 5 and 6. Our DCSs for 100, 500, and 1000 eV are in good agreement with the results of Gregory and Fink [30], but the same disparity in the forward direction that we observed for beryllium in comparison of our results with those of Gregory and Fink [9], exists here again since the calculations of Gregory and Fink [30] do not account for polarization and exchange; hence the same explanations for the disagreements in the forward direction given in the previous subsection apply here as well. At 100 eV impact energy, our DCS is in excellent agreement with experimental data of Predojević et al. [26] in the forward direction but in the middle and backward scattering angles, though following congruently, our values generally stay above those of the experiments. This gap is almost non-existent at 80 eV as our values and those of Zatsarinny et al. [35] follow the experiment closely. Nonetheless, our DCS values indicate a slightly earlier minimum compared to those by Zatsarinny et al. [35], which is also visible at 100 eV. The disagreement on the positions of DCS minima among most theoretical works is more evident in the comparisons in Figure 6. As it can be seen in Figure 6, while the agreement between our DCS data and the experimental data of Williams and Trajmar [25] at 10 and 20 eV is quite good, the comparison at 40 eV is not very promising. In fact, our DCS data visibly favor the experimental values of Predojević et al. [26] at 40 eV. In addition, the DCS data from the close-coupling calculations of Fabrikant [29] at 10 and 20 eV do not agree

very well with those given by us and the experimental works. The DCS provided by the nonrelativistic partial-wave calculations of Khare et al. [31] at 10 eV is, on the other hand, nowhere near any other available data for that energy. In all comparisons of our DCS data with the BSR-37 data of Zatsarinny et al. [35] in Figures 5 and 6, there exist disagreements on the positions of DCS minima. These discrepancies become more prominent at lower energies and at large scattering angles.

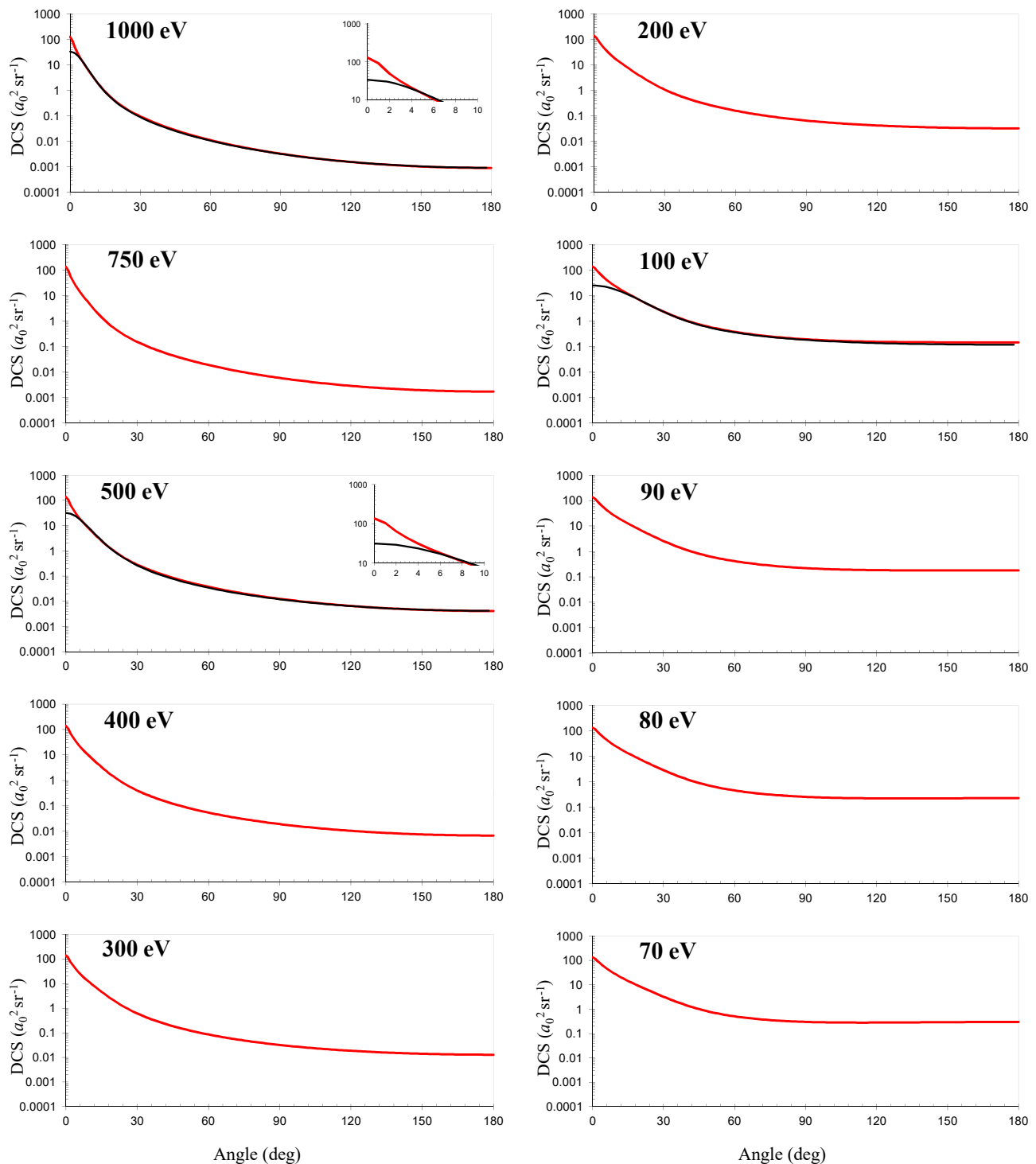


Figure 1. Differential cross sections for elastic electron scattering from beryllium at energies between 70 and 1000 eV: red solid line, present work; Other theoretical: black solid line, Fink and Ingram [9].

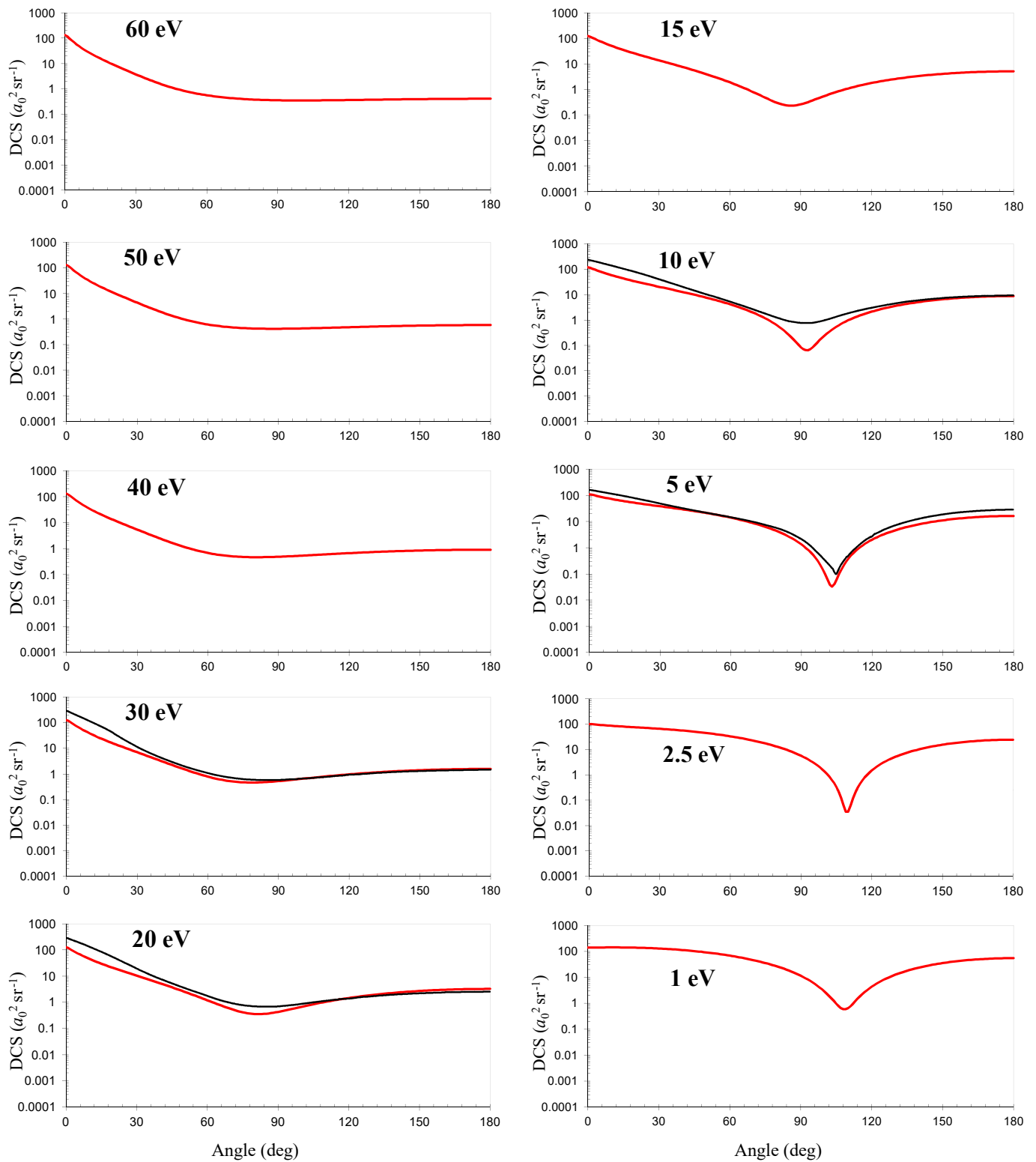


Figure 2. Differential cross sections for elastic electron scattering from beryllium at energies between 1 and 60 eV: red solid line, present work; Other theoretical: black solid line, Kaushik et al. [11].

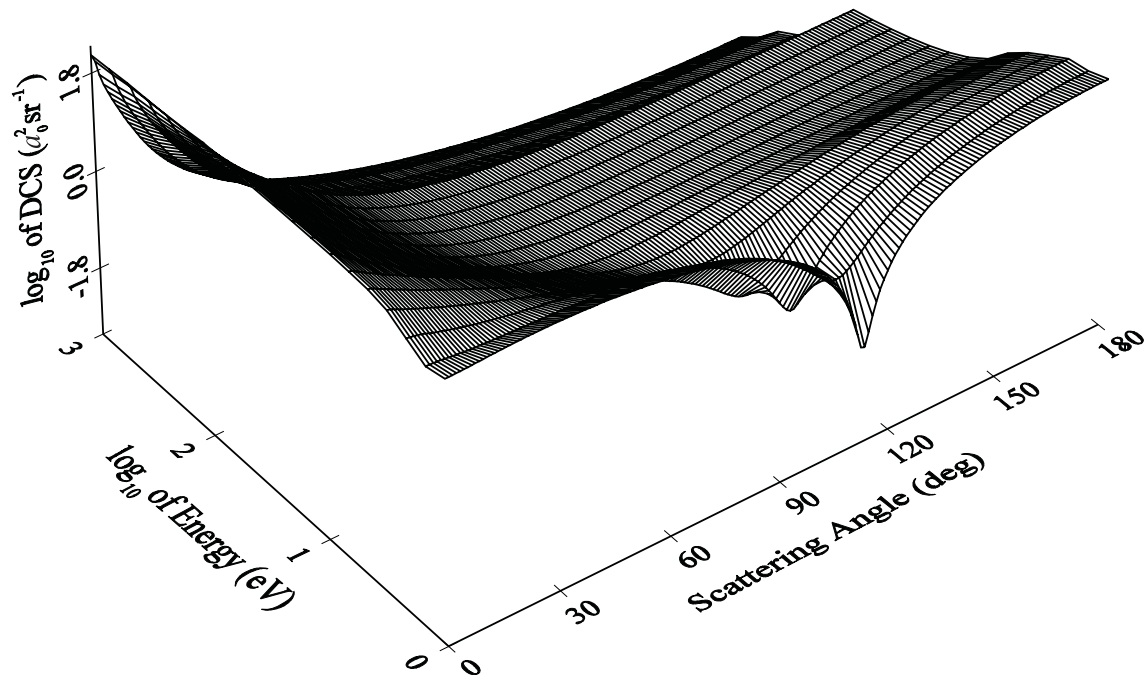


Figure 3. A three—dimensional view of the differential cross section for elastic electron scattering from beryllium.

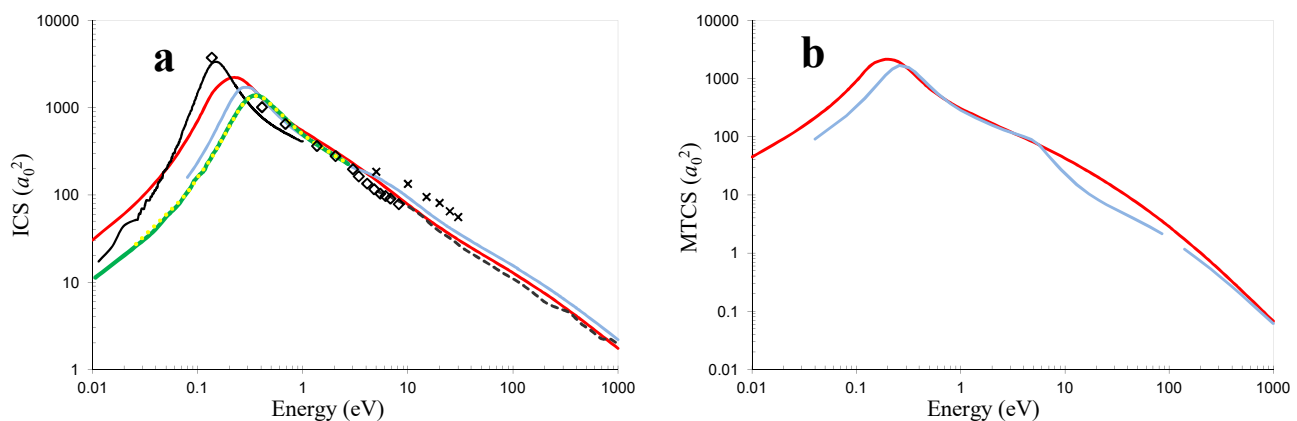


Figure 4. Integrated (a) and momentum transfer (b) cross sections for elastic electron scattering from beryllium: red solid line, present work; Other theoretical: black solid line, Yuan and Zhang [12]; $\times$, Kaushik et al. [11]; $\diamond$, Fabrikant [10]; dashed black line, Fursa and Bray [5,6]; blue solid line, McEachran et al. [14]; green solid line, BSR-660 data of Zatsarinny et al. [13]; thick dotted yellow line, CC-409 data of Zatsarinny et al. [13].

Like beryllium, a 3D graph of magnesium's DCS for energies between 1 and 1000 eV is given in Figure 7. Magnesium's 3D graph demonstrates a more complex pattern compared to beryllium's, which reflects the difference in the atomic structure, e.g., the number of filled shells. In Figure 8, we present our elastic ICS and MTCS results for magnesium. The agreement between our ICS and MTCS values and the experimental data of Williams and Trajmar [25] is satisfactory except for the data point of 40 eV, at which the DCSs also differed from each other in general but most notably in the backward direction. This difference can be explained knowing that the experimental ICS and MTCS of Ref. [25] have been obtained by the integration of the actual experimental DCSs and those obtained from the extrapolation to small and large scattering angles. The extrapolated DCSs for the large scattering angles, reported in Ref. [25], do not bounce back and instead follow a downward path. Consequently, the discrepancy between our large-angle DCS values and

the extrapolated DCSs of Williams and Trajmar [25] reaches an extreme, where ours is larger by a factor of 100. Obviously, such discrepancy between the DCSs can cause a difference in ICS and MTCS values since these quantities involve integrals of DCS over the angles. By the same reasoning, we can see why there is a marginal agreement between the present ICS value at 40 eV, and that of Predojević et al. [26].

Our ICS values are in very good agreement with those of McEachran et al. [36] for energies between 5 and 1000 eV. That is also, more or less, the case for other theoretical values except those of Zatsarinny et al. [35], which are consistently lower than our values. This is not surprising as Ref. [35]’s corresponding DCS values are also consistently smaller than ours over large intervals of scattering angles, if not all. Our low-energy ICS values are in agreement with the results of Yuan and Zhang [12] down to 0.7 eV energy, below which our values are markedly higher. The ICS values of McEachran et al. [36] deviate from our values below 4 eV and develop a maximum at almost 0.1 eV higher than ours. The present data observed a Ramsauer–Townsend (RT) minimum in the elastic ICS data for magnesium at just above 0.01 eV impact energy, below which the cross section rises very rapidly.

Our MTCS values are in excellent agreement with two experimental values of Williams and Trajmar [25] at 10 and 20 eV; however, not at 40 eV as was the case for the ICS data. The difference between our MTCS and the experimental MTCS at 40 eV is noticeably larger than the corresponding disparity in the ICS values. To understand this, one notices that the mathematical expression for MTCS has an extra factor of $(1 - \cos \theta)$ compared to that of ICS. This extra factor can contribute to this larger difference as it is small in the forward direction but becomes greater than 1 for $\theta > 90^\circ$, where the present DCS values are maximally higher than those obtained by the extrapolation of the experimental DCS at 40 eV. The agreement between our MTCS data and that of McEachran et al. [36] is inconsistent over a wide energy range. Angular dependence of the DCS function at each projectile energy must be the contributing factor to the difference between our MTCS values and those of McEachran et al. [36]. We observe a disagreement on the position of MTCS maximum (which existed in ICS data as well) between the only two theoretical values for magnesium.

2.3. Calcium

Our DCS results, and comparison with other calculations, are shown in Figures 9 and 10. They display noticeable diffraction oscillations, which are expected from a medium or heavy atom. These pronounced minima and their energy evolution can be seen readily in Figure 11, where we present a 3D graph of calcium’s DCS. As can be seen in Figure 9, there is a good agreement between our DCSs and those of Gregory and Fink at 100, 500, and 1000 eV, while the aforementioned disparity in the forward direction still exists. The comparisons with the DCSs of Khare et al. [40] show agreements at 40 and 100 eV but strong disagreements at 10 and 500 eV impact energies. Our DCS values at 1, 5, and 10 eV also differ from the results of Yuan [42]. Our DCS values are in very good agreement at 100 eV with those of Zatsarinny et al. [47] but at 60, 40, and 20 eV, impact energies are generally larger and in mild disagreement on the position of the minima of DCS values with those of Ref. [47]. These disagreements with Ref. [47] are most apparent at 10 eV. The same disagreements exist with the DCSs of Wei et al. [48] at 40, 20, and 10 eV. The comparisons of our DCS data with the only experimental work, by Milisavljević et al. [39], show general agreement in both magnitude and angular dependency and disagreement at 10 eV. Interestingly, similar discrepancies exist between the experimental values of Ref. [39] and other theoretical works. Further precision experimental investigations of elastic scattering of electrons off calcium atoms would certainly be helpful.

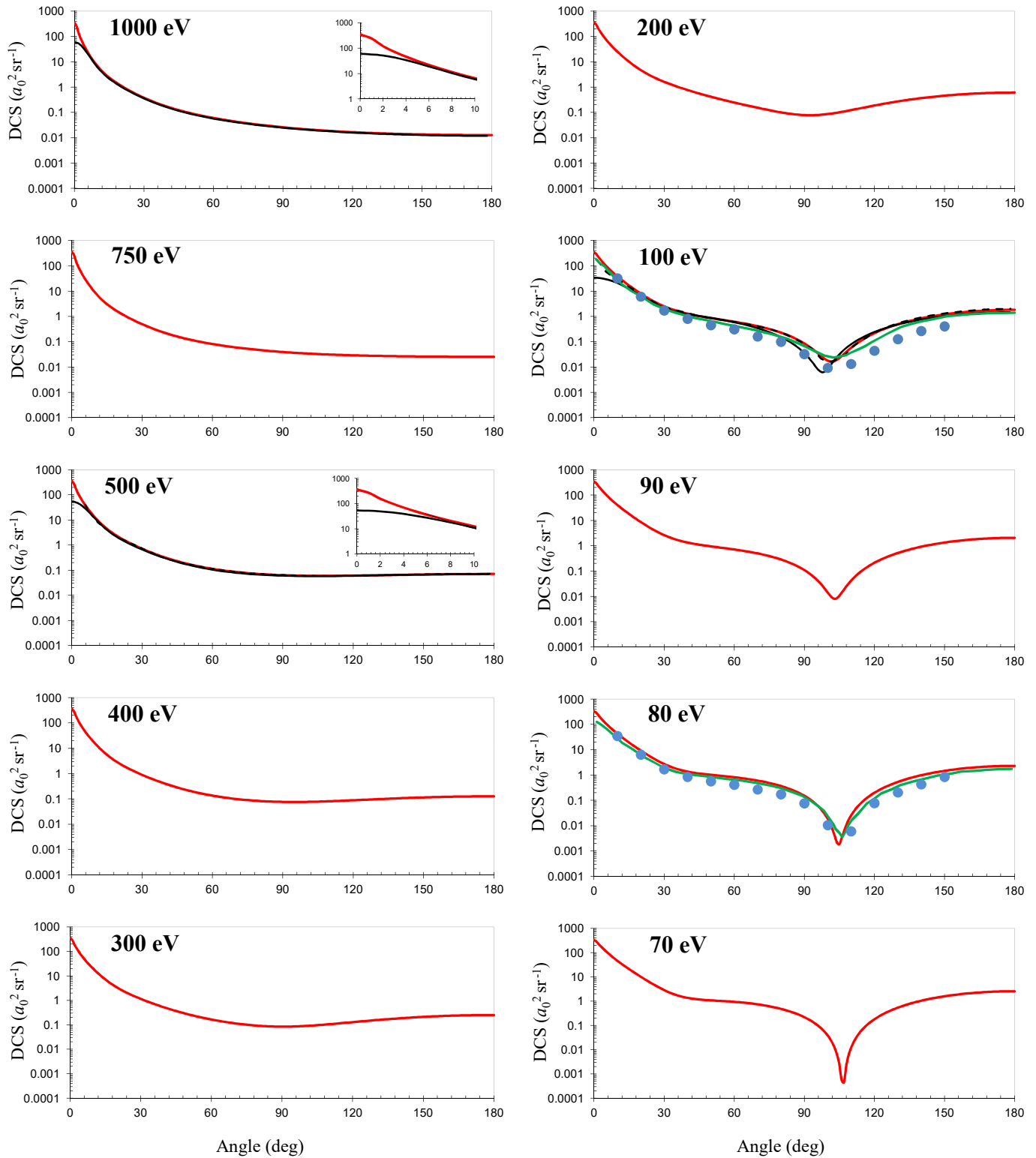


Figure 5. Differential cross sections for elastic electron scattering from magnesium at energies between 70 and 1000 eV: red solid line, present work; Experimental data: ●, Predojević et al. [26]; Other theoretical: black solid line, Gregory and Fink [30]; black dashed line, Khare et al. [31]; green solid line, BSR-37 data of Zatsarinny et al. [35]. Note that the size of the marker for the experimental data is indicative of its error.

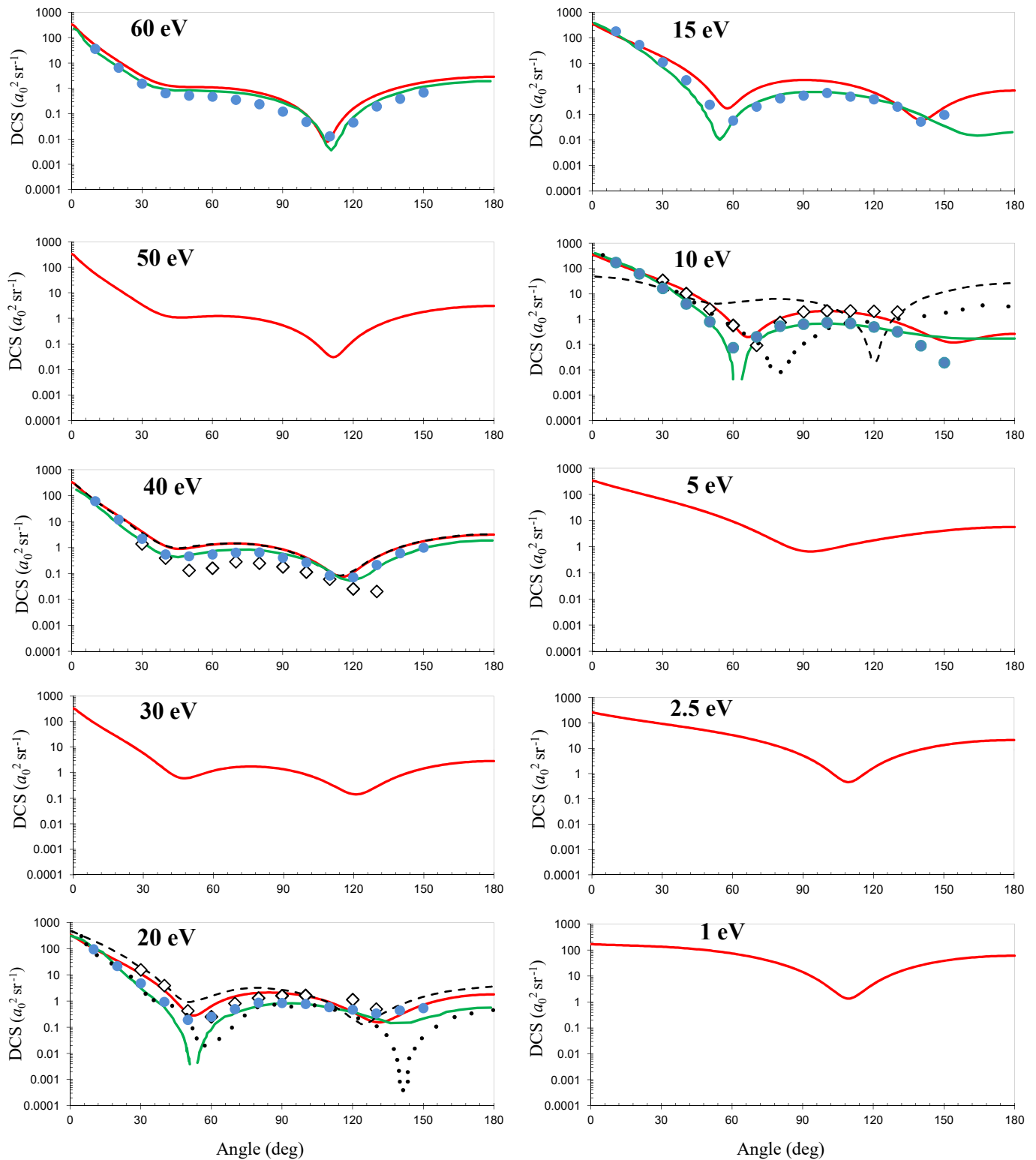


Figure 6. Differential cross sections for elastic electron scattering from magnesium at energies between 1 and 60 eV: red solid line, present work; Experimental data: ●, Predojević et al. [26]; ◇, Williams and Trajmar [25]; Other theoretical: black solid line, Gregory and Fink [30]; dotted black line, Fabrikant [29]; black dashed line, Khare et al. [31]; green solid line, BSR-37 data of Zatsarinny et al. [35]. Note that the size of the marker for the experimental data is indicative of its error.

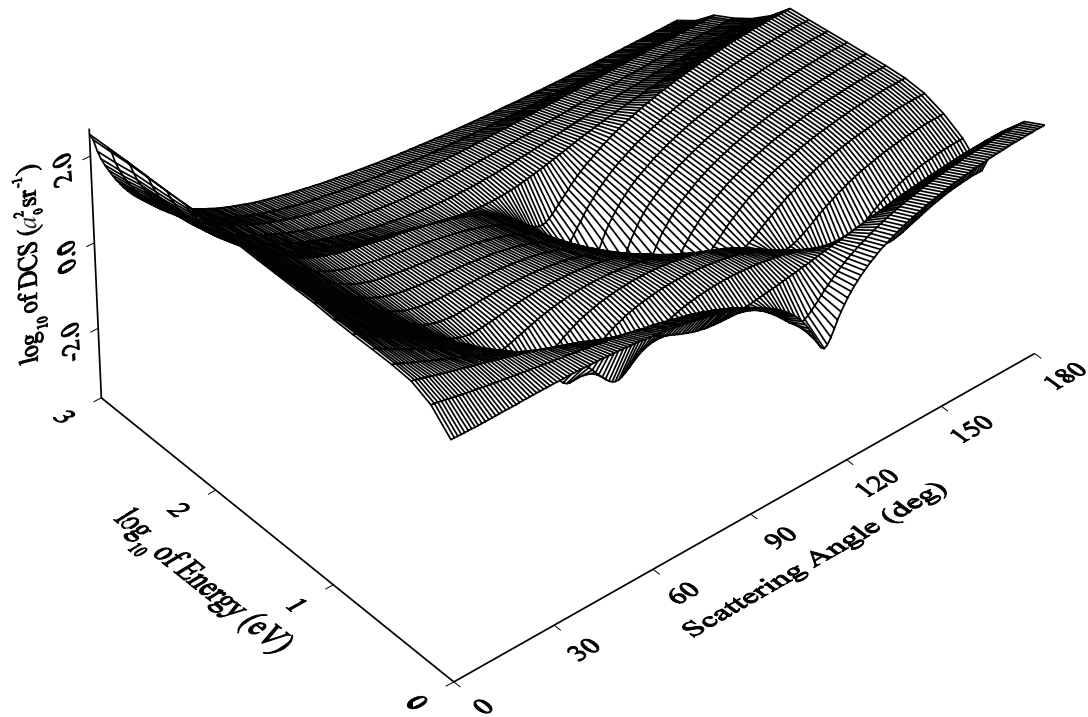


Figure 7. A three-dimensional view of differential cross section for elastic electron scattering from magnesium.

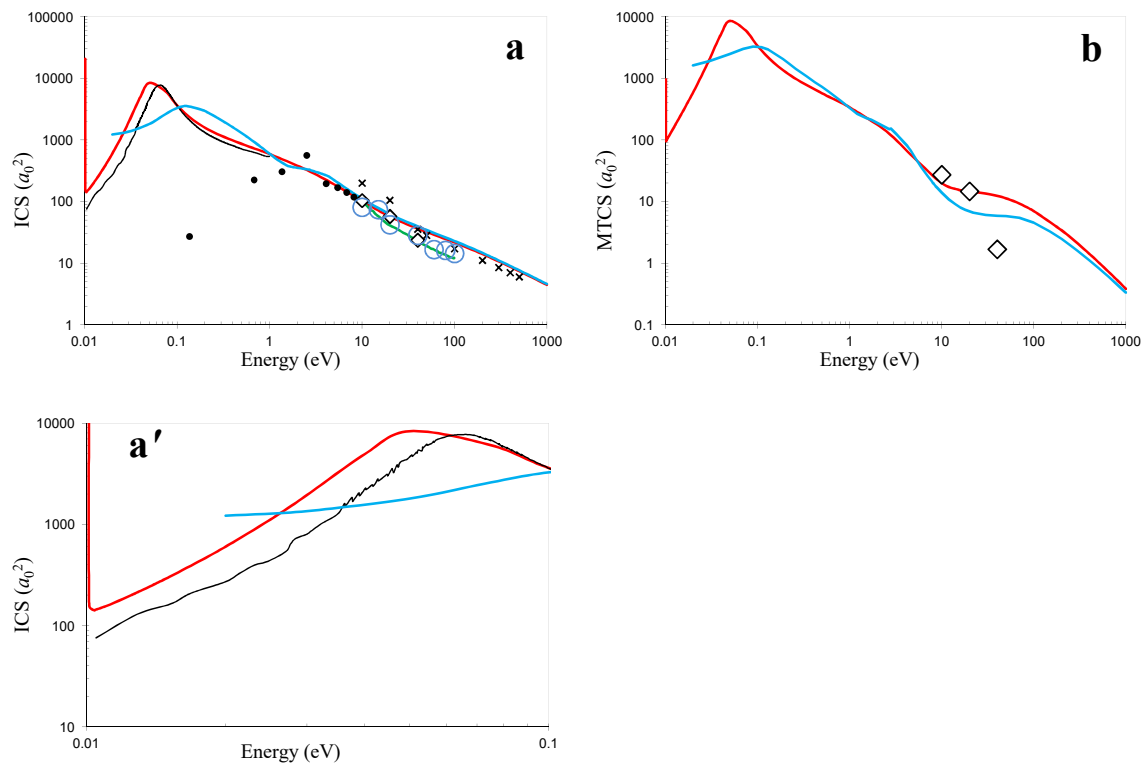


Figure 8. Integrated (a,a') and momentum transfer (b) cross sections for elastic electron scattering from magnesium: red solid line, present work; Experimental data: $\bigcirc$, Predojević et al. [26]; $\diamond$, Williams and Trajmar [25]; Other theoretical: black solid line, Yuan and Zhang [12]; $\times$, Khare et al. [31]; $\bullet$, Fabrikant [10,28]; blue solid line, McEachran et al. [36]; green solid line, BSR-37 data of Zatsarinny et al. [35]. Note that the size of the marker for the experimental data is indicative of its error.

Our ICS and MTCS data for calcium are presented in Figure 12. There is a partial agreement with the ICS values of Khare et al. [40] for energies between 10 and 500 eV. Present ICS values demonstrate a good agreement with the ICSs of Yuan [42] for energies below 0.5 eV but differ from them strongly at larger energies. The ICSs of Fabrikant [10] also disagree with those of Yuan [42] at energies larger than 0.5 eV, while they somehow agree with ours. The experimental ICS values of Milisavljević et al. [39] agree with our values at 100 and 20 eV, while those at other energies sit lower than ours. This is not surprising as our DCS values are also generally higher than those of Ref. [39]. Our TCS values are also higher than those of the BSR-438 data of Zatsarinny et al. [47] between 3 and 20 eV and those of Wei et al. [48].

The only experimental ICS data set at low energies [38] follow a complex path, which seems to prefer the low energy theoretical data of Zatsarinny et al. [46] down to 0.7 eV before the points suddenly rise (which implies a relative minimum in ICS function). The estimated error in the experimental ICS values of Ref. [38] is not known to the authors, and for that reason, the size of the markers does not represent anything. Unfortunately, the ICS values of Zatsarinny et al. [46] do not extend to lower energies to check the existence of an RT minimum, which our data and that of Yuan [42] indicate at around 0.05 eV.

Our MTCS values follow a similar curve for low-impact energies when compared to those of the theoretical work of Cribakin et al. [41], but they are generally lower than the values of Ref. [41] by almost a factor of two. Present MTCS values only agree with the experimental work of Milisavljević et al. [39] at 10 eV and not the rest. This agreement may be due to the excellent agreement of our DCS values in the backward direction with those of Milisavljević et al. [39] at 10 eV, which is not replicated at other energies to that degree (see the last paragraph of the previous subsection for more on this).

In addition to cross sections, we also present Sherman functions for elastic electron scattering from calcium in Figures 13 and 14. The magnitude of the Sherman function, $S(\theta)$, gives the degree of polarization of an unpolarized beam after scattering, given the direction of polarization being perpendicular to the scattering plane, the so-called up/down asymmetry. Furthermore, it can describe the left/right asymmetry in the scattering of a polarized beam. The sign of $S(\theta)$, on the other hand, indicates whether the spin-up states are preferentially populated, in which case it is positive, or the spin-down states are more occupied, in which case it is negative. The comparisons of our Sherman function results with those of Gregory and Fink [30], at 100, 500, and 1000 eV, indicate a very good agreement, while comparisons with the results of Yuan [42] at 1, 5, and 10 eV show some disagreements. This is not surprising, however, if we recall the differences in the DCSs at those energies. In Figure 15, we compare our Sherman functions with some of those given in the paper by Khare et al. [40]. Generally, there is a mixed agreement between our data and those of Khare et al. [40]. The Sherman functions provided by Ref. [40] do not span the whole angular range; therefore, a thorough comparison is not possible. Even though Khare et al. [40] do not give Sherman functions at 100 and 500 eV, they mention a disagreement with the results of Gregory and Fink [30] at those energies, with theirs being larger by a factor of two at all angles. Since our Sherman functions agree with those of Gregory and Fink [30], the Sherman functions of Ref. [40] at 100 and 500 eV, then, would have been larger than ours by a factor of two, as well.

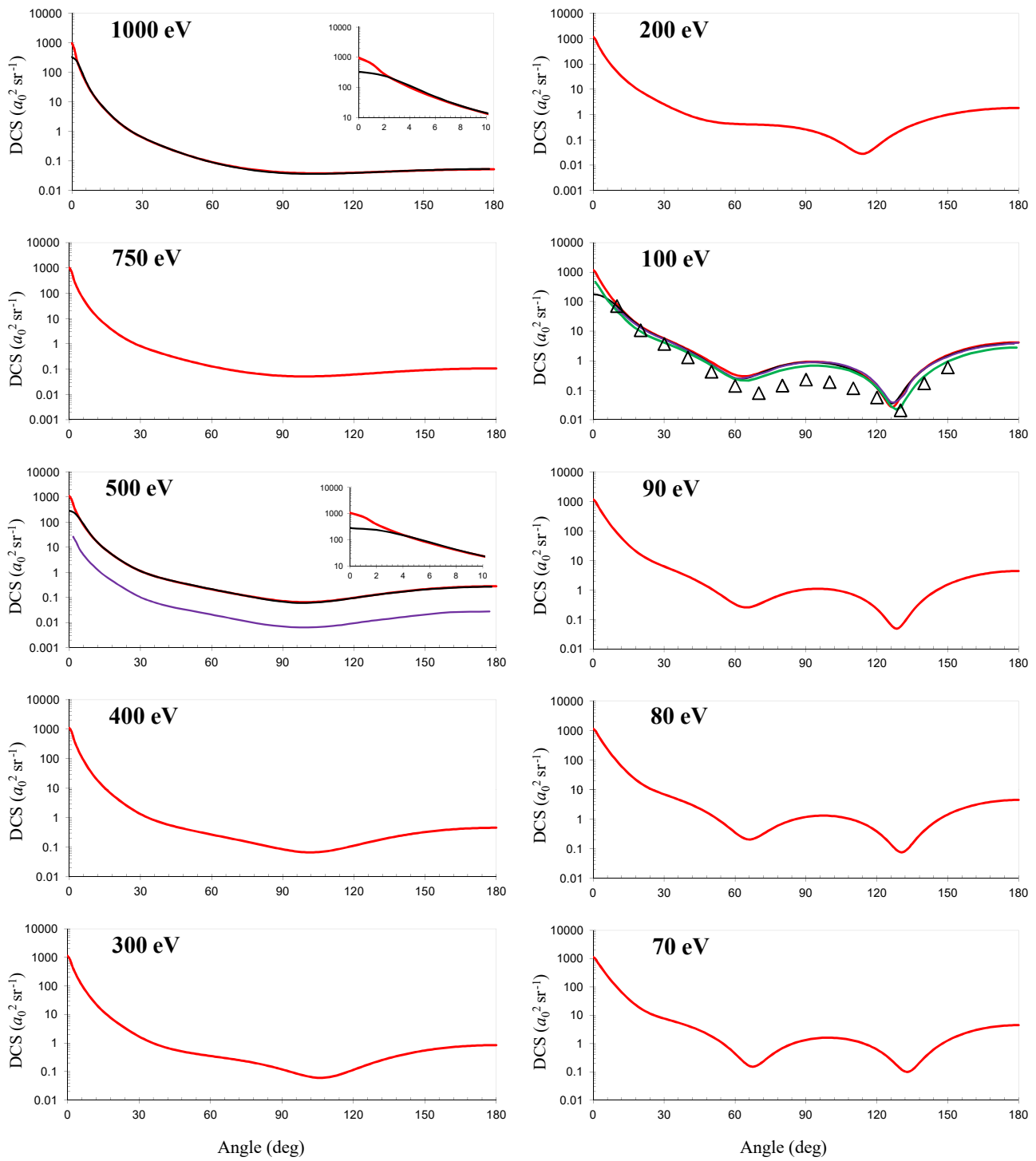


Figure 9. Differential cross sections for elastic electron scattering from calcium at energies between 70 and 1000 eV: red solid line, present work; Experimental data: $\triangle$: Milisavljević et al. [39]; Other theoretical: black solid line, Gregory and Fink [30]; purple solid line, Khare et al. [40], green solid line, Zatsarinny et al. [47]. Note that the size of the marker for the experimental data is indicative of its error.

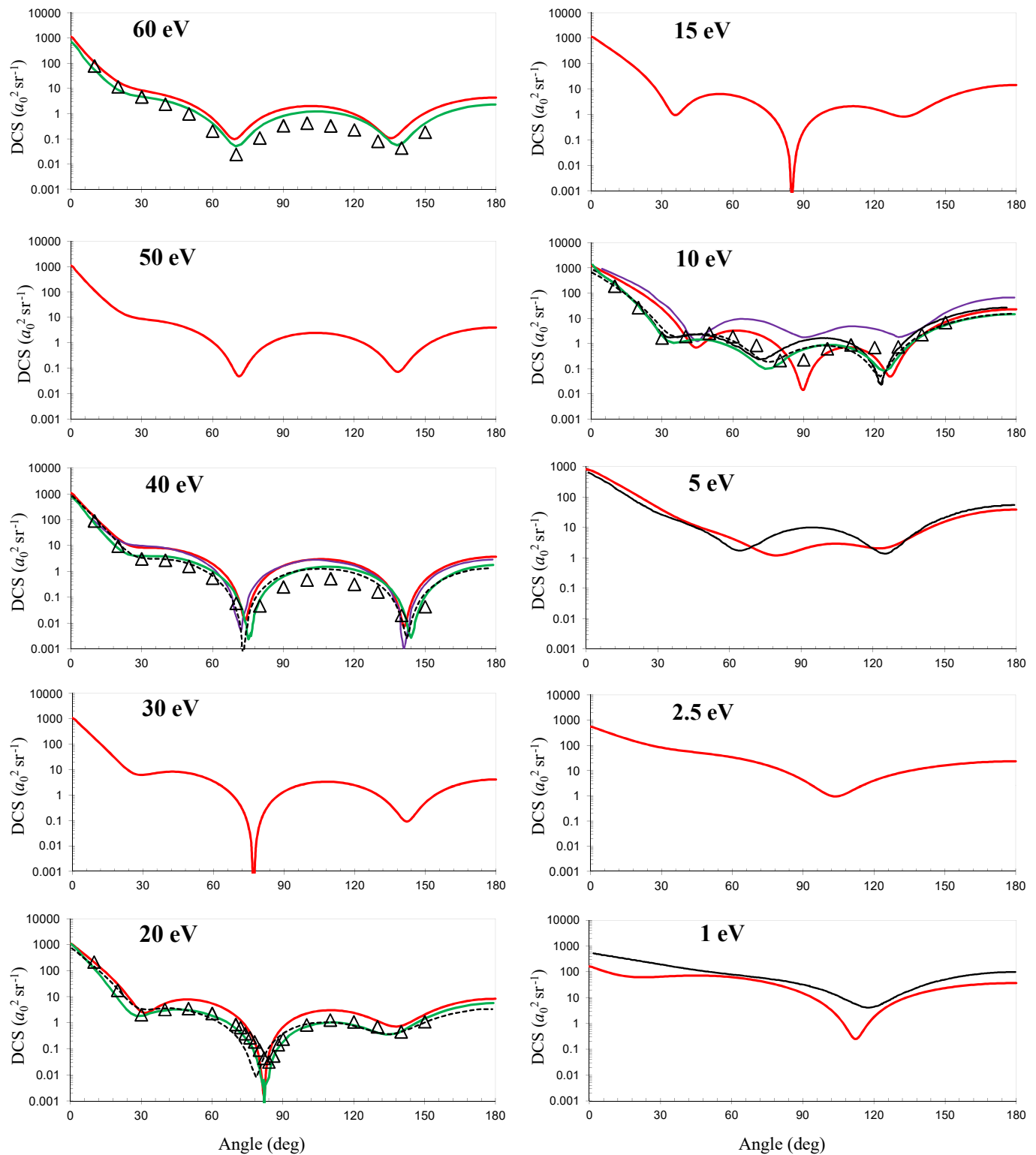


Figure 10. Differential cross sections for elastic electron scattering from calcium at energies between 1 and 60 eV: red solid line, present work; Experimental data: $\triangle$, Milisavljević et al. [39]; Other theoretical: black solid line, Yuan [42]; purple solid line, Khare et al. [40], green solid line, BSR-438 data of Zatsarinny et al. [47], black dashed line, Wei et al. [48]. Note that the size of the marker for the experimental data is indicative of its error.

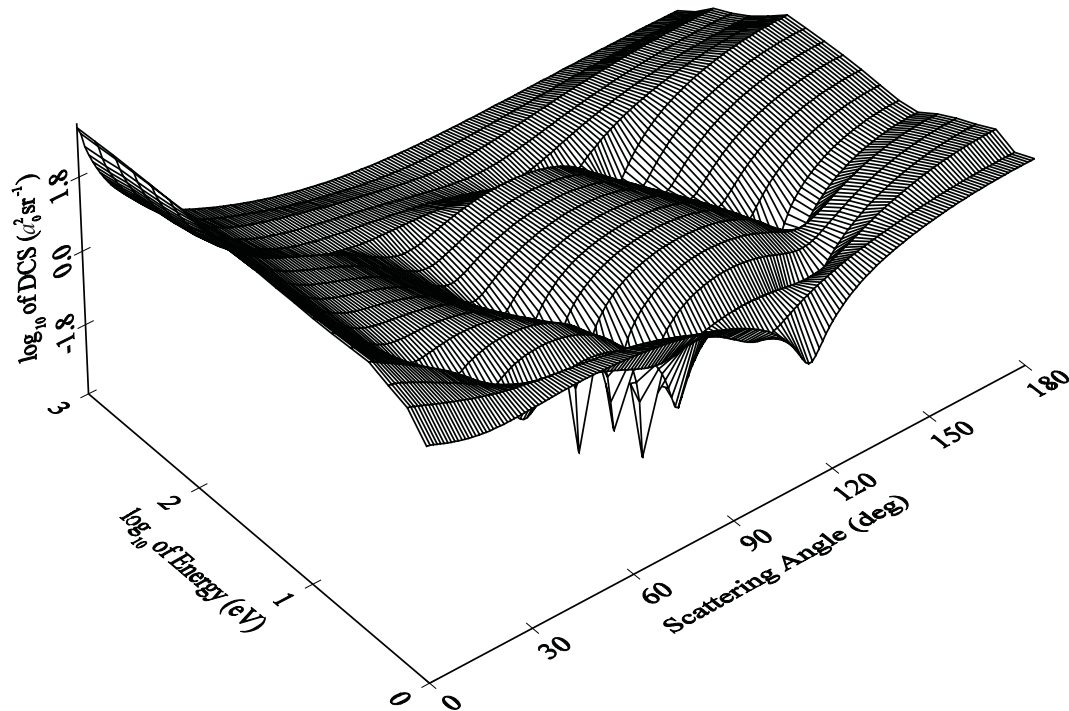


Figure 11. A three-dimensional view of differential cross section for elastic electron scattering from calcium.

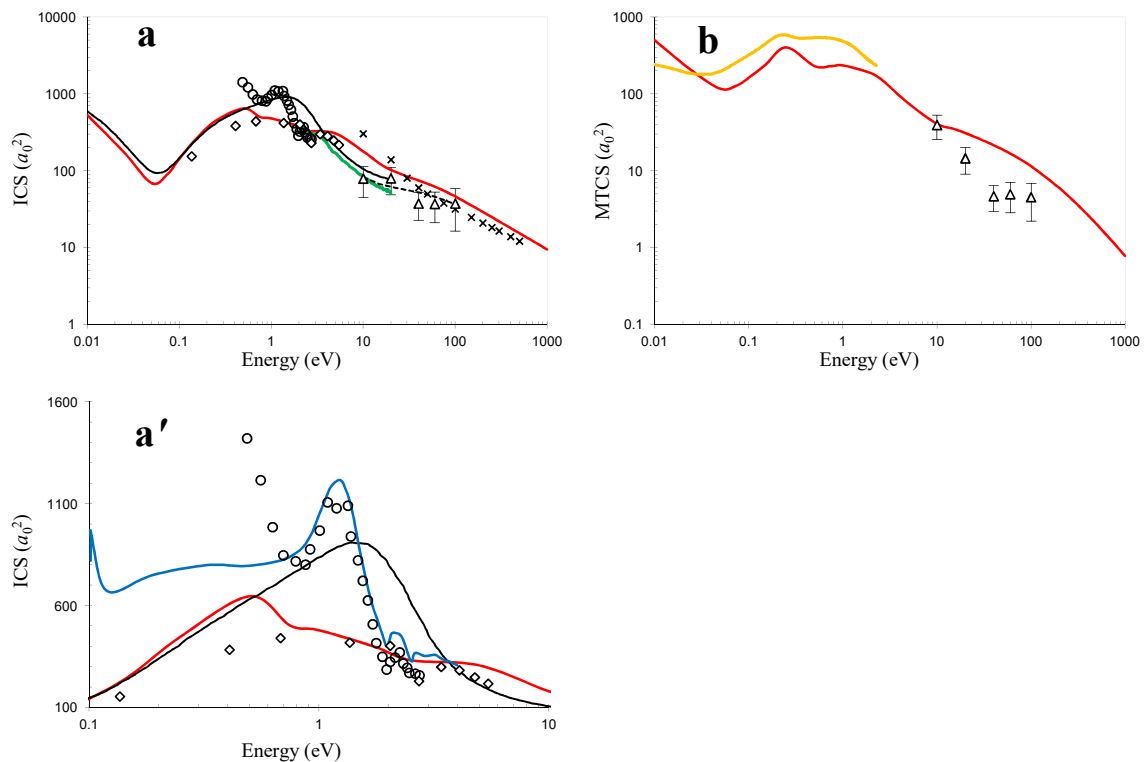


Figure 12. Integrated (a,a') and momentum transfer (b) cross sections for elastic electron scattering from calcium: red solid line, present work; Experimental data: $\circ$, Romanyuk et al. [38], $\triangle$, Milisavljević et al. [39]; Other theoretical: black solid line, Yuan [42]; $\diamond$, Fabrikant [10]; $\times$, Khare et al. [40], green solid line, BSR-438 data of Zatsarinny et al. [47], blue solid line, BSR-39 data of Zatsarinny et al. [46], amber solid line, Cribakin et al. [41], black dashed line, Wei et al. [48].

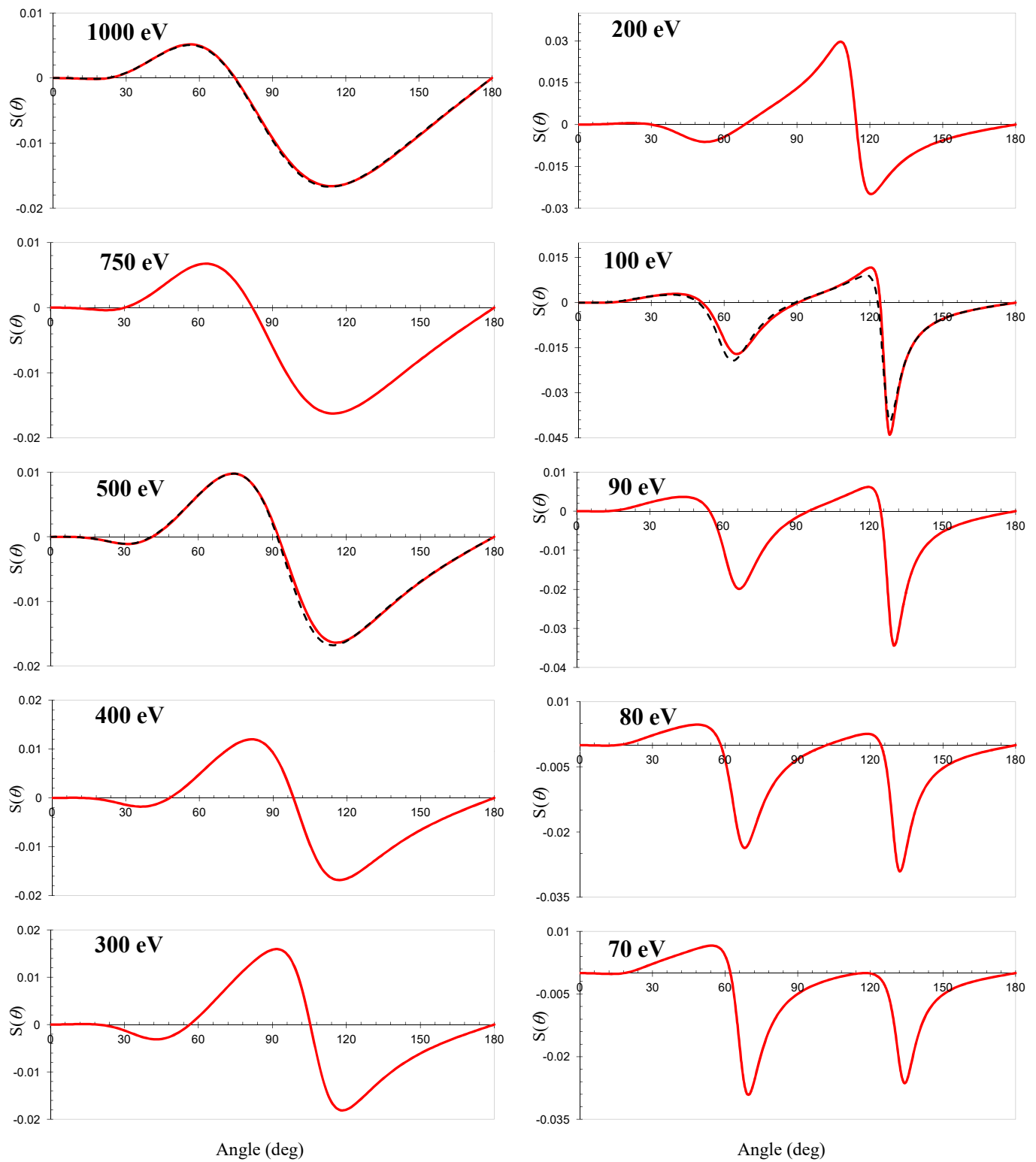


Figure 13. Sherman functions for elastic electron scattering from calcium at energies between 70 and 1000 eV: red solid line, present work; Other theoretical: black dashed line, Gregory and Fink [30].

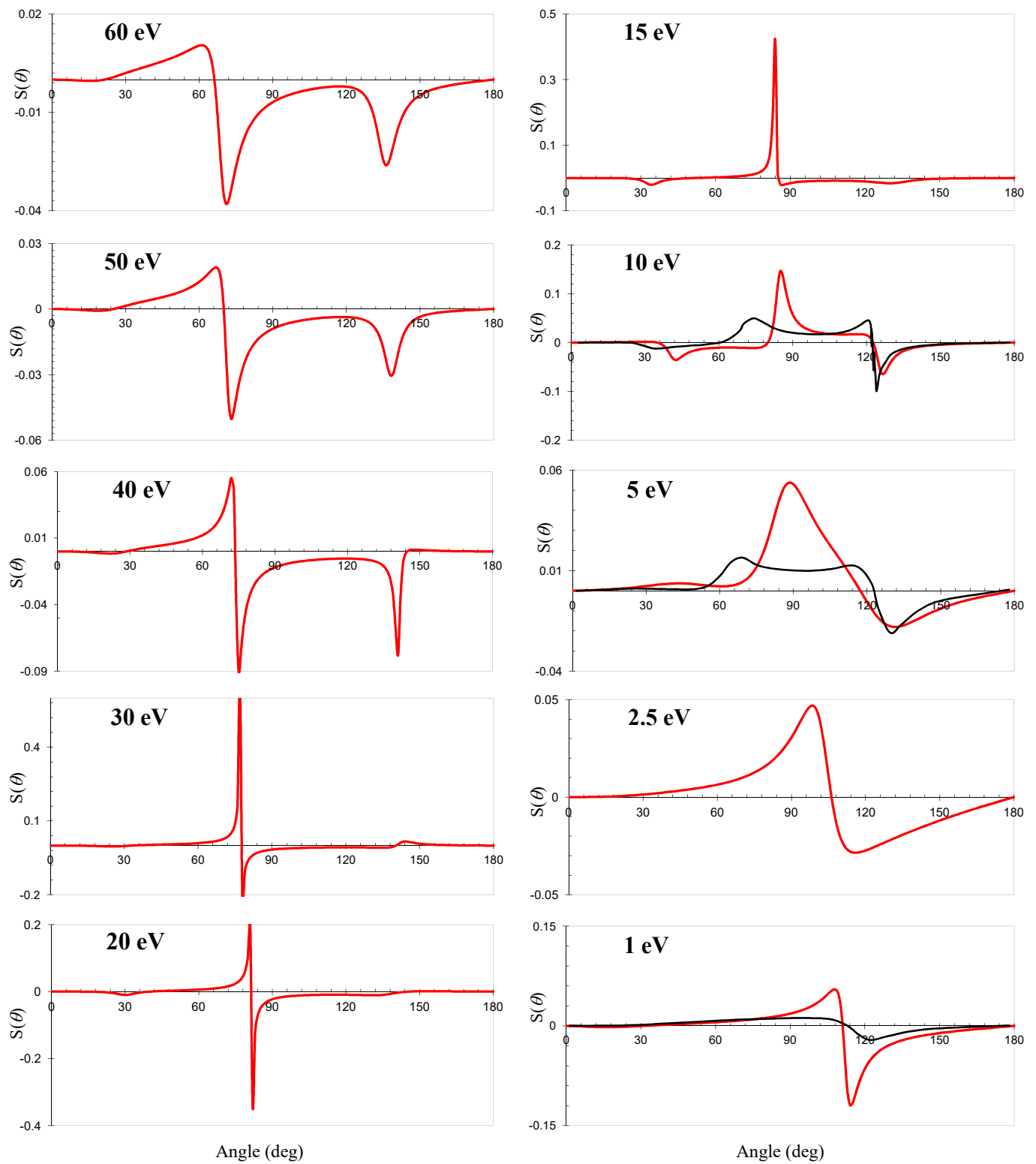


Figure 14. Sherman functions for elastic electron scattering from calcium at energies between 1 and 60 eV: red solid line, present work; Other theoretical: black solid line, Yuan [42].

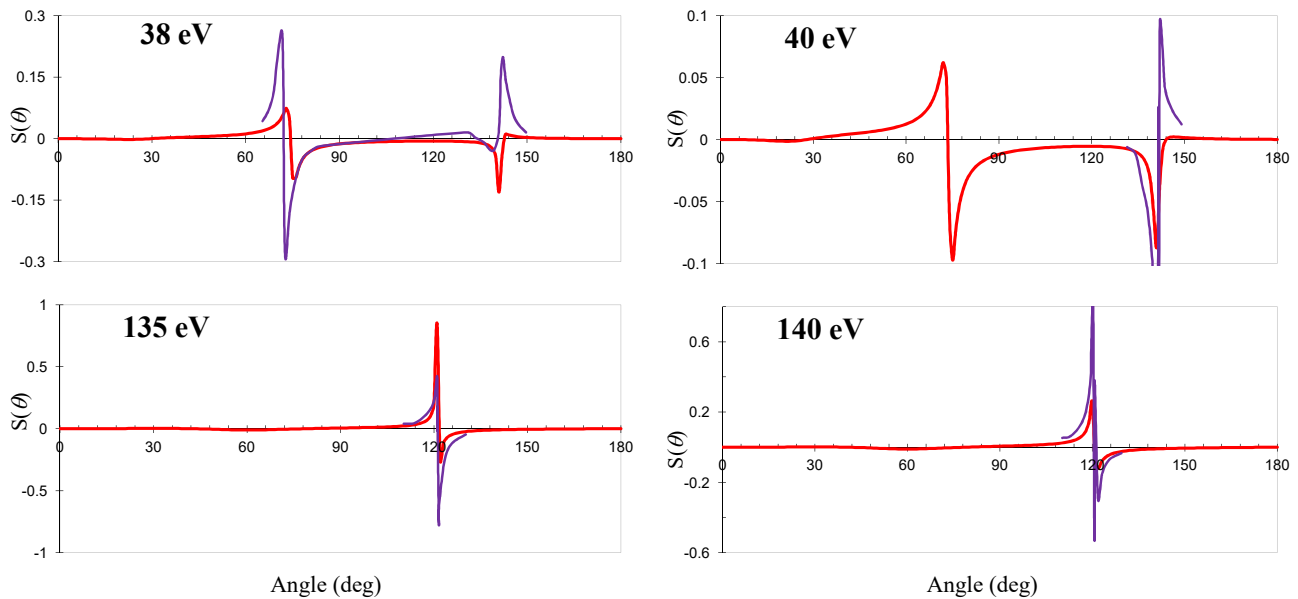


Figure 15. Comparisons of Sherman functions for elastic electron scattering from calcium at various energies: red solid line, present work; Other theoretical: purple solid line, Khare et al. [40].

3. Materials and Methods

The method of calculations of the present work is the same as that described in our previous papers [1,2], which can be consulted for more details. In summary, we followed the standard method of partial-wave expansion in potential scattering, where the phase shifts were obtained by solving the stationary Dirac equation. The choices for central static atomic, exchange, and polarization potential in Dirac Hamiltonian that were used in this work are the same as those of Ref. [1].

We arrived at that combination for potentials by exhaustive analysis and comparison with the collection of all appropriate experimental and theoretical works on elastic electron scattering by Ba and Sr (and previously by inert gases).

Through such analysis of the behavior of differential and integrated cross sections in response to several combinations of the components of the effective potential, we were able to find the best combination of the central static atomic, exchange, and polarization potentials that could produce a consistent agreement between the calculated cross sections and reliable experimental and theoretical results at different collision energies.

Although we have adopted the potential choices of Ref. [1] in this work, we applied the same methodology to Be, Mg, and Ca to confirm our choices and to obtain the only free parameter in this work: the cutoff radius of the polarization potential. This was carefully performed, in particular for beryllium, since its simple atomic structure warrants more elaboration in the choices we make for exchange and polarization potentials. At the end and for all three atoms, the Dirac-Slater atomic potential, the semi-classical exchange potential expression by Furness and McCarthy [49] and the Buckingham-type II polarization potential in the form

$$V_P(r) = -\frac{\alpha_d}{2(r^2 + r_c^2)^2}, \quad (1)$$

were used in the current work. In the above equation, α_d and r_c are the static atomic polarizability and the cutoff radius, respectively. The static polarizabilities used in polarization potential were taken from the theoretical values of Kolb et al. [50].

Similar to our previous works, to determine the cutoff radius, we demanded r_c to be a smooth, continuous, and finite function of the scattered electron energy E . We further confirmed the functional behavior of this energy-dependent cutoff radius to be similar to those we used for barium and strontium [1] through comparisons with dependable

theoretical and experimental data, as scarce as they are for Be, Mg, and Ca. Therefore, the cutoff radius for beryllium was assumed to be (in atomic units)

$$r_c(E) = \begin{cases} \frac{1}{3} \ln\left(\frac{E}{\mathcal{R}}\right) + \langle r \rangle_{2s} & E > 30 \text{ eV}, \\ 2.75 & E \leq 30 \text{ eV}, \end{cases} \quad (2)$$

for magnesium,

$$r_c(E) = \begin{cases} \frac{1}{3} \ln\left(\frac{E}{\mathcal{R}}\right) + \langle r \rangle_{3s} & E \geq 20 \text{ eV}, \\ 3.1 & E < 20 \text{ eV}, \end{cases} \quad (3)$$

and for calcium,

$$r_c(E) = \begin{cases} \frac{1}{3} \ln\left(\frac{E}{\mathcal{R}}\right) + \langle r \rangle_{4s} & E \geq 10 \text{ eV}, \\ 3.7 & E < 10 \text{ eV}. \end{cases} \quad (4)$$

Here E is the energy of the incident electron in eV, $\mathcal{R}$ is the Rydberg constant ($\mathcal{R} = 13.605\,691\,72 \text{ eV}$), and $\langle r \rangle_{2s} = 2.61 a_0$, $\langle r \rangle_{3s} = 3.12 a_0$ and $\langle r \rangle_{4s} = 3.98 a_0$ are the expectation values of the beryllium's 2s shell, magnesium's 3s shell, and calcium's 4s shell radii, respectively. The cutoff radii for low energies are set to constant values to avoid the anomaly caused by the logarithmic term. For more on this constant value and its behavior below an energy threshold, the reader may consult with Ref. [1]. That said, in the absence of experimental data for beryllium, the low energy constant value for r_c was determined through careful analysis and comparisons with accurate theoretical data for the integrated cross section.

In addition to cross section values, with the relativistic treatment, we are also able to compute the Sherman function, which describes the measured spin-up and spin-down asymmetries in the number of scattered electrons [51,52]. The present work only provides Sherman function values for calcium. Throughout this work and for all considered energies, we used up to 150 partial-wave phase shifts, which caused the last spin-up or spin-down phase shift to be less than 10^{-6} .

4. Conclusions

We now have extended our method of calculating elastic electron scattering for inert gases to all alkaline-earth-metal atoms. Our DCSs compared well with available experimental DCS data, which were available only for magnesium and calcium. The present ICS values also produced agreements and disagreements with experimental and other theoretical results, such as B-spline, CCC, and ROP calculations. We also studied the spin polarization of the scattered electrons from the calcium atom and gave Sherman functions for an extensive energy range. Comparisons between our Sherman functions and prior theoretical results generated mixed outcomes, which, in the absence of experimental data or other precise calculations, yield no final conclusion.

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