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Ionization and single electron capture in collision of highly charged Ar^{16+} ions with helium*

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This paper uses the two-centre atomic orbital close-coupling method to study the ionization and the single electron capture in collision of highly charged Ar^{16+} ions with He atoms in the velocity range of 1.2–1.9 a.u.. The relative importance of single ionization (SI) to single capture (SC) is explored. The comparison between the calculation and experimental data shows that the SI/SC cross section ratios from this work are in good agreement with experimental data. The total single electron ionization cross sections and the total single electron capture cross sections are also given for this collision. The investigation of the partial electron capture cross section shows a general tendency of capture to larger n and l with increasing velocity from 1.2 to 1.9 a.u..

Keywords: close-coupling method, electron capture, highly charged ions
PACC: 3400, 5220H

1. Introduction

Ionization and electron capture in ion-atom collision have been investigated experimentally and theoretically not only for interest in atomic physics, but also for their importance in fields such as astrophysics, laser physics and plasma physics. When charged ions collide with neutral targets, ionization and electron capture compete in the collisions. At low velocity, ionization involving highly charged ions is a weak process with small transition probabilities, and the dominant target electron removal process is single electron capture. It is desirable to find out the relative importance of the ionization process to the dominant charge transfer process. Wu *et al*[1,2] first measured single ionization (SI) and single capture (SC) cross sections in collisions of C^{6+}, N^{7+}, O^{8+}, Ar^{16+}, I^{16+}, Xe^{30+} on helium at low velocity (0.2 to 1.7 a.u.). Later, Wang and Lin *et al*[3] calculated the ionization and charge transfer in slow collisions between highly charged C^{6+}, N^{7+}, O^{8+} projectiles and helium atoms by using the two-centre atomic orbital close-coupling method. Their theoretical results are in good agreement with the experimental results by Wu *et al.* Cassimi *et al*[4] reported the state-selective electron capture in the collision of Ar^{18+} on He using recoil ion momentum spectroscopy. Recently, Cai *et al*[5] measured the transfer ionization to SC ratios for Ar^{8+} ions on He, Ne and Ar atoms by using position sensitive and time-of-flight techniques[6,7].

Highly charged Argon ions could carry intense fields and large potential energy into the collisions, which strongly perturb the target. The collision system, a challenge not only to experimental but also to theoretical, is quite complex since many electrons can participate. To our knowledge, there have been only a few calculations on ionization and electron capture of two-electron targets by multiply charged Argon ions. The close-coupling method is one of the most reliable and powerful theoretical approaches to study the atomic collision in the intermediate- or low-energy region, where the perturbative approaches are not applicable. In this work, the close-coupling method where the wave functions are expanded in terms of atomic orbitals on the two collision centres has been used to calculate the cross section of ionization and electron capture in collisions of multiply charged Ar^{16+} ions with helium atoms over a broad range of energies. The ratio of the SI cross section ($\sigma_{\rm SI}$) to the SC cross section ($\sigma_{\rm SC}$) has been investigated for He by Ar^{16+} projectiles to compare with experiment. The total single electron ionization cross sections and the total single electron capture cross sections are given for collision of Ar^{16+} with He. The main partial elec-

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tron capture cross sections are also calculated for the collision. These available data will give us a better understanding of the experimental data in the future.

2. Method

The multistate close-coupling method[8,9] is used to solve the time-dependent Schrodinger equation and obtain the one-electron transition probabilities. The time-dependent Schrodinger equation is given by

$$\left(\mathrm{i}\frac{\partial}{\partial t} - H\right)\Psi\left(\boldsymbol{r},t\right) = 0, \tag{1}$$

with

$$H = -\frac{1}{2}\Delta_r^2 + V_{\mathrm{T}}\left(r_{\mathrm{T}}\right) + V_{\mathrm{P}}\left(r_{\mathrm{P}}\right). \tag{2}$$

Where r_{P}, r_{T} are the electron coordinates measured from the target and projectile nucleus, respectively. The time-dependent electronic wave function for the collision system is expanded in terms of atoms orbitals centred on the two heavy nuclei as

$$\begin{aligned}\Psi\left(\boldsymbol{r},t\right) = {} & C\sum_{i=1}^{N_{\mathrm{T}}} a_i\left(t\right)\psi_i^{\mathrm{T}}\left(\boldsymbol{r}_{\mathrm{T}},t\right) \\ & + \sum_{i=N_{\mathrm{T}}+1}^{N} a_i\left(t\right)\psi_i^{\mathrm{P}}\left(\boldsymbol{r}_{\mathrm{P}},t\right).\end{aligned} \tag{3}$$

Where $\psi_i^{\mathrm{T}}\left(\boldsymbol{r}_{\mathrm{T}},t\right)$ and $\psi_i^{\mathrm{P}}\left(\boldsymbol{r}_{\mathrm{P}},t\right)$ are the target and the projectile atomic orbital with appropriate electron translation factors, respectively. The eigenfunctions of each centre are further expanded in terms of the Slater-type orbitals (STOs) as

$$\phi_{nlm}\left(\boldsymbol{r}\right) = \sum_{\nu} c_{\nu}^{(nl)}\mathrm{e}^{-\alpha_\nu r}r^l Y_{lm}\left(\boldsymbol{r}\right). \tag{4}$$

In each case, the coefficients $c_\nu^{(nl)}$ are determined by diagonalizing the atomic Hamiltonian of the target and the projectile. The effective potential for the helium atom is of the form

$$V_{\mathrm{T}}\left(r_{\mathrm{T}}\right) = -\frac{1}{r_{\mathrm{T}}} - \left(1 + 0.4143r_{\mathrm{T}}\right)\frac{\mathrm{e}^{-2.499r_{\mathrm{T}}}}{r_{\mathrm{T}}}. \tag{5}$$

Since the excited electrons of Li-like Ar^{15+} ion remain far away outside the closed $1s^2$ core, the excited electrons are supposed to move in the effective potential generated by inner electrons and the nucleus. The effective potential for the Argon ion is of the form

$$V_{\mathrm{P}}\left(r_{\mathrm{P}}\right) = -\frac{z_0}{r_{\mathrm{p}}} - \left(z_1 + z_2 r_{\mathrm{p}}\right)\frac{\mathrm{e}^{-z_3 r_{\mathrm{P}}}}{r_{\mathrm{p}}}, \tag{6}$$

where $z_0 = 16$, $z_1 = -2$, $z_2 = -20.99$, and $z_3 = 20.99$ in this work. These parameters z_0, z_1, z_2, and z_3 are adjustable parameters, whose optimum values can be selected by solving the one electron Schrodinger equation by using the potential Eq.(6).

3. Results and discussion

In this work, the two-centre atomic orbital close-coupling method is used to calculate the cross section of ionization and electron capture in collisions of highly charged Ar^{16+} ions with helium atoms at low velocity. In order to account for electron capture into the dominant excited states of the projectile, we used a fairly large STO-type basis which contains exact states up to $n = 8$ with maximum angular momentum $l = 5$ on the Ar^{16+} centre. Table 1 has shown us the comparison between the calculations of energies of the bond states $1s^2nl$ (n = 2–8, l = 0–5) for Li-like Ar^{15+} and the experimental data.[10] From Table 1,

Table 1. Energies of the bond states for Li−like Ar^{15+} ($1s^2nl$). (in a.u.)

n \ l	s	p	d	f	g	h
2	−33.733	−32.567				
Exp.[10]	−33.737	−32.527				
3	−14.712	−14.337	−13.976			
Exp.[10]	−14.701	−14.411	−14.228			
4	−8.198	−7.994	−7.832	−5.359		
Exp.[10]	−8.088					
5	−5.217	−5.061	−5.001	−3.058	−3.120	
6	−4.153	−3.455	−3.455	−1.920	73.611	53.764
7	−3.452	−2.454	−2.502	28.083	311.639	169.561
8	−2.438	−2.030	−1.854	147.029		471.959

we know that our theoretical results are in good agreement with the experimental. In this work, a great number of pseudostates were employed to represent the projectile continuum. For the target He centre, the basis includes $l = 0$, $l = 1$, and $l = 2$ states obtained from the effective potential Eq.(5).

The competition between ionization and the dominant charge transfer processes in slow collisions is a rather intriguing subject. The ratio of the SI cross section (σ_{SI}) to the SC cross section (σ_{SC}) has been explored for the Ar^{16+}-He collisions. Figure 1 shows us the apparent onset in the velocity dependence of the cross section ratio between ionization and charge transfer. In the velocity range of 1.2–1.8 a.u., the SI/SC cross section ratio increases slowly with the increase of velocity. From $v = 1.8$ a.u., the increase of the ratio with the increase of velocity becomes more and more rapid, which is caused by the strong onset of the target direct ionization. The calculated curve of SI/SC ratio with the velocity variety in this work has been compared with the experimental data for the velocity range of 1.2–1.6 a.u. of Wu *et al*,[1] whose measurement cannot reach the classical Bohr–Lindhard velocity limit for ionization due to the limitation of experimental condition. Figure 1 shows that the curve from this work are in good agreement with the experimental curve from $v = 1.2$ to 1.6 a.u.. Our theoretical results will be very useful for further understanding the ionization and electron capture process in the collision of highly charged argon ions on He atoms.

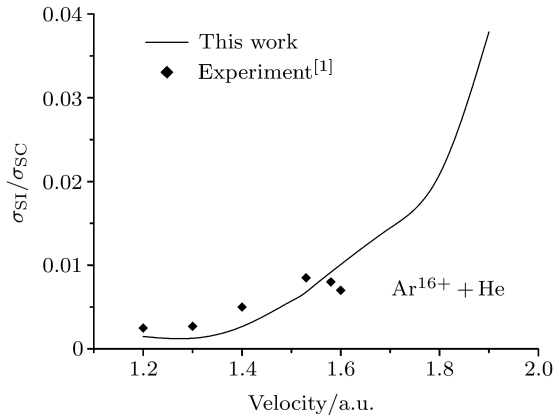


Fig.1. The ratio of the SI cross section (σ_{SI}) to the SC cross section(σ_{SC}) for He by Ar^{16+} projectiles.

In Fig.2, the total single electron ionization cross sections and the total single electron capture cross sections are also given for Ar^{16+}-He collisions, respectively. The ionization cross section increases rapidly with the increase of velocity. The capture cross section is relatively constant from $v = 1.2$ to 1.9 a.u. In Fig.3, the main theoretical partial electron capture cross section of Ar^{15+} ions has shown us a general tendency of capture to larger n and l with increasing velocity from 1.2 to 1.9 a.u.. According to our calculations, $3l$ states are the most important final states captured into by projectile, and $5l$ states, including 5d, 5f and 5g states, would be more and more important with the increase of velocity. To our knowledge, no other results of the partial electron capture cross section are available for the Ar^{16+}-He collisions. Our theoretical results would be useful for further investigating the collisions between highly charged ions and atoms in the future.

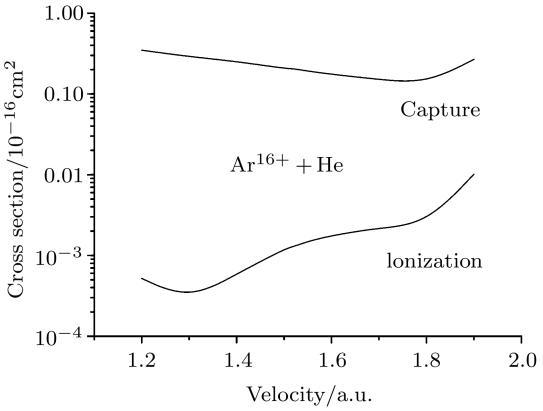


Fig.2. Total single electron ionization cross sections and total single electron capture cross sections for Ar^{16+}- He collisions.

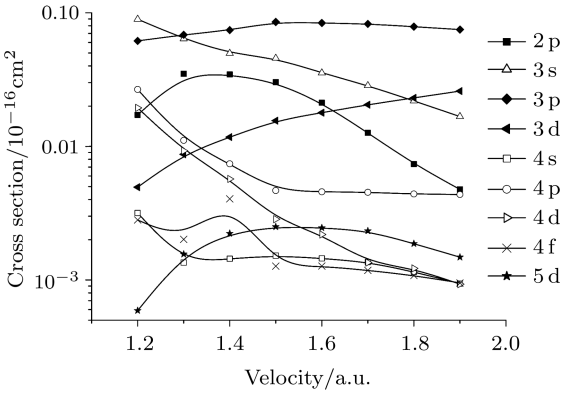


Fig.3. Theoretical partial electron capture cross section to $1s^2nl$ states of Ar^{15+} ions.

4. Conclusion

In this work, we investigated the relative importance of SI to SC for the Ar^{16+}-He collisions. The comparison between our calculation and experimental data shows that the curve of the SI/SC cross section ratio from this work is in good agreement with experimental data. The total single electron ionization cross sections and the total single electron capture cross sections are also given for this collision. From our work, it is the most important SC for Ar^{16+}–He collisions to capture electrons to $1s^2 3l$ states at the velocity range of 1.2–1.9 a.u. However, larger n or l states will become important states captured into by projectiles with the increase of velocity.

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