Polarization effect in (e, 2e) reaction process for Ar (3s) in coplanar asymmetric geometry*

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The (e, 2e) triple differential cross sections (TDCSs) of Ar (3s) are calculated by using distorted-wave Born approximation under coplanar asymmetric geometry. The incident electron energy is 113.5 eV, and the scattering electron angle θ_1 is -15°. The ejected electron energy is set at 10 eV, 7.5 eV, 5 eV, and 2 eV, respectively. The polarization effects have been discussed and the polarization potential $V_{\rm pol}$ changing from a second-order to a fourth-order term has been analyzed. Our calculated TDCSs have been compared with reported experimental and theoretical results, and the calculated TDCSs of polarization potential up to the fourth order could give a good fit with experimental results in the binary region, but fail to predict the correct recoil-to-binary ratio in most cases.

Keywords: (e, 2e) reaction, distorted-wave Born approximation, triple differential cross sections, polarization effect

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1. Introduction

The single ionization of atom and molecule by electron impact is well known as the (e, 2e) coincidence technique. The triple differential cross section (TDCS) of the (e, 2e) reaction can provide abundant information about the target structure and the complex dynamic interaction involved in a collision. Up to now, a large number of (e, 2e) reactions have been studied, including hydrogen,[1,2] inert gas atoms,[2–6] alkali and alkali earth atomics,[6–8] biological macromolecules,[9,10] atoms on the surface,[11] etc. According to research purposes (structural or dynamic analyses), researchers designed different measurement geometries. Among them, coplanar asymmetrical geometry is a common choice in (e, 2e) dynamic research. Under this geometry, the incident electron, scattering electron and ejected electron are in the same geometric plane. The angle of scattering electron is fixed, and the TDCSs of (e, 2e) reaction is detected at different angles of the ejected electron. The theory of plane wave impulse approximation is in good accordance with the experimental results at high incident electron energy, but with low incident electron energy, some effects ignored under high incident electron energy become very important, such as the distorted wave effect, exchange effect, polarization effect, post collision interaction (PCI), etc. It is a great challenge for theory to obtain an accurate description of TDCS's under low incident electron energy.[12–16] Among various theoretical methods, distorted-wave Born approximation (DWBA) is a widely used theory to deal with (e, 2e) reaction. In this method, two effects, i.e., polarization and PCI, could be added to improve the accordance between experimental and theoretical results under low incident electron energy.[4,5,12–15]

As is well known, the PCI and polarization effects play important roles in the study of electron–atom scattering.[4,5,12–15] The DWBA calculations including PCI of some inert gas atoms indicated the theoretical results have relatively good accordance with experimental data.[4,5] The polarization effect is commonly considered by adding polarization potential $V_{\rm pol}$ on the distorting potential, and $V_{\rm pol}$ approximately equals the first item of the second-order perturbation expansion formula, which has been used in most treatments.[8,15] However, this method fails to represent the true short-range behavior of the full effective potential since they diverge at the origin.[16] In order to correct this deviation, some methods have been proposed. Gianturco *et al.* presented two kinds of polarization potential.[16,17] One of them was obtained from a semiclassical perturbation model and several damping functions were devised, and they calculated the integral and differential elastic cross sections for Ne and Ar targets using this method.[16] The other was obtained via the density functional theory.[17] Hu *et al.*[13,18] used such a model in the near-target region to calculate the TDCS's of Ar (3s, 2p), and their calculations improve the accordance between calculation and experimental results. In 2009, Purohit *et al.*[12] reported their calculation of TDCS's of Ar (3s) using a modified DWBA theory, and they called it DWBACPE (distorted wave Born approximation with exchange including correlation-polarization potential). In the near target region, this DWBACPE theory includes a correlation polarization potential which is a function of the electron density parameter. The calculated results of DWBACPE show a better agreement with experimental results in comparison to the standard DWBA calculation. All the research on the polarization effect

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showed its importance in the (e, 2e) reaction.

As for Ar (3s), aside from the above studies on the polarization effect, a DWB2-2st-MC (DWB2-second order distorted wave Born approximation; 2st-2 states; MC-multi-configuration) calculation was carried out by Bartschat *et al.* to study the target structure, channel coupling, and nonlocal exchange in an (e, 2e) reaction.[14] These calculated results improved the agreement between theoretical and experimental results. However, there were still some discrepancies between these theoretical results and the experimental results.

In this paper, we further investigate the polarization effect in the (e, 2e) reaction of Ar (3s). Based on the experimental conditions reported by Haynes and Lohmann,[19,20] we calculated the (e, 2e) TDCSs of Ar (3s) using DWBA theory under coplanar asymmetric geometry. The incident electron energy is 113.5 eV, and the scattering electron angle is set at $\theta_1 = -15^\circ$. The ejected electron energy is set at 10 eV, 7.5 eV, 5 eV, and 2 eV, respectively. Here, we use the $V_{\rm pol}$ obtained from the semiclassical perturbation model proposed by Gianturco *et al.*[16] to study the polarization effect under low incident electron energy, and the polarization potential $V_{\rm pol}$ changing from second-order to fourth-order term has been analyzed. Our calculated TDCSs have been compared with experimental[19,20] and some theoretical results,[12–14] such as calculations using the DWBACPE,[12] DWBA calculations using polarization potential via DFT,[13] and the DWBA results using DWB2-2st-MC.[14] Our calculated results show that the present DWBA calculation under the fourth-order potential can improve the accordance with experimental data in the binary region.

2. Theory

Considering an atom target ionized by an incident electron with momentum k_0 followed by two outgoing electrons with momenta k_1 and k_2, the TDCS for such a process could be described by DWBA theory as follows:[21]

$$\frac{{\rm d}^3\sigma^{\rm DWBA}}{{\rm d}\Omega_1\,{\rm d}\Omega_2\,{\rm d}E_1} = (2\pi)^4\frac{k_1k_2}{k_0}\sum_{\rm av}\left[|f|^2+|g|^2-{\rm Re}(f^*g)\right], \quad (1)$$

$$f = \left\langle \chi^{(-)}(k_1,r_1)\chi^{(-)}(k_2,r_2)\left|\frac{1}{r_{12}}\right|\chi^{(+)}(k_0,r_0)\psi_{nl}\right\rangle, \quad (2)$$

$$g = \left\langle \chi^{(-)}(k_1,r_2)\chi^{(-)}(k_2,r_1)\left|\frac{1}{r_{12}}\right|\chi^{(+)}(k_0,r_0)\psi_{nl}\right\rangle, \quad (3)$$

where $\sum_{\rm av}$ represents the sum over final and average over the initial magnetic and spin degeneracy, ψ_{nl} is the orbital of the target, $\chi^{(+)}$ denotes the distorted wave of incident electron generated in the equivalent local ground state potential $V_{\rm D}$ of an atom, and $\chi^{(-)}$ is the distorted wave of outgoing electrons generated in the equivalent local ground state potential of an ion; $\chi^{(+)}$ and $\chi^{(-)}$ are both orthogonal to ψ_{nl}. The equivalent local ground state potential $V_{00}(r)$, i.e., distorting potential, is the sum of direct potential $V_{\rm D}$ and exchange potential $V_{\rm E}$. The direct potential $V_{\rm D}$ is obtained from the target radial orbital $u_{nl}(r)$[21]

$$V_{\rm D}(r) = \sum_{nl}N_{nl}\int {\rm d}r'[u_{nl}(r')]^2/r_>, \quad (4)$$

where $r_>$ is the greater one between r and r', and N_{nl} is the electron number of orbital ψ_{nl}. The spin average static exchange potential $V_{\rm E}$ is given by[22]

$$V_{\rm E}(r) = 0.5\left\{E - V_{\rm D}(r) + \frac{3}{10}[3\pi^2\rho(r)]^{2/3}\right\} - 0.5\left\{\left[E - V_{\rm D}(r) + \frac{3}{10}[3\pi^2\rho(r)]^{2/3}\right]^2 + 4\pi\rho(r)\right\}^{\frac{1}{2}}, \quad (5)$$

where $\rho(r)$ is the electron density. The equivalent distorting potential $V_{00}(r)$ could be described as

$$V_{00}(r) = V_{\rm D}(r) + V_{\rm E}(r). \quad (6)$$

Here, the effects of PCI and polarization are considered, respectively.

As to the effect of PCI on TDCS, it has been taken into account by multiplying a parameter $M_{\rm ee}$, defined as[23]

$$M_{\rm ee} = \frac{\pi\exp(-\pi/k_3)}{k_3\left[1-\exp(-\pi/k_3)\right]}\left|{}_1{\rm F}_1(-{\rm i}V, 1, -2{\rm i}k_3r_{3\rm ave})\right|^2,$$
$$V = -1/|\boldsymbol{k_1}-\boldsymbol{k_2}|,$$
$$k_3 = |\boldsymbol{k}_1-\boldsymbol{k}_2|/2,$$
$$r_{3\rm ave} = \frac{\pi^2}{16\varepsilon}\left(1+\frac{0.627}{\pi}\sqrt{\varepsilon}\ln\varepsilon\right), \quad (7)$$
$$\varepsilon = \left(k_1^2+k_2^2\right)/2. \quad (8)$$

Then, the TDCS can be described as

$$\frac{{\rm d}^3\sigma}{{\rm d}\Omega_1\,{\rm d}\Omega_2\,{\rm d}E_1} = M_{\rm ee}\frac{{\rm d}^3\sigma^{\rm DWBA}}{{\rm d}\Omega_1\,{\rm d}\Omega_2\,{\rm d}E_1}. \quad (9)$$

As to the effect of polarization on TDCS, it has been taken into account by the addition of polarization potential $V_{\rm pol}$ on $V_{00}(r) = V_{\rm D}(r) + V_{\rm E}(r)$ (Eq. (6)). The polarization potential $V_{\rm pol}$ is described as follows:[17,24]

$$V_{\rm pol}(r) = V_{\rm pol}^{(2)} + V_{\rm pol}^{(3)} + V_{\rm pol}^{(4)} + \cdots, \quad (10)$$

$$V_{\rm pol}^{(2)}(r) = -f_4(r)\frac{\alpha_{\rm D}}{2r^4} - -f_6(r)\frac{\alpha_{\rm Q}}{2r^6} - -f_8(r)\frac{\alpha_{\rm O}}{2r^8}, \quad (11)$$

$$V_{\rm pol}^{(3)}(r) = -f_6(r)\frac{B}{2r^7}, \quad (12)$$

$$V_{\rm pol}^{(4)}(r) = -f^{(4)}(r)\frac{\gamma}{24r^8}, \quad (13)$$

where

$$f_{2l+2}(r) = \frac{\int_0^r\rho(r_{\rm b})r_{\rm b}^{2l+2}{\rm d}r_{\rm b}}{\int_0^\infty\rho(r_{\rm b})r_{\rm b}^{2L+2}{\rm d}r_{\rm b}}, \quad (14)$$

$$f^{(4)}(r) = \frac{\int_0^r\rho(r_{\rm b})r_{\rm b}^6{\rm d}r_{\rm b} - \frac{40\pi}{9Z}\left[\int_0^r\rho(r_{\rm b})r_{\rm b}^4{\rm d}r_{\rm b}\right]^2}{\int_0^\infty\rho(r_{\rm b})r_{\rm b}^6{\rm d}r_{\rm b} - \frac{40\pi}{9Z}\left[\int_0^\infty\rho(r_{\rm b})r_{\rm b}^4{\rm d}r_{\rm b}\right]^2}. \quad (15)$$

The coefficients $\alpha_{\rm D}$, $\alpha_{\rm Q}$, and $\alpha_{\rm O}$ are the dipole, quadrupole, and octupole static polarisabilities of the target atom, re-

spectively. B and γ are the dipole–dipole–quadrupole and dipole–dipole–dipole–dipole hyperpolarisability of the target, respectively. For target atom Ar, α_D, α_Q, α_O, B, and γ are $11.1e^2a_0^2E_h^{-1}$, $48e^2a_0^4E_h^{-1}$, $418e^2a_0^8E_h^{-1}$, $-164.3e^3a_0^4E_h^{-2}$, and $1083e^4a_0^4E_h^{-3}$, respectively.[25,26] These Hartree atomic units e, a_0, and E_h have been shown in Table 1.

Table 1. Conversion factors from Hartree atomic units to SI units.[26]

Quantity	Atomic unit	SI equivalent
energy	E_h	$4.3597482 \times 10^{-18}$ J
distance	a_0	$5.29177249 \times 10^{-11}$ m
charge	e	$1.60217733 \times 10^{-19}$ C

3. Results and discussion

Figure 1 presents the (e, 2e) TDCSs of Ar (3s) under coplanar asymmetric geometry including our calculated results and reported experimental[19,20] and theoretical results.[12–14] In order to compare these results, the intensity of the binary peak in all theoretical and experimental results is normalized to unity. In this (e, 2e) reaction, the incident electron energy is set at 113.5 eV, and the scattering electron angle θ_1 is set at $-15°$. Figures 1(a)–1(d) illustrate the TDCSs with different ejected electron energy of 10 eV, 7.5 eV, 5 eV, and 2 eV, respectively. In our calculation (Eq. (10)), the TDCS's are calculated ignoring little perturbation item. In Figs. 1(a)–1(d), the solid curve, dashed curve, and dotted curve show our calculated results with different approximation up to the fourth order, second order and the first item of the second order in Eq. (10), respectively. Except these three curves, other curves present the reported DWBACPE calculations of Purohit *et al.* (dash-dotted),[12] DWBA calculations using polarization potential via the DFT of Hu *et al.* (dash-dot-dotted),[13] and the DWB2-2st-MC results of Bartschat *et al.* (short dashed).[14]

The calculated TDCSs of Ar (3s) with the ejected electron energy of 10 eV is shown in Fig. 1(a). From Fig. 1(a), it can be seen that the recoil-to-binary ratio of the experimental data

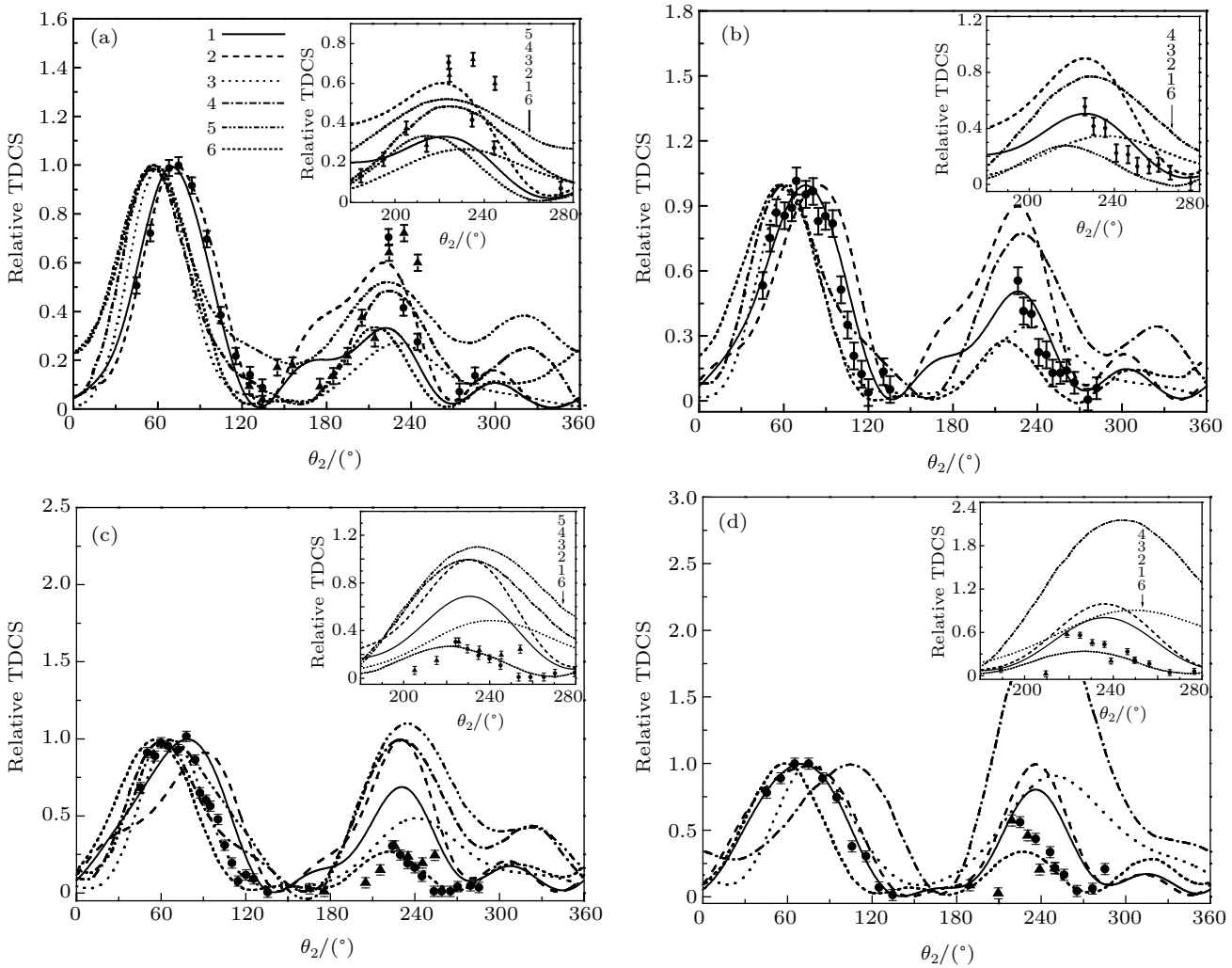


Fig. 1. TDCSs of Ar (3s) under coplanar asymmetric geometry with a scattering electron angle of $-15°$, incident electron energy of 113.5 eV, and different ejected electron energy: (a) 10 eV, (b) 7.5 eV, (c) 5 eV, (d) 2 eV. The solid circles and triangles are experimental data reported by Lohmann *et al.*[19,20] Solid curve (1): our DWBA calculation, polarization with contributions up to the fourth order. Dashed curve (2): our DWBA calculation, polarization with contributions up to the second-order potential. Dotted curve (3): our DWBA calculation, polarization with contributions to the first term of the second-order potential. Dash-dotted curve (4): DWBACPE calculations of Purohit *et al.*[12] Dash-dot-dotted curve (5): DWBA calculations using the polarization potential via DFT of Hu *et al.*[13] Short dashed curve (6): the DWB2-2st-MC results of Bartschat *et al.*[14]

is about 0.67, while the ratio of the theoretical results underestimated it on the whole. Our DWBA calculation with polarization potential up to the second order gives the best prediction of the recoil-to-binary ratio among all theoretical curves, which is about 0.6. As to the recoil peak and binary peak, all theoretical curves predict the position of the recoil peak quite well. Our calculations with the polarization potential up to the fourth-order potential and second-order potential with all three terms fit well with the experimental results in the binary peak region. The other four curves are incapable of correctly predicting the position of the binary peak.

Furthermore, it can be seen that there is a shoulder at $\theta_2 = 155^\circ$ in experimental TDCSs, and our calculation with the polarization potential up to the fourth order and the second order also show this shoulder, which suggests that the shoulder may be ascribed to the polarization effect. Theoretical lines exhibit another peak at about 300°, while the experimental data are lacking in this range. The shoulder at 300° may attribute to one kind of double-binary collision,[27,28] as shown in Fig. 2. In this double-binary collision, the incident electron is first scattered elastically off the nucleus, then collides with the orbital electron, and subsequently emerges at angle θ_1.

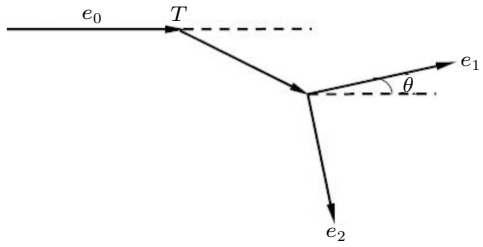


Fig. 2. One kind of double-binary collision process. T denotes the target nucleus.

The calculated TDCSs of Ar (3s) with an ejected electron energy of 7.5 eV is shown in Fig. 1(b). It can be seen that a well fitting with experimental data has been given by our DWBA calculation of the polarization potential up to the fourth order. Our DWBA calculation of the polarization potential up to the second order and DWBACPE calculation[12] both predict a larger recoil peak than experimental results, and other calculations give lower intensity than experimental results in the recoil peak region. As shown in Fig. 1(a), our calculations of the polarization potential up to the fourth order and second order show a shoulder between the binary and recoil peaks. However, there are no experimental data in this region to compare.

The calculated TDCSs of Ar (3s) with an ejected electron energy of 5 eV is shown in Fig. 1(c). The experimental recoil-to-binary ratio decreases to 0.3 at this ejected electron energy. The DWB2-2st-MC calculation[14] can give the best prediction of recoil-to-bianry ratio compared with other theoretical curves, but this method fails to predict the correct position of the binary peak. In the binary peak region, our DWBA calculation with the first item of the second-order potential fits well with experimental data both in position and intensity. Other theoretical curves cannot predict the correct position of the binary peak. In the region of the recoil peak, the DWB2-2st-MC calculation[14] gives the best fitting with experimental results, and other theoretical curves give a higher intensity than experimental results.

The calculated TDCSs of Ar (3s) with an ejected electron energy of 2 eV is shown in Fig. 1(d). It is worthwhile to see in the binary peak region that, there is a very good accordance of our DWBA calculation of the polarization potential up to the fourth order and the experimental result, but this theoretical curve gives a higher intensity in the region of the recoil peak. For the recoil-to-binary ratio, experimental data show it is 0.6, the present DWBA calculation result of the polarization potential up to the fourth order and the DWB2-2st-MC calculation predict it as 0.8 and 0.25 respectively, and these two theoretical curves approach the experimental results best compared with other theoretical calculations.

4. Conclusions

In this article, we calculate the (e, 2e) TDCSs of Ar (3s) using DWBA theory under coplanar asymmetric geometry. The incident electron energy was 113.5 eV, and the ejected electron energy is 10 eV, 7.5 eV, 5 eV, and 2 eV, respectively. The scattering electron angle θ_1 is set at -15°. The present calculations consider the polarization effect by adding a polarization potential $V_{\rm pol}$ on the distorting potential, and the polarization potential $V_{\rm pol}$ changing from the second-order to the fourth-order term (Eq. (10)) has been analyzed. Our calculated TDCSs of the different order polarization potential have been compared with reported experimental[19,20] and theoretical results.[12–14] We found that our DWBA calculation of the polarization potential up to the fourth order is able to improve the agreement with experimental data in the binary region, but fail to predict the correct recoil-to-binary ratio in most cases. The reported DWB2-2st-MC calculation, which treats the projectile–target interaction up to the second order, can give a better recoil-to-binary ratio. However, in most cases, it shows a little discrepancy in the position of the binary peak between theoretical and experimental results.[14] Moreover, our calculation up to the fourth-order polarization potential and other DWB1 (first-order-DWBA) calculations[14] can show that the shoulder between binary and recoil peaks at ejected electron energy equals 10 eV, while DWB2-2st-MC calculation cannot. The above discussion indicates that the second-order effect of the projectile-target interaction and the polarization effect are both important, and that further theoretical research may combine these two aspects.

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