Vol 13 No 11, November 2004
1009-1963/2004/13(11)/1857-05

Chinese Physics

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Theoretical calculation of triple differential cross sections of 3s orbital of argon in coplanar symmetric (e, 2e) reaction*

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(Received 27 February 2004; revised manuscript received 24 April 2004)

The triple differential cross section for the low-energy electron impact ionization of inner-valence 3s orbital of argon has been calculated using the modified distorted wave Born approximation in coplanar symmetric energy-sharing geometry. Satisfactory agreement between theory and experiment is achieved when the polarization and post-collisional interaction (PCI) are included in the calculations. It is shown that the polarization and PCI effects play a very important role in the case of argon at low incident energies.

Keywords: (e, 2e), distorted wave Born approximation, polarization, coplanar symmetric geometry
PACC: 3480D, 3450H

1. Introduction

(e, 2e) processes provide detailed information on the ionization mechanism as well as dynamics of three charged particles moving in the three-body continuum. In particular, in low-energy ionization collisions, many-body effects, polarization effects, correlation effects, exchange effects and the long-range effects of the Coulomb potentials are all very important and act together to make the problems more complicated and interesting. There have been continued experimental and theoretical efforts in the study of low-energy (e, 2e) processes. Extensive studies[1−7] have been performed on hydrogen and helium targets in a variety of collision geometries. Coplanar symmetric experiments[1−3] have yielded a wealth of interesting results and theory is still struggling to give a satisfactory description. At intermediate and high energies (e.g. with excess energies of 100eV and above), the distorted-wave Born approximation (DWBA) gives a reasonable description of the triple differential cross section (TDCS).[8] Below 100eV, the DWBA including polarization and post-collisional interaction (PCI) has been effective in reproducing the qualitative features of the TDCS for hydrogen and helium.[9,10,11]

In order to obtain more information on the role of dynamical effects, studies have been extended to heavier noble gas targets. DWBA with initial channel polarization and final channel PCI included has been used to calculate the TDCSs for 2s and 2p shells of neon[12,13] and 3p shell of argon[14] in coplanar symmetric geometry. It was found that the inclusion of polarization and PCI leads to some improvement in the overall agreement with experimental data. This suggested that the two effects are very important in the low energy (e, 2e) processes. Recently, Haynes and Lohmann[15] presented the first symmetric measurements for low-energy ionization of inner-valence 3s shell of argon. The experimental TDCSs generally show two peaks: the binary peak at forward angles and the recoil peak at backward angles, and the intensity ratio of recoil to binary peak increases with decreasing incident energy. Subsequently, Biava *et al*[16] have investigated the effects of electron exchange on

*Project supported by the National Natural Science Foundation of China (Grant No 10134010), and by the Natural Science Foundation of Anhui Province, China (Grant No 03046203) and the Natural Science Foundation of Education Commission of Anhui Province, China (Grant No 2001KJ262).

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low energy electron ionization of 3s and 3p shells of argon using DWBA. They pointed out that exchange scattering is important for 3s ionization. But, their results are not in satisfactory agreement with the experiment of Haynes and Lohmann. In this paper, we have modified the DWBA by adding polarization and PCI effects to calculate TDCSs of 3s orbital of argon in coplanar symmetric geometry at incident energies of 129.3, 69.3, 49.3 and 37.3 eV. Through the comparison of calculated results and the available experimental data,[15] we have further investigated the role of polarization and PCI effects in the (e, 2e) processes.

2. Theory

Considering an argon atom singly ionized by impact of an electron with incident momentum $\boldsymbol{k}_0$, in the spin averaged static exchange DWBA (referred to as 'standard' DWBA for simplicity),[17] the TDCS for coincident detection of two continuum electrons escaping with momenta $\boldsymbol{k}_1$, $\boldsymbol{k}_2$ and emerging into directions defined by solid angles Ω_1 and Ω_2 takes the form (in atomic unit):

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

where we assume that the ionized target electron comes from the ψ_{nl} orbital of the atom. The amplitudes f, g are given by

$$f \equiv \left\langle \chi^{(-)}(\boldsymbol{k}_1,\boldsymbol{r}_1)\chi^{(-)}(\boldsymbol{k}_2,\boldsymbol{r}_2)\left|\frac{1}{r_{12}}\right| \times \chi^{(+)}(\boldsymbol{k}_0,\boldsymbol{r}_1)\psi_{\mathrm{nl}}(\boldsymbol{r}_2)\right\rangle, \quad (2a)$$

$$g \equiv \left\langle \chi^{(-)}(\boldsymbol{k}_1,\boldsymbol{r}_2)\chi^{(-)}(\boldsymbol{k}_2,\boldsymbol{r}_1)\left|\frac{1}{r_{12}}\right| \times \chi^{(+)}(\boldsymbol{k}_0,\boldsymbol{r}_1)\psi_{\mathrm{nl}}(\boldsymbol{r}_2)\right\rangle, \quad (2b)$$

where $\sum_{\mathrm{av}}$ represents the sum over final and average over initial magnetic and spin degeneracy. $\chi^{(+)}$ is the distorted wave for incident electron generated in the equivalent local ground state potential of atom and $\chi^{(-)}$ denotes the distorted waves for outgoing electrons generated in the equivalent local ground state potential of ion. $\chi^{(+)}$ and $\chi^{(-)}$ are both orthogonalized to ψ_{nl}. The spin averaged static exchange potential taken in the equivalent local approximation[18] is given as

$$V_{\mathrm{E}}(r) = 0.5(E_0+V_{\mathrm{D}}(r)-\{[E_0+V_{\mathrm{D}}(r)]^2 - 2\pi\rho(r)\}^{\frac{1}{2}}), \quad (3)$$

where $\rho(r)$ is the electron density. The direct distorting potential $V_{\mathrm{D}}(r)$ for the incident electron is obtained from the target-atom radial orbitals $u_{\mathrm{nl}}(r)$ as[17]

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

where $r_>$ is the greater of r and r', N_{nl} is the number of electrons in each orbital nl. For the outgoing electrons, direct distorting potential $V_{\mathrm{D}}(r)$ is obtained from the ion radial orbitals. The equivalent local ground state potential V_{00} (i.e. distorting potential) is the sum of exchange and direct potentials:

$$V_{00} = V_{\mathrm{D}}(r)+V_{\mathrm{E}}(r). \quad (5)$$

As formulated above, the DWBA does not include the effects of electron–electron repulsion in the final state or polarization. In order to include few-body effects in both the incident and final channels, the DWBA was modified through adding polarization potentials and including PCI effects.

The PCI effect is considered by multiplying by a Gamow factor M_{ee}.[19] The TDCS was then defined as

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\mathrm{d}\Omega_2\mathrm{d}E_1} = M_{\mathrm{ee}}\frac{\mathrm{d}^3\sigma^{\mathrm{DWBA}}}{\mathrm{d}\Omega_1\mathrm{d}\Omega_2\mathrm{d}E_1}. \quad (6)$$

The polarization potential V_{pol} is added into the distorting potential V_{00} to calculate $\chi^{(+)}$ and $\chi^{(-)}$, which takes the form[12]

$$V_{\mathrm{pol}} = -f_2(r)\frac{\alpha_1}{2r^4}, \quad (7)$$

where α_1=11.1, which is the dipole polarizability of argon.[20] The damping function is given by[21,22]

$$f_2(r) = \frac{\int_0^r \rho(r_{\mathrm{b}})r_{\mathrm{b}}^4\mathrm{d}r_{\mathrm{b}}}{\int_0^\infty \rho(r_{\mathrm{b}})r_{\mathrm{b}}^4\mathrm{d}r_{\mathrm{b}}}. \quad (8)$$

The orbital ψ_{nl} in Eq.(2) is taken from the Hartree–Fock wavefunction given by Clementi and Roetti.[23] The parameters such as the maximum orbital angular momenta in the partial wave expansions and mesh size of the integration have been optimized in order to satisfactorily converge the cross-sections.

3. Results and discussions

We have calculated the TDCS for electron impact ionization of inner valence 3s orbital of argon using the DWBA methods in coplanar symmetric energy-sharing geometry at incident energies of 129.3, 69.3, 49.3 and 37.3eV. The results are given in Fig.1(a)–(d) for four different variants of DWBA calculations: (1) standard DWBA, (2) DWBA with polarization only, (3) DWBA with PCI only, (4) DWBA with both polarization and PCI. For the sake of comparison with the experimental data in Ref.[15], the calculated results are normalized (arbitrarily) for the best visual agreement with the experiment.

The dashed curves in Fig.1(a)–(d) present the calculated results using the standard DWBA with neither polarization nor PCI effects included. As shown in Fig.1(a)–(c), in the region of the forward angles $\theta < 90°$, the TDCS calculated using the standard DWBA increases monotonically as the angle decreases and would not vanish as $\theta \to 0°$. This is not reasonable because the calculation was performed in coplanar symmetric energy-sharing geometry in which both final state electrons have the same energy and are observed at the same scattering angles on opposite side of the beam direction. When the scattering angle θ becomes very small ($\sim 0°$) or very large ($\sim 180°$), the repulsion between the two outgoing electrons after the ionization is very strong, and so the TDCS should go to zero for 0° and 180° scattering.[12,16] On the other hand, in the case of the incident energy of 37.3eV in Fig.1(d), the standard DWBA calculation does have two peaks, but the position of the recoil peak is shifted to a larger angle by about 35° from experiment, and the calculated ratio of recoil to binary peak is much smaller than that of experiment. In general, the standard DWBA model is not enough to explain the measurements.

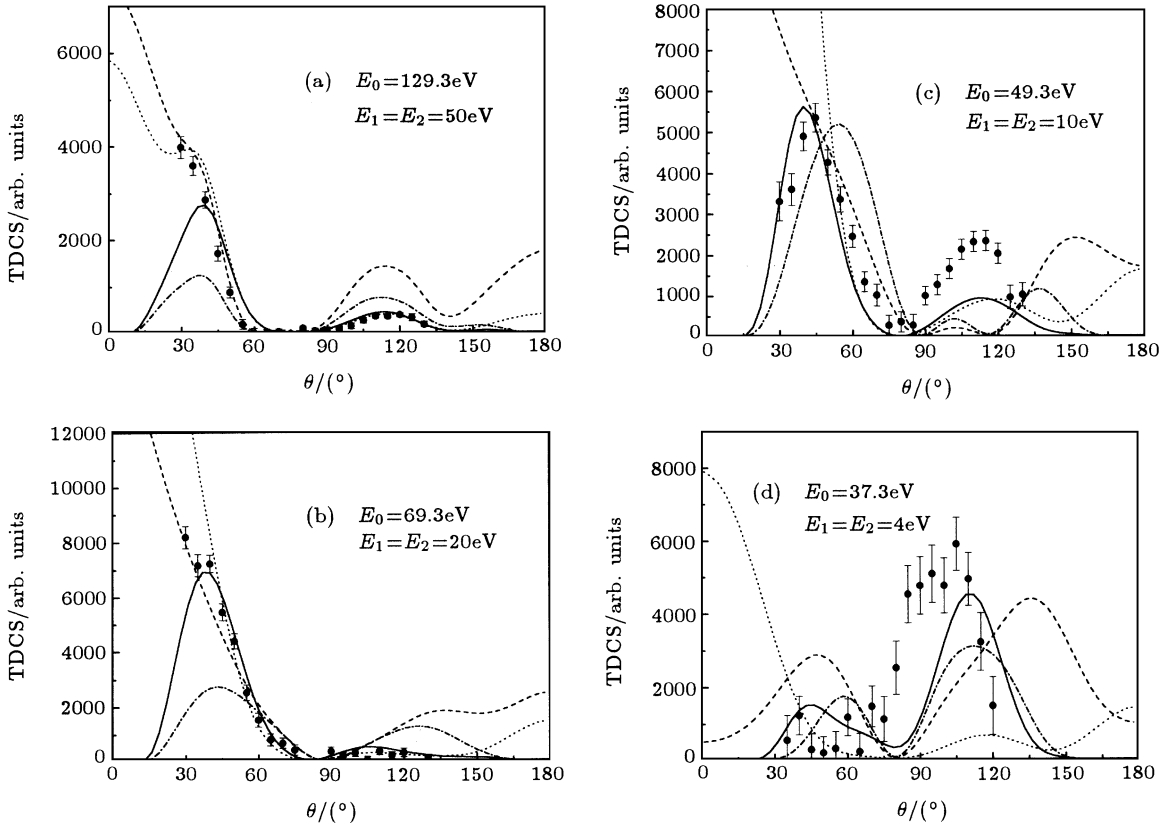


Fig.1. TDCSs in coplanar energy sharing symmetric geometry for ionization of Ar(3s) at incident energy of (a) 129.3eV, (b) 69.3eV, (c) 49.3eV, and (d) 37.3eV. • experiment.[15]. DWBA calculations: - - - standard; ····· including polarization effects; —·— including PCI effects; — including PCI and polarization effects. The theoretical results are normalized to the experimental data.

As seen from the dotted curves in Fig.1, the inclusion of only polarization effect in the DWBA calculation leads to some improvement in the agreement with experiment in the region of intermediate scattering angles from 35°, 40°, 50° and 50° to 130° for incident energies of 129.3, 69.3, 49.3 and 37.3eV, respectively. However, for very small and very large angles, the theoretical calculation with only polarization included are not reasonable, owing to the fact that significant repulsion between the outgoing electrons are not taken into account.

When only PCI was included into the DWBA calculation through multiplying by the M_{ee} factor, which is designed to take account of final state electron–electron repulsion, the improvement in the overall agreement between theory and experiment was obvious (shown as dash-dotted curves in Fig.1). The observed main feature of two peaks is generally reproduced. This indicates that the PCI effect is very important and should be taken into account in the theoretical calculation for low-energy (e, 2e) processes in coplanar symmetric energy-sharing geometry. But significant discrepancies between theory and experiment were still found. For the case of incident energies of 129.3 and 69.3eV, the ratios of recoil to binary peaks are much larger than that of experiment while it is smaller for incident energy of 37.3eV. Particularly for incident energy of 49.3eV in Fig.1(c), the calculation predicted two peaks in the region of backward angles where one recoil peak was observed by experiment.

The solid curves in Fig.1(a)–(d) present the results calculated using the DWBA method with both polarization and PCI included. We can see that they give satisfactory agreement with experiment. The two peaks observed by experiment are well reproduced. The calculation indicates that the intensity ratio of recoil to binary peak generally increases with decreasing incident energy. The binary peak at forward angle is the dominant structure at incident energy of 129.3eV, while the recoil peak at backward angle has become the dominant one at incident energy of 37.3eV. This is in good agreement with experiment and can be interpreted by that with the incident energy decreased, the elastic cross section for backscattering from the nucleus increases and the double-scattering process should become more dominant.[3] It is shown that both of polarization and PCI effects play important roles in the processes of low-energy electron impact ionization of inner valence 3s orbital of argon in coplanar symmetric energy-sharing geometry.

The DWBA with PCI and polarization gives quite a good overall fit to the experiment. However, some discrepancies between theory and experiments still remain as shown in Fig.1(c). The calculated intensity ratio of recoil to binary peaks is smaller than that of the experiment. The treatment of the PCI and polarization in a simple way should be responsible for some of the observed discrepancies.

In conclusion, we have calculated the TDCSs for low-energy (e, 2e) on Ar(3s) target using the DWBA method with and without polarization and/or PCI. Only when both polarization and PCI are included into the DWBA calculation, do we get satisfactory agreement with experiment. It is demonstrated that polarization and PCI effects play a very important role in the case of 3s orbital of argon in coplanar symmetric energy-sharing geometry at low incident energies.

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