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# Polarization effect in (e, 2e) collisions of argon

Xiao-Ying Hu *, Ya-Jun Zhou, You-Qi Ke, Guang-Jun Nan

*Institute of Atomic and Molecular Physics, Jilin University, Changchun 130012, PR China*

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**Abstract**

Calculations of the triple differential cross section (TDCS) for electron impact ionization of the Ar(2p) orbital in a highly asymmetric geometry, using modified distorted wave Born approximation (DWBA) methods, are reported. The role of the polarization effect in (e, 2e) collisions of Ar(2p) is considered in the calculations, and the calculated results shows that the polarization potential is particularly important.


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*Keywords:* (e, 2e) reaction; Polarization potential; Distorted wave Born approximation

## 1. Introduction

In recent years, a number of new directions have been pursed in (e, 2e) investigations of electron-impact ionization processes. Much attention has been concentrated on atomic outer shells, particularly with simple targets, and the less bound intermediate shells of atoms and molecules. However, because of the smallness of the cross section the core region has been the subject of fewer studies, although the dynamical studies of inner-shell ionization in neon, argon [1–3] and xenon [4] revealed a number of interesting features of the scattering which were distinctly different to outer-shell ionization.

Experiment results [5,6] were reported for (e, 2e) ionization of the argon 2p orbital in a highly asymmetric geometry, which showed that the theoretical results obtained using the DWBA method had significant differences, compared with experimental data, in the overall shape and magnitude of the triple differential cross section. The recoil-to-binary ratio in relative TDCS for the Ar(2p) ionization was significantly underestimated by the DWBA calculations. The double peaks using the standard DWBA calculations were approximately symmetric about the direction of momentum transfer $\pm\vec{K}$, while the experimental results did not show this feature clearly. The calculated binary and recoil peaks showed no structure where the

* Corresponding author.
*E-mail address:* xiaoying-hu@tom.com (X.-Y. Hu).

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experiments might possibly show some. All of these differences present a substantial challenge to theory. The discrepancy is probably due to neglecting to consider the higher-order electron–electron correlations in the DWBA method. Thus, a new dynamical mechanism and the modification of the DWBA method are needed to explain the experimental data properly.

In order to test the significance of polarization, Whelan et al. [7] modified the DWBA calculations by introducing an ad hoc polarization potential $V_{\rm pol}$ in (e, 2e) collisions of He. In this Letter, we have extended the model proposed by Whelan et al. [7] and added another potential $V_{\rm dft}$ via density-functional theory (DFT) [8] for argon. We aim at showing the influence of the polarization potential [9] on the calculated TDCS of Ar(2p). In order to test the validity of our model, we have calculated the TDCS with the incident energy of 8256 and 5720 eV, respectively, in a highly asymmetric geometry. The calculated results have been compared with those obtained by the standard DWBA and the experimental data [5,6].

## 2. Theory

The triple differential cross section in the distorted-wave Born approximation is given by [10]

$$\frac{d^3\sigma}{d\Omega_f\, d\Omega_s\, dE_0} = (2\pi)^4 \frac{k_f k_s}{k_0} \sum_{\rm av} \left|\langle \vec{k}_f \vec{k}_s | T | \alpha \vec{k}_0 \rangle\right|^2, \tag{1}$$

where the subscript $f$ and $s$ represent the fast and slow electrons, respectively. $E$ is kinetic energy, $\vec{k}$ momentum, $E_0$ the kinetic energy of the incident electron. The incident electron with momentum $\vec{k}_0$ incidents on an uncharged system consisting of electron $s$ bound to the core in the state $\alpha$ with separation energy $\varepsilon_\alpha$. The notation $\sum_{\rm av}$ represents a sum over the final state and average over the initial magnetic and spin degeneracy state. In the calculation, the atomic units ($\hbar = m_e = e = 1$) are used.

The DWBA T-matrix element is

$$\langle \vec{k}_f \vec{k}_s | T | \alpha \vec{k}_0 \rangle = \left\langle \chi^{(-)}(k_f) \chi^{(-)}(k_s) \middle| v_{fs} \middle| \alpha \chi^{(+)}(k_0) \right\rangle, \tag{2}$$

where $v_{fs}$ is the interaction potential between the fast and slow electron. $|\chi^{(-)}(k_f)\rangle$, $|\chi^{(-)}(\vec{k}_s)\rangle$ and $|\chi^{(+)}(\vec{k}_0)\rangle$ are the distorted waves at different asymptotic conditions. The superscripts refer to the outgoing and incident waves, respectively.

The partial-wave expansions of the distorted waves can be written as

$$\left\langle \chi^{(-)}(\vec{k}) \middle| r \right\rangle = \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{kr} \sum_{LM} i^{-L} e^{i\sigma_L} u_L(k,r) Y_{LM}(\hat{k}) Y^*_{LM}(\hat{r}), \tag{3}$$

$$\left\langle \vec{r} \middle| \chi^{(+)}(\vec{k}) \right\rangle = \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{kr} \sum_{LM} i^{L} u_L(k,r) Y^*_{LM}(\hat{k}) Y_{LM}(\hat{r}), \tag{4}$$

where $\sigma_L$ is the Coulomb phase shift.

The coordinate representation of the orbital $|\alpha\rangle$ is

$$\langle \vec{r} | \alpha \rangle = r^{-1} u_{nl} Y_{LM}(\hat{r}), \tag{5}$$

and the partial wave $\mu_L(k,r)$ can be obtained by solving the differential equation as follows:

$$\left(\frac{d^2}{d\rho^2} - \frac{L(L+1)}{\rho^2} - \frac{\eta}{\rho} - \frac{v(r) + V_P(r)}{E} + 1\right) u_L(k,r) = 0, \tag{6}$$

where the potential $v(r)$ includes the direct distorting potentials $V_D(r)$ and the spin-averaged static-exchange potential $V_E(r)$, $\rho = kr$, $\eta = -Z/k$, $E = \frac{1}{2}k^2$, $V_P(r)$ is the polarization potential which we introduce in our calculations.

The asymptotic form of the adiabatic polarization potential is simply given by the well-know second-order perturbation expansion formula [11,12].

$$V_p^T(r) \underset{r\to\infty}{\sim} -\sum_{l=1}^{\infty} \frac{\alpha_l}{2r^{2l+2}}, \quad \text{for } r > r_0, \tag{7}$$

$\alpha_l$ is the multipolar polarizability of the target atom and $r_0$ separates the outer region from the inner short-range region.

In the near-target region, the main drawback of the expansion (7) is that it grossly overestimates polarization and incorrectly diverges near the origin of the force field. According to Whelan et al. [7], we only consider the dipole term. Hence the polarization po-