Distorted Wave Born and Optical Potential Calculation Methods for Electron-Sodium Elastic Scattering Cross-section at Intermediate Energies

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The first order distorted wave Born approximation (DWBA) and the optical potential (OP) method are systematically compared in the calculation of differential cross sections and integral cross sections in the elastic scattering of electrons by sodium atom at the intermediate energies range10 – 150eV using the same distorting potential. It is found that the difference between the two methods increases with a decrease in electron-impact energy and decreases as the distorting potential becomes more accurate. A comparison with available experimental and theoretical results shows the need to use a complex distorting potential to account for loss of flux in inelastic channels.

1. Introduction

Since the development of quantum mechanics close to a century ago, many attempts have been made to formulate quantum mechanical approaches for solving electron-atom scattering problems that yield results in agreement with experimental data, which have consistently been made available over a wide range of energies and for a variety of target atoms. These are broadly classified into perturbation methods based on Born approximation and non-perturbation methods based on close-coupling. Two perturbation approaches that have been developed are the first order distorted wave Born approximation (DWBA) and the optical potential (OP) method. These methods are capable of giving reliable scattering cross section data and require minimal computational resources.

The theoretical approach that has been widely used to study elastic scattering of electrons by atoms at the intermediate energy range above the ionization threshold of the atom is the OP method, which was first formulated by Mittlemann and Watson [1]. As noted by Yaqiu et al. [2], the most straight forward theoretical approach that has produced reliable results for inelastic processes is the DWBA method especially at high electron impact energies. Very few calculations for elastic scattering process have been made using the DWBA method. In using the DWBA method the form of distorting potentials adopted is vital and various formulations exist (Itikawa [3]). In principle, the choice of the distorting potential is rather arbitrary but various forms, such as the ground state average of the projectile – target potential, or a linear combination with the excited state average of the interaction potential, have been found to yield good agreement with experimental results. The DWBA method has an advantage over the OP method in that it can be used to study elastic as well as inelastic processes. However, for a given effective potential while the DWBA method is accurate to first order of perturbation theory, the OP method is valid to infinite order (Madison et al. [4]).

In this paper, we compare the OP and the DWBA methods in the problem of elastic scattering of intermediate energy electrons by the sodium atom. While the OP and DWBA methods have been widely applied in the study of elastic and inelastic scattering problems, respectively, there has been no systematic study to compare both these methods for the elastic scattering process in which both are applicable. Also alkali atoms, such as sodium and potassium, have a relatively simple atomic structure and are adequately described using the Hartree-Fock approximation. However, numerous theoretical approaches for calculation of scattering cross sections (Teubner et al., McCarthy et al., Mitroy et al., Balashov et al., Bray et al., Bray et al., Madison et al., Bray [5-12]) have yielded results that are not in complete agreement with absolute measurements (Teubner et al., Srivastava and Vuskovic, Allen et al., Marinkovic et al. [5,13-15]). This indicates the need for continued work to better understand how these

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atoms interact with energetic electrons especially at intermediate energies above the ionization threshold.

We have reformulated the polarization potential used previously to study noble gas atoms (Bartschat et al. [16,17]) and applied it to alkali atoms. In previous studies, the real part of the non-local polarization potential was found not to adequately describe the polarization process and was replaced by the local potential obtained using the polarized-orbital method. In the present study, we have used the real non-local polarization potential and since for alkali atoms inelastic processes play an important role in the scattering process above the ionization threshold, we have accounted for these processes using the local absorption potential of Staszewska et al. [18]

2. Theory

In the DWBA method, the transition matrix element [19] is given by

$$T^{DWBA}{}_{fi} = \left\langle \chi_f{}^{(-)}\varphi_f \left| U \right| \beta\varphi_i \right\rangle + \left\langle \chi_f{}^{(-)}\varphi_f \left| V - U \right| \mathrm{A}\chi_i{}^{(+)}\varphi_i \right\rangle \tag{1}$$

Where, $|\beta\rangle$ is the plane wave function of the incident electron, $|\chi_i{}^{(+)}\rangle\left(\ |\chi_f{}^{(-)}\rangle\right)$ is the initial (final) distorted wave of the projectile electron satisfying outgoing (incoming) spherical wave boundary conditions, $|\varphi_i\rangle\left(\ |\varphi_f\rangle\right)$ is the initial (final) target atom state, V is the electron-atom interaction potential, U is the distorting potential, and A is the anti-symmetrization operator. For elastic scattering $|\varphi_i\rangle = |\varphi_f\rangle = |\varphi\rangle$ and the first term in equation (1) corresponds to the transition matrix element in the OP method given as

$$T_{fi}{}^{OP} = \left\langle \chi_f{}^{(-)} \left| U \right| \beta \right\rangle \tag{2}$$

The differential cross section is given in terms of the transition matrix element by

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \frac{k_f}{k_i} \left| T_{fi} \right|^2 \tag{3}$$

Where, $k_f(k_i)$ is the final (initial) momentum (in atomic units) of the scattered electron. The integral cross sections is defined as follows

$$\sigma = \iint \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi \tag{4}$$

And, the total cross sections are obtained using the optical theorem

$$\sigma = -(2/k_i)(2\pi)^3 \ \mathrm{Im}\, T_{00} \tag{5}$$

In coordinate representation

$$\langle r|\beta\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{k_i r} \sum_{l_i m_i} i^l f_{l_i}(k_i, r) Y_{l_i m_i}(\hat{r}) Y^*{}_{l_i m_i}(\hat{k}_i) \tag{6}$$

$$\left\langle r \left| \chi_f{}^{(-)} \right\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{r} \sum_{l_f m_f} i^{l_f} e^{-i\delta_{l_f}} \chi_{l_f}(k_f, r) Y_{l_f m_f}(\hat{r}) Y^*{}_{l_f m_f}(\hat{k}_f) \right. \tag{7}$$

and

$$\left\langle \chi_f{}^{(-)} \right| r \rangle = \sqrt{\frac{2}{\pi}} \frac{1}{r} \sum_{l_f m_f} i^{-l_f} e^{i\delta_{l_f}} \chi_{l_f}(k_f, r) Y^*{}_{l_f m_f}(\hat{r}) Y_{l_f m_f}(\hat{k}_f) \tag{8}$$

Where, f_l are the regular Ricatti-Bessel functions and χ_l are radial distorted (partial) waves, which satisfy the Schrödinger equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + 2\left(E - V_{opt}\right) \right] \chi_l = 0 \tag{9}$$

And $E = k^2/2$ is the energy of the incident electron. In Eqn. (9) $V_{opt} \equiv U$ is the complex non-local optical potential given by

$$V_{opt}\chi_l = V_{st}(r)\chi_l + V_{ex}(r)\chi_l + V_{pol}(r)\chi_l + iV_{abs}(r)\chi_l \tag{10}$$

In Eqn. (10), V_{st} is the static potential

$$V_{st}(r) = \langle 0|V|0\rangle = -\frac{Z}{r} + \sum_{n_a l_a} 2(2l_a + 1) \int_0^\infty dr' \frac{P_{n_a l_a}{}^2(r')}{r_>} \tag{11}$$

Where, V_{ex} is the Furness-McCarthy [20] exchange potential

$$V_{ex}(r,E)=$$
$$\frac{1}{2}\left\{(E-V_{st}(r))-\left[(E-V_{st}(r))^2+4\pi\rho(r)-(-1)^S 2R_j^2\right]^{\frac{1}{2}}\right\} \quad (12)$$

The third and fourth terms are the non-local polarization and absorption potentials [16] given, respectively, as

$$V_{pol}(r)\chi_l+iV_{abs}(r)\chi_l= -2\sum_{n\neq 0}V_{on}(r)\int_0^\infty dr' G_0^{(+)}(\bar{k};r,r')\,V_{no}(r')\chi_l(k,r') \quad (13)$$

Eqn. (13) implies a sum over all the discrete intermediate states of the target atom and integration over the continuum states of the atom, whereas the complex free particle Green's function $G_o^{(+)}(\bar{k},r,r')$ is given in terms of the regular and irregular Ricatti-Bessel functions f_l and g_l by

$$G_0^{(+)}(\bar{k};r,r')=\frac{1}{\bar{k}}f_l(\bar{k}r_<)\left[g_l(\bar{k}r_>)+if_l(\bar{k}r_>)\right] \quad (14)$$

Further, $\bar{k}=\left[k^2-2\Delta\right]^{\frac{1}{2}}$, where for discrete states Δ is the energy gap between the ground and nth excited (intermediate) state. In Eqn. (13) $V_{on}(r)$ is the direct coupling matrix element defined by

$$V_{on}(r)=\langle 0|V|n\rangle \quad (15)$$

The interaction potential V is

$$V=-\frac{Z}{r}+\sum_{i=1}^{N}\frac{1}{|r_i-r|} \quad (16)$$

For single determinant atomic wave functions the direct matrix element reduces to the matrix element of V between the initial $|\alpha\rangle$ and $|\beta\rangle$ final states of the active target electron are

$$V_{on}(r)=\left\langle\alpha\left|\frac{1}{|r-r'|}\right|\beta\right\rangle \quad (17)$$

Then, coupling the angular momenta of the active target electron and that of the scattered electron, we write

$$|\alpha\rangle=|n_\alpha l_\alpha m_\alpha l_i m_i\rangle \quad (18a)$$

$$|\beta\rangle=|n_\beta l_\beta m_\beta l_f m_f\rangle \quad (18b)$$

And, using

$$\frac{1}{|r-r'|}=\sum_{\lambda\mu}\frac{r_<^\lambda}{r_>^{\lambda+1}}(-1)^\mu C_\mu^\lambda(\hat{r})C_{-\mu}^\lambda(\hat{r}') \quad (19)$$

Eqn. (17) becomes

$$V_{on}(r)=\int_0^\infty dr'\frac{r_<^\lambda}{r_>^{\lambda+1}}P_{n_\alpha l_\alpha}(r')P_{n_\beta l_\beta}(r')\times\sum_{\lambda\mu}(-1)^\mu\int d\hat{r}Y^*{}_{l_f m_f}(\hat{r})C_{-\mu}^\lambda(\hat{r})Y_{l_i m_i}(\hat{r})\int d\hat{r}'Y^*{}_{l_\beta m_\beta}(\hat{r}')C_\mu^\lambda(\hat{r}')Y_{l_\alpha m_\alpha}(\hat{r}') \quad (20)$$

Now using

$$\begin{aligned}\sum_\mu(-1)^\mu\int d\hat{r}Y^*{}_{l_f m_f}(\hat{r})C_{-\mu}^\lambda(\hat{r})Y_{l_i m_i}(\hat{r})\int d\hat{r}'Y^*{}_{l_\beta m_\beta}(\hat{r}')C_\mu^\lambda(\hat{r}')Y_{l_\alpha m_\alpha}(\hat{r}')&=\sum_\lambda\left\langle l_f l_\beta m_f m_\beta\left|C^\lambda\cdot C^\lambda\right|l_i l_\alpha m_i m_\alpha\right\rangle\\ &=\sum_{J'M'}\sum_{JM}C^{J'M'}_{l_f l_\beta m_f m_\beta}C^{JM}_{l_i l_\alpha m_i m_\alpha}\delta_{J'J}\delta_{M'M}(-1)^{l_i+l_\beta+J}[J]^{1/2}\begin{Bmatrix}l_f & l_\beta & J\\ l_\alpha & l_i & \lambda\end{Bmatrix}\\ &\times(-1)^{l_f}[l_f,l_i]^{1/2}(-1)^{l_\beta}[l_\beta,l_\alpha]^{1/2}\begin{pmatrix}l_f & \lambda & l_i\\ 0&0&0\end{pmatrix}\begin{pmatrix}l_\beta & \lambda & l_\alpha\\ 0&0&0\end{pmatrix}\end{aligned} \quad (21)$$

Where, C^λ is a spherical tensor operator. And, since $l_\alpha=0, m_\alpha=0$ for the valence electron in alkali atoms, we have

$$\begin{Bmatrix}l_f & l_\beta & J\\ l_\alpha & l_i & \lambda\end{Bmatrix}=\delta(l_f l_\beta J)\delta_{l_\beta\lambda}\delta_{l_i J}\frac{(-1)^{l_f+l_\beta+J}}{[l_\beta,J]^{1/2}} \quad (22)$$

Eqn. (21) then becomes

$$\sum_{\lambda}\left\langle l_f l_\beta m_f m_\beta \left| C^{\lambda}\cdot C^{\lambda}\right| l_i l_\alpha m_i m_\alpha \right\rangle = \sum_{JM} C^{JM}_{l_f l_\beta m_f m_\beta} C^{l_i m_i}_{l_i 0 m_i 0}\delta_{Jl_i}\delta_{Mm_i}(-1)^{l_i+l_\beta} \times\left[l_f, l_i\right]^{1/2}\begin{pmatrix} l_f & l_\beta & l_i \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_\beta & l_\beta & 0 \\ 0 & 0 & 0\end{pmatrix}\delta\left(l_f l_\beta J\right)\delta_{l_\beta\lambda}\delta_{l_i J} \quad (23)$$

Writing

$$F^{\lambda}_{n_\alpha l_\alpha n_\beta l_\beta}(r)=\int_0^\infty dr'\frac{r_<^{\lambda}}{r_>^{\lambda+1}}P_{n_\alpha l_\alpha}(r')P_{n_\beta l_\beta}(r') \quad (24)$$

And, using Eqns. (23) and (24) in (20) we obtain

$$V_{on}(r)=F^{l_\beta}_{n_\alpha l_\alpha n_\beta l_\beta}(r)\sum_{m_i} C^{l_i m_i}_{l_f l_\beta m_f m_\beta}(-1)^{l_i+l_\beta}\left[l_f, l_i\right]^{1/2}\begin{pmatrix} l_f & l_\beta & l_i \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_\beta & l_\beta & 0 \\ 0 & 0 & 0\end{pmatrix}\delta\left(l_f l_\beta l_i\right) \quad (25)$$

Finally, applying the orthogonality property of Clebsch-Gordan coefficients we get

$$V_{on}(r)V_{n0}(r')=F^{l_\beta}_{n_\alpha l_\alpha n_\beta l_\beta}(r)F^{l_\beta}_{n_\alpha l_\alpha n_\beta l_\beta}(r')\frac{1}{2l_f+1}\sum_{l_f=|l_\beta-l_i|}^{l_\beta+l_i}\left[l_f, l_i\right]\begin{pmatrix} l_f & l_\beta & l_i \\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix} l_\beta & l_\beta & 0 \\ 0 & 0 & 0\end{pmatrix}^2 \quad (26)$$

The polarization potential of the sodium atom is dominated by excitation to the 3^2P state and consequently we have included only a few low-lying states, 3^2P, 3^2D, 4^2P, and 4^2S, to obtain the polarization potential in Eqn. (13). However, since the imaginary part in Eqn. (13) converges slowly, we have replaced it by the absorption potential of Staszewska et al. [18], version 2, to take into account excitation to discrete states as well ionization of the target atom. For the Δ parameter in the absorption potential, we have used the average of the energy gap between the first excited state and the ground state and the ionization potential of the sodium atom thus

$$\Delta=\left(E_{3p}-E_{3s}+I_{pot}\right)/2 \quad (27)$$

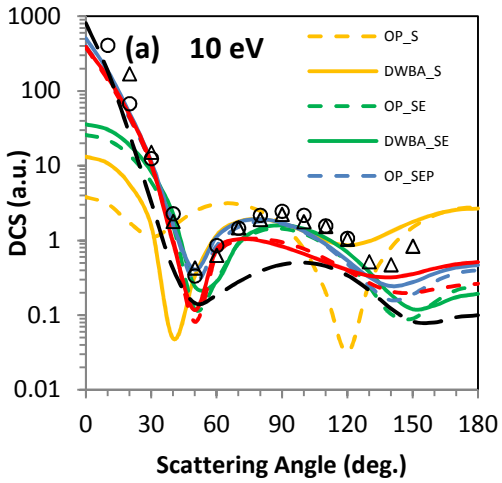
3. Results and Discussion

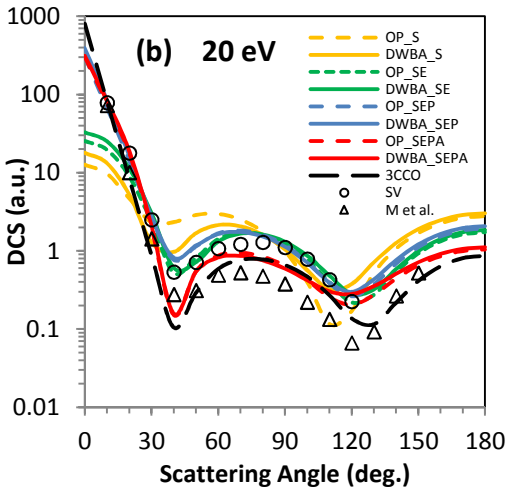
The present differential cross sections for elastic scattering of electrons by sodium atom are given in Fig. 1. The present OP and DWBA calculations are carried out using the static (S), static-exchange (SE), static-exchange-polarization (SEP), and static-exchange-polarization-absorption (SEPA) potential.

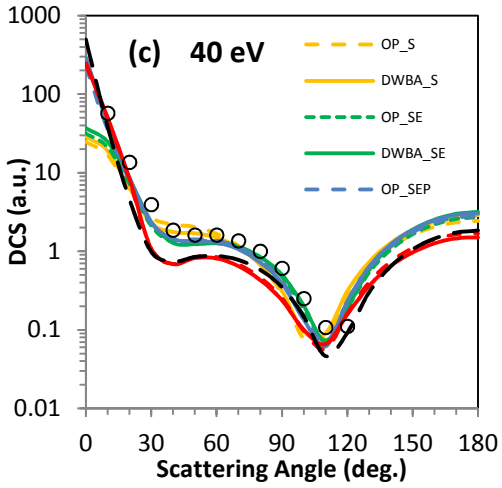
At 10eV, the present DWBA_S differential cross section results at intermediate scattering angles are in better agreement with the experimental results of Srivastava and Vuskovic [13] as compared to the present OP_S results since the DWBA_S calculation includes exchange effects in the form of the exchange T-matrix element. The present DWBA_SE and OP_SE results are in qualitative agreement indicating that the exchange potential, which has been used in both calculations, has a significant effect in accounting for the exchange process. Inclusion of the polarization potential has a large effect on the differential cross sections particularly at small scattering angles as can be seen in the present DWBA_SEP, and OP_SEP results. The present DWBA_SEPA and OP_SEPA results are in very close agreement with each other indicating that as the potential becomes more accurate the extra terms in the DWBA transition matrix element become less significant. The present result obtained using a static-exchange-polarization potential tend to give the best agreement with the experimental results of Srivastava and Vuskovic [13] and Marinkovic et al. [15]. The present results obtained using an absorption potential are generally higher than the results of Bray et al. [10].

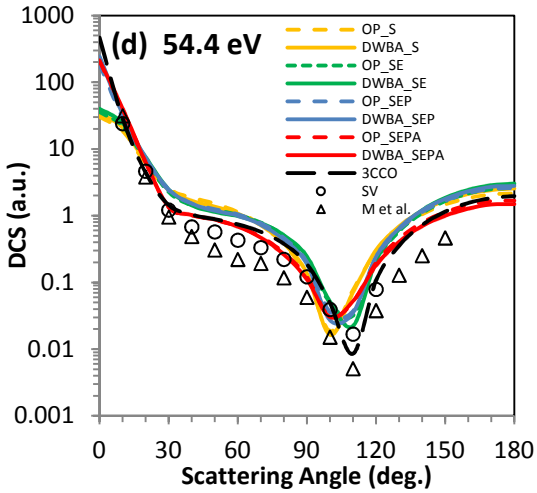
At 20eV, the present DWBA_S and OP_S differential cross sections are in better qualitative agreement with each other indicating that exchange effects become less significant as the electron impact energy increases. Inclusion of the exchange potential however gives DWBA_SE and OP_SE results that are in better agreement with the experimental results of Srivastava and Vuskovic [13] at intermediate scattering angles. With addition of the polarization potential, the DWBA_SEP and OP_SEP results are in very good agreement with the experimental results of Srivastava and Vuskovic [13] at all scattering angles, but are higher than the experimental results

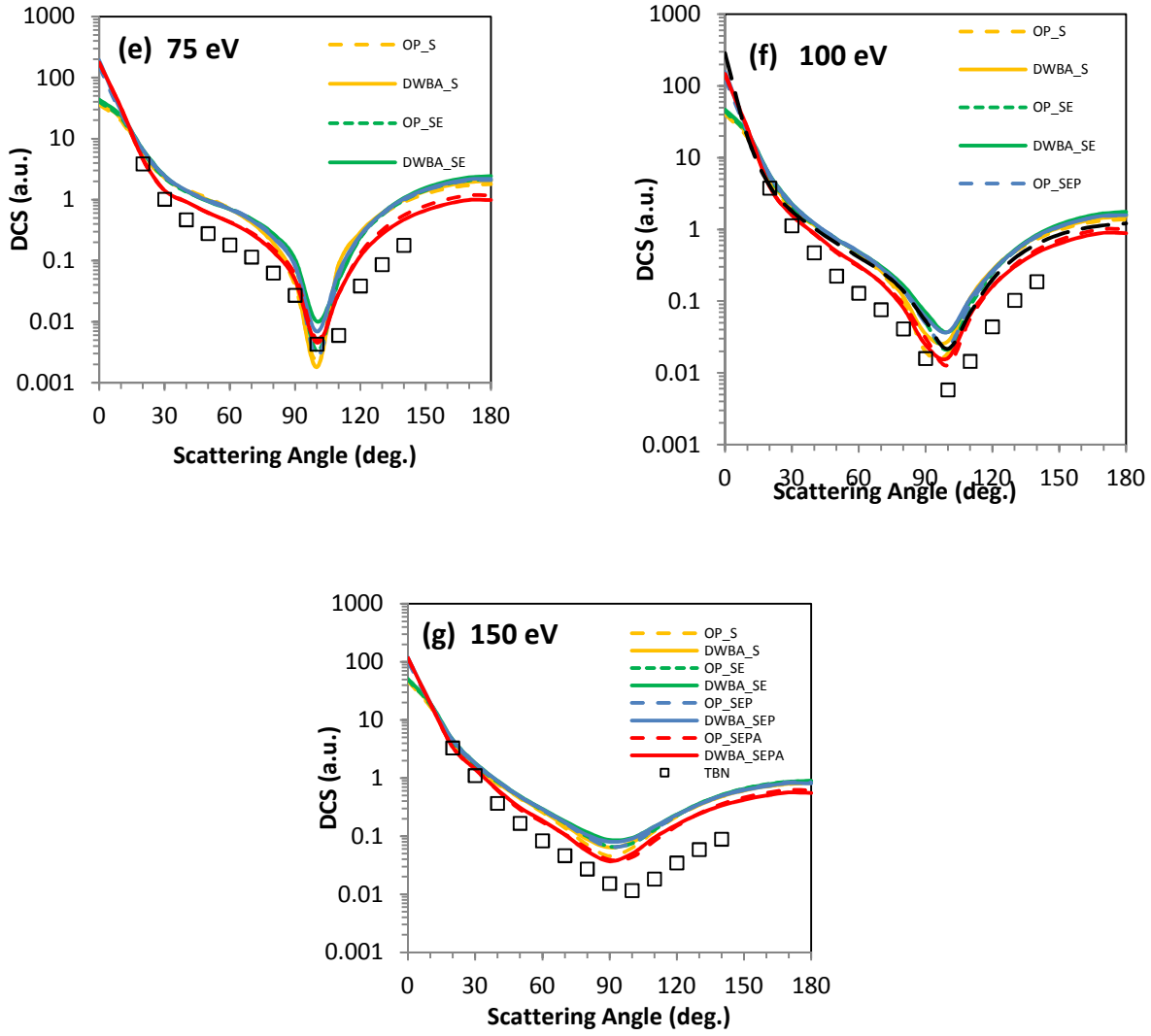
of Marinkovic et al. [15] at intermediate to large scattering angles. The inclusion of the absorption potential, which accounts for excitation and ionization of the target atom, leads to the DWBA_SEPA and OP_SEPA results that are in closer agreement with the experimental results of Marinkovic et al. [15] and the calculated results of Bray et al. [10].











Figures 1(a) – 1(g) show the differential cross sections for electron-sodium elastic scattering at 10–150eV.
Theory: OP, present optical potential calculation; DWBA, present first order distorted-wave Born approximation; 3CCO, coupled-channels optical calculation of Bray et al. [10].
Experiment: SV, Srivastava and Vuskovic [13]; TBN, Teubner et al. [5]; M et al., Marinkovic et al. [15].

At 40eV, the six sets of present results without absorption are in close agreement with each other at intermediate to large scattering angles, but at small angles the DWBA_SEP and OP_SEP results are significantly larger due to the polarization potential that greatly influences small angle scattering. The results are also in close agreement with the experimental results of Srivastava and Vuskovic [13]. This would suggest that absorption effects are not important at this energy. However, inclusion of the absorption potential gives DWBA_SEPA and OP_SEPA results which together with the theoretical results of Bray et al. [10] seem to suggest otherwise.

Fig. 1(d) shows the present results at 54.4eV. The SEPA results give the closest agreement with the experimental results of Srivastava and Vuskovic [13] but are appreciably higher than the experimental data of Marinkovic et al. [15] especially at large scattering angles. If we assume that the experimental results of Marinkovic et al. [15] are correct, then this implies that the absorption potential does not adequately account for inelastic processes at this energy. Alternatively the experimental results could suffer from systematic errors.

In Fig. 1(e) we see that at 75eV the present results without absorption are very close for intermediate to large scattering angles but at small angles the SEP results are larger due to the effect of the polarization potential. As expected, the SEPA results are lower than the results obtained without

absorption but are slightly higher than the experimental differential cross section results of Teubner et al. [5]. The situation at 100eV and 150eV is very similar, as shown in Figs. 1(f) and 1(g). An exact treatment of the non-local absorption potential including discrete and continuum states would most likely improve the agreement with experimental data at these high energies. However, more experimental results are desirable in order to reach an objective conclusion.

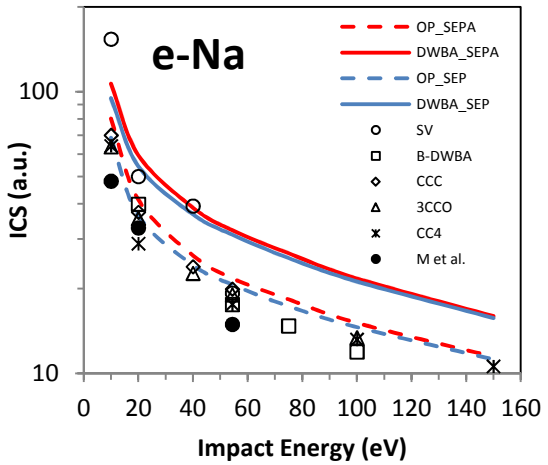


Fig.2: Integral Cross Sections for elastic scattering of electrons by Sodium atom at 10 - 150 eV electron impact energies.
Theory: OP, present optical potential method, DWBA, present first order distorted-wave Born approximation, B-DWBA, distorted wave Born approximation of Balashov et al. [8]; 3CCO, 3-state coupled channels optical method [10]; CCC, convergent close-coupling method [12]; CC4, 4-state close-coupling approximation [7].
Experiment: SV, Srivastava and Vuskovic [13].

Fig. 2 shows the integral (total elastic) cross sections obtained using the SEP and the SEPA potentials for both the OP and DWBA calculations. For the OP_SEP method agreement with the CC4 [7], B-DWBA [8], 3CCO [10], and CCC [12], calculations is very good. This indicates that the polarization potential used in the present calculations is quite accurate as this potential affects small-angle scattering significantly. The DWBA_SEP method yields higher ICS results at all electron-impact energies considered due to the additional direct and exchange terms in the T-matrix element. The present DWBA_SEP results are in good agreement with the experimental results of Srivastava and Vuskovic [13] at 20 and 40eV but not at 10 and 54.4eV. As expected, the effect of the absorption potential on the total elastic cross sections is small. In figure 3, the present grand total (elastic + inelastic) cross sections at 10 -150eV obtained using the SEPA potential are shown. These results are seen to be significantly lower than earlier theoretical and experimental results at all electron impact energies considered. This suggests that the absorption potential used in the present calculations does not adequately describe small-angle scattering that leads to lower total cross sections.

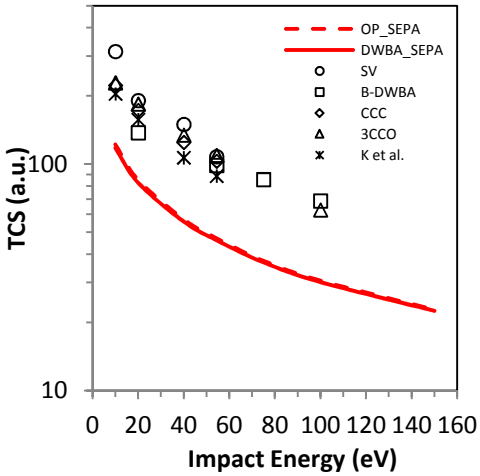


Fig.2: Total Cross Sections for elastic scattering of electrons by Sodium atom at 10 - 150 eV electron impact energies.
Theory: OP, present optical potential method, DWBA, present first order distorted-wave Born approximation, B-DWBA, distorted wave Born approximation of Balashov et al. [8]; 3CCO, 3-state coupled channels optical method [10]; CCC, convergent close-coupling method [12].
Experiment: SV, Srivastava and Vuskovic [13]; K et al., Kwan et al. [21].

4. Conclusions

We have compared the first order distorted wave Born approximation and the optical potential method in calculation of electron-sodium elastic scattering at intermediate energies using various levels of approximation for the distorting/effective potential. The difference between the two methods is significant at low energies, especially when the exchange potential is not included, but decreases as the accuracy of the potential improves. Use of the exact non-local absorption potential including all discrete and continuum states is likely to improve agreement with experiment and we intend to carry out such calculations in the future. To this end, more experimental data for comparison with theoretical calculations, especially at high energies, is desirable.

Acknowledgements

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