(e, 2e) triple-differential cross sections for Ag^+(4p, 4s) in coplanar symmetric geometry*

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The (e, 2e) triple-differential cross sections of Ag^+(4p, 4s) were calculated based on the three-body distorted-wave Born approximation considering post-collision interaction in coplanar symmetric geometry. The energy of outgoing electron was set to be 50, 70, 100, 200, 300, 500, 700, and 1000 eV, and the intensity and splitting of forward and backward peaks were discussed in detail. Some new structures were observed around 15° and 85° for 4p and 4s orbitals. Structures in triple-differential cross sections at 15° have been reported for the first time. A double-binary collision was proposed to explain the formation of such structures. The structures at 85° were also considered as the result of one kind of double-binary collision.

Keywords: (e, 2e) process, distorted-wave Born approximation, triple-differential cross section, coplanar symmetric geometry

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1. Introduction

Electron-impact ionization of atoms or ions is a fundamental process in atomic physics, which provides detailed information about ionization mechanism and dynamics of three charged particles moving in three-body continuum. Such impacting process so-called (e, 2e) reaction were extensively investigated experimentally and theoretically.

Coplanar symmetric geometry is one kind of geometry often used. For this geometry, two peaks called forward peak and backward peak in (e, 2e) triple-differential cross sections (TDCSs) have been well distinguished. The forward peak could be ascribed to a single binary collision, and a usual-double binary collision results in the backward peak. In such a usual-double binary collision, the incident electron first recoils from the impact with target ions, and then knocks out orbital electrons. The intensity and position of forward and backward peaks have been widely studied for He, Ne, Ar, Kr, H, alkali, and alkali earth atoms.[1−11]

In addition to forward and backward peaks, a new structure in the TDCS of Ne has been found by Rioualt *et al.*[4] They reported their experimental and theoretical (e, 2e) research and found a new structure at a symmetric scattering angle of 85°. They ascribe such structure to the fact that the outgoing electrons experience an elastic scattering with target ion by 90°, following by a direct collision. Murray[10] and Hitawala *et al.*[11] reported the experimental and theoretical (e, 2e) TDCSs for Na, K, Mg, and Ca in coplanar symmetric geometry. The TDCSs showed shallow dips at about 70° for K atom, which were attributed to the interplay of various contributions in the scattering amplitude. Furthermore, they argued that the three-peak structures in the theoretical profiles near 80° for Ca and K atoms may be due to the presence of open 3d shell for these targets.

The (e, 2e) research for ion targets plays an important role in the fields of astrophysics, plasma physics, and fusion. Up to now, the experimental measurements of (e, 2e) reaction in coplanar symmetric geometry for ionic targets have not been reported. Several pieces of theoretical research have been reported.[12,13] In these studies, the (e, 2e) TDCSs in coplanar or perpendicular plane geometry were calculated for outer valence orbitals of Li^+, Na^+, K^+, Rb^+, Cs^+, and Cu^+.

In this paper, the (e, 2e) TDCSs of 4p and 4s orbitals of Ag^+were firstly calculated under coplanar symmetric geometry with different outgoing energies. The intensity and splitting of the forward and backward peaks were discussed in detail. Aside from for-

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ward and backward peaks, we also found some new structures in TDCSs for 4p and 4s orbitals at around 15° and 85°. Two kinds of double-binary collision were proposed to explain these new structures.

2. Theory

Consider an Ag^+ ion ionized by impact with an incident electron with momentum $\boldsymbol{k}_0$, followed by two outgoing electrons with momenta $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$, the TDCS for such a process can be described via the distorted-wave Born approximation (DWBA) theory as[14]

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

where

$$f = \left\langle \chi^{(-)}(\boldsymbol{k}_1,r_1)\chi^{(-)}(\boldsymbol{k}_2,r_2)\left|\frac{1}{r_{12}}\right|\chi^{(+)}(\boldsymbol{k}_0,r_0)\psi_{nl}\right\rangle, \quad (2)$$

$$g = \left\langle \chi^{(-)}(\boldsymbol{k}_1,r_2)\chi^{(-)}(\boldsymbol{k}_2,r_1)\left|\frac{1}{r_{12}}\right|\chi^{(+)}(\boldsymbol{k}_0,r_0)\psi_{nl}\right\rangle. \quad (3)$$

In Eq. (1), $\sum_{\mathrm{av}}$ represents the sum over final and average over initial magnetic and spin degeneracy, ψ_{nl} is the orbital of Ag^+, $\chi^{(+)}$ denotes the distorted wave of incident electron generated in the equivalent local ground state potential of Ag^+ ion, and $\chi^{(-)}$ is the distorted wave of outgoing electrons generated in the equivalent local ground state potential of ion in final channels. Both $\chi^{(+)}$ and $\chi^{(-)}$ are orthogonal to ψ_{nl}.

The equivalent local ground state potential $V_{00}(r)$ (i.e., distorting potential) is the sum of direct potential V_{D} and exchange potential V_{E}. The direct potential V_{D} is obtained from the target–ion radial orbital $u_{nl}(r)$ as[14]

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

where $r_> = \max[r,r']$, and N_{nl} is the number of electrons in orbital nl. The spin average static exchange potential V_{E} is given by[15]

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

where E is the total energy, and $\rho(r)$ is the electron density. Then, the equivalent distorting potential $V_{00}(r)$ can be described as

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

The effect of post-collision interaction (PCI) has been taken into account by introducing a parameter M_{ee}[16]

$$\begin{aligned} M_{\mathrm{ee}} &= \frac{\pi\exp(-\pi/k_3)}{k_3[1-\exp(-\pi/k_3)]} \times |{}_1F_1(-\mathrm{i}V,1,-2\mathrm{i}k_3r_{3\mathrm{ave}})|^2, \quad (7)\\ V &= -1/|\boldsymbol{k}_1-\boldsymbol{k}_2|,\\ k_3 &= |\boldsymbol{k}_1-\boldsymbol{k}_2|/2,\\ r_{3\mathrm{ave}} &= \frac{\pi^2}{16\varepsilon}\left(1+\frac{0.627}{\pi}\sqrt{\varepsilon}\ln\varepsilon\right),\\ \varepsilon &= \left(k_1^2+k_2^2\right)/2. \quad (8) \end{aligned}$$

Then, TDCS can be expressed as

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

3. Results and discussion

Figure 1 shows the TDCSs of electron-impact ionization of $Ag^+(4p)$ in coplanar symmetry geometry under different outgoing energies.

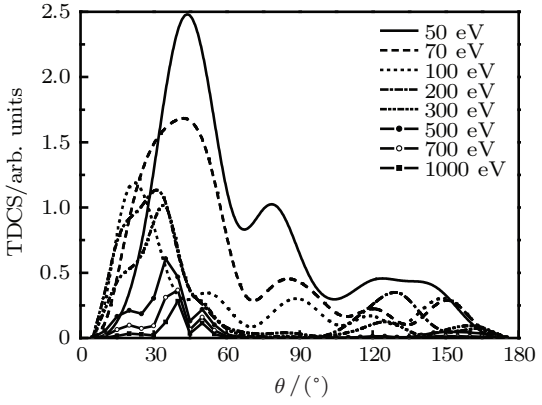


Fig. 1. TDCSs of electron impact ionization for $Ag^+(4p)$ at different outgoing energies in coplanar symmetric geometry.

In Fig. 1, it can be seen that the forward peaks appear at outgoing angle $\theta \approx 45°$, and split into two peaks when outgoing energy increases up to 100 eV. However, as for the backward peaks in the region of 105°–165°, all backward peaks split. The splitting of forward and backward peaks can be attributed to the

electron momentum distribution of p orbital.[4] The intensity of the forward peak is always higher than that of the backward peak.

In addition to the forward and backward peaks, some new structures appear at $\theta \approx 15°$ and $\theta \approx 85°$. The former structure does not appear until the outgoing energy reaches 100 eV. When the outgoing energy increases to 200 eV, a noticeable shoulder appears. It becomes more obvious as the outgoing energy further increases. This structure has not been explained yet. Assume that a double-binary collision has happened. Such double-binary collision process can be described in Fig. 2. The incident electron ionizes the target atom and the two outgoing electrons exit in the symmetry directions relative to the incident electron. Then the outgoing electrons are elastically scattered by the target ion. Therefore, the outgoing electrons appear at smaller angles. This is the reason why this structure appears at smaller outgoing angle than the forward peak. From Fig. 2, we can conclude that the outgoing angle θ will be close to the forward peak as the outgoing energy increases. These phenomena indeed happen in Fig. 1. The latter structure at $\theta \approx 85°$ has been explained by Rioualt *et al.*[4] They demonstrated that the outgoing electrons experience an elastic scattering with the target ion by 90°, following by a direct collision with target atom.

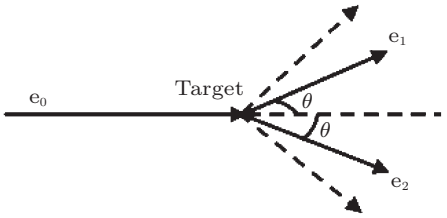


Fig. 2. Schematic of double-binary collision process of (e, 2e) reaction in coplanar symmetry geometry.

Figure 3 shows the TDCSs of electron impact ionization of $Ag^+(4s)$ in coplanar symmetry geometry. The ratio of forward peak to backward peak is smaller than one at the outgoing energy of 50 and 70 eV. The ratio exceeds one when the outgoing energy increases to 100 eV. Another difference from 4p orbital is that the forward peaks of 4s orbital does not show splitting. This difference can be ascribed to the difference of electron momentum distribution between 4s and 4p orbitals.[4]

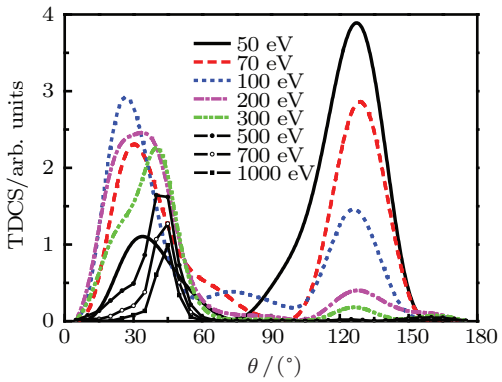


Fig. 3. (colour online) TDCSs of electron impact ionization for $Ag^+(4s)$ at different outgoing energies in coplanar symmetric geometry.

Note the structures at $\theta \approx 15°$ and $\theta \approx 85°$. The former structure at $\theta \approx 15°$ only appears at outgoing energies of 200, 300, and 500 eV, whereas the latter structure at $\theta \approx 85°$ only appears at outgoing energies of 70 and 100 eV, and most of them only show a small shoulder. Such phenomenon indicates that double-binary collisions seldom occur for 4s orbital.

4. Conclusion

The TDCSs of Ag^+ (4p, 4s) have been calculated using the three-body distorted-wave Born approximation under different outgoing energies in coplanar symmetric geometry. The intensity and splitting of the forward and backward peaks have been studied. We also found some new structures appearing at about 15° and 85° for 4p and 4s orbitals. These structures were more obvious for 4p orbital, which suggests that the double-binary collisions seldom occur for 4s orbital. We used a double-binary collision to explain the structures at about 15°. The structures at about 85° are also probably related to one kind of double-binary collision.

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