

Multiple ionization cross sections of atoms by swift ions in the independent electron model

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The impact-parameter-dependent ionization probability is obtained from consideration of the Coulomb-Born ionization cross section together with the energy transfer to the atomic electrons. Different from the conventional perturbative treatments, this ionization probability is found to satisfy the unitarity even for highly charged projectiles. Using this quantity, the multiple ionization cross sections of Ne and Ar atoms by fast-ion impact are calculated in two kinds of the independent electron models (IEM's). One is that the orbital energies of neutral atoms are used. The other is that the orbital energies are changed successively as the degree of ionization increases one by one. By comparison, the latter model was found to provide the better agreement with the data.

1. Introduction

The ionization process of atom and molecule by fast ion impact has been one of the fundamental and important problems in the ion-material interaction. So far a lot of works have been carried out. For light targets, the multiple ionization of He atom was investigated in detail by several theoretical and experimental scientist [1-5]. For heavier targets, Tawara et al.[6], Tonuma et al.[7,8], and Matsuo et al.[9] reported the experimental data of the multiple ionization cross sections of Ar and Ne atoms by the 1.05 MeV/amu Ar^{Z_1+} and Ne^{Z_1+} ($Z_1=4,6,8$) impact[5-9]. Saito et al. measured the ionization cross section of Ar atom impacted by the 2 MeV C^{3+} [10]. Moreover, they have simultaneously investigated the electron capture process. In recent years, Melo et al. systematically measured the multiple ionization cross sections of He, Ne, Ar, Kr, and Xe by a proton and an antiproton with 2 MeV impact[11].

On the other hand, the theoretical studies for the multiple ionization probability of an atom have been mainly done both by the independent electron model(IEM) [12] and by the statistical energy deposition model(SED) [13,14]. The calculation based on the IEM needs the impact-parameter-dependent ionization probability and the ionization energies of neutral atoms or the ionization energies for the individual ionized states. In most cases, this model is based on the perturbative treatment, so that the ionization probability exceeds unity and some artificial treatments will be needed. The calculation based on the SED, on the other hand, needs the impact-parameter-dependent energy loss and the ionization energies of individual ionized states. In this model, the ionization probabilities are governed by the factor fitted to the existing data. Itoh calculated the differential ionization cross section as a function of the scattering angle[15,16] with Kaneko's ionization probability[17].

The aim of this paper is to investigate the multiple ionization process by the IEM without any fitting parameters or corrections. Here, the impact-parameter-dependent ionization probability is obtained

from single ionization cross section with the impact-parameter-dependent energy transfer. The multiple ionization probability for two cases is calculated with the ionization energies of neutral atoms[18] and of ionized[19] states. In sec. 2, the ionization probability is derived from the single ionization cross section. Section 3 is devoted to the treatment of the multiple ionization probability and the comparison of theoretical results with experimental data. In sec. 4, we give a conclusion. Throughout the paper, e , m_e , a_B , v_B and \hbar denote the elementary charge, the electron rest mass, the Bohr radius, the Bohr velocity and the Planck constant divided by 2π , respectively.

2. Ionization Probability

We consider the ionization of an atom colliding with the fast ion. We assume that the projectile is the point charge, with the incident velocity faster than the mean orbital velocity of the target electron. The charge exchange processes are assumed not to occur during the passage. For simplicity, we first consider the cross section for ionizing the hydrogenlike atomic electron in the Born approximation. According to quantum-mechanics, the ionization cross section by the point charge projectile with charge, Z_1e , can be analytically obtained. Here, the initial and the final states are the 1s-state and the continuous-state eigenfunctions of a pure Coulomb field. the differential cross section, $d\sigma$, for exciting from the 1s to the $\vec{\kappa}$ state is expressed as

$$d\sigma = \frac{8\pi Z_1^2 e^4}{q^3 v^2 \hbar^2} |\langle \vec{\kappa} | \exp(-i\vec{q}\vec{r}) | 1s \rangle|^2 dq d\vec{\kappa}, \quad (1)$$

where $\hbar\vec{q}$, v and $\vec{\kappa}$ denote, respectively, the momentum transfer vector, the incident velocity and the wave number of the emitted electron. The wave function of the initial and the final states are expressed as

$$\psi_{1s} = \frac{1}{\sqrt{\pi a^3}} \exp\left(-\frac{r}{a}\right), \quad (2)$$

$$\psi_{\kappa} = \frac{1}{(2\pi)^{3/2}} \exp\left(\frac{\pi}{2a\kappa} + i\vec{\kappa}\vec{r}\right) \Gamma\left(1 + i\frac{1}{a\kappa}\right) F\left(-i\frac{1}{a\kappa}, 1, -i(\kappa r + \vec{\kappa}\vec{r})\right) \quad (3)$$

where, Γ and F are the gamma function and the confluent hypergeometric function. The constant a is the 1s orbital radius determined by the binding energy ϵ as $a = \hbar/\sqrt{2m_e\epsilon}$. After integration, the ionization cross section using these is expressed as

$$\begin{aligned} \sigma &= \int_0^\infty dE \int_{aq_{(min)}}^{aq_{(max)}} d(aq) \frac{2^{11} \pi a^4 Z_1^2 m_e}{(v/v_B)^2 (aq)(\hbar)^2} \\ &\times \frac{\{(aq)^2 + \frac{1+(a\kappa)^2}{3}\} \exp[-\frac{2}{a\kappa} \tan^{-1} \frac{2a\kappa}{(aq)^2 - (a\kappa)^2 + 1}]}{\{(aq + a\kappa)^2 + 1\}^3 \{(aq - a\kappa)^2 + 1\}^3 (1 - e^{-2\pi/a\kappa})} \end{aligned} \quad (4)$$

where $E (= \hbar^2 \kappa^2 / 2m_e)$ is the energy of the emitted electron and the value of \tan^{-1} ranges from 0 to π .

Here we introduce the impact dependent energy transfer, derived in the classical Rutherford scattering. In derivation, the binding effect is neglected so that one can connect this energy transfer with the kinetic energy of the ionized electron. Then we have

$$E = \frac{2Z_1^2 e^4}{m_e v^2} \frac{1}{b^2 + a^2 + (Z_1 e^2 / m_e v^2)^2} \quad (5)$$

whrer b denotes the impact parameter. Here, we adopt $b^2 + a^2$ instead of b^2 because the uncertainty of the target electron is taken into account.

Once this relation is used, we rewrite the ionization cross section in the form of the impact-parameter expression with the classical energy transfer. Then, by comparing the formal expression for the ionization cross section

$$\sigma = 2\pi \int db b P(b). \quad (6)$$

with the modified expression using eq.(5), the impact-parameter-dependent ionization probability $P(b)$ is finally derived as

$$P(b) \equiv \int_{aq(min)}^{aq(max)} d(aq) \frac{2^{12} (a/a_B)^4 Z_1^4}{(v/v_B)^4 (aq) \{ (\frac{Z_1}{(v/v_B)^2})^2 + (b/a_B)^2 \}^2} \times \frac{\{(aq)^2 + \frac{1+(a\kappa)^2}{3}\} \exp[-\frac{2}{a\kappa} \tan^{-1} \frac{2a\kappa}{(aq)^2 - (a\kappa)^2 + 1}]}{\{(aq + a\kappa)^2 + 1\}^3 \{(aq - a\kappa)^2 + 1\}^3 (1 - e^{-2\pi/a\kappa})}, \quad (7)$$

where $q_{(min)} = (E + \epsilon)/\hbar v$ with E in eq.(5) (ϵ : ionization energy) and $q_{(max)} = \infty$. The derived probability eq.(7) does not exceed unity even for highly charged projectiles and satisfies the unitarity.

3. Multiple Ionization

In this section, we consider the multiple ionization on the basis of the expression eq.(7) together with two types of the independent electron models. One is that the ionization energies for the atomic states are used[18]. The other is that the ionization energies are changed, depending on the degree of ionization[19].

In the first case, the n -th multiple ionization probability for a given shell is expressed as

$$P_n(b) = \binom{N}{n} P(b)^n (1 - P(b))^{N-n} \quad (8)$$

where N is the number of the target electrons in the shell of interest, and n is the number of the emitted electrons among them.

If we extend this method to the cases for more atomic shells taking part in the n -th multiple ionization probability is written as

$$P_n(b) = \sum_{j=0}^n P_{n-j}^A(b) P_j^B(b) \quad (9)$$

where, P^A and P^B are the ionization probability for the shell A and the shell B, respectively. Figure 1 shows the multiple ionization cross sections of Ar atom by the 1.05 MeV/amu Ar^{Z_1+} ($Z_1=4,6,8$) impact. The solid symbols connected by solid lines show the theoretical results. The open symbols connected by dashed lines show the experimental data[7]. The ionization energies of neutral atoms in ref.[18] are used. On the other hand, the squares, triangles and circles show the experimental data for the cases of $Z_1=4, 6$, and 8 , respectively. These experimental data are well considered to be the direct ionization cross section without the charge changing process. At a glance, the cross sections for the small charge states are well reproduced but for the large charge states there is an unnegligible discrepancy.

In the second case, we assume that the electrons are ionized one by one and the rest electrons immediately move to the transient ground state. Moreover, the electrons in the inner shells are assumed not to be ionized till the electrons in the outer shells are all ionized. Then, the n -th multiple ionization probability for each shells is expressed as (When n -th electrons are ionized till α shell)

$$P_n(b) = \binom{N_\alpha}{n_\alpha} P(b, \epsilon_1) P(b, \epsilon_2) \cdots P(b, \epsilon_n) (1 - P(b, \epsilon_{n+1}))^{N_\alpha - n_\alpha} / C, \quad (10)$$

where N_α denotes the number of electron in the shell α and n_α denotes the number of emitted electrons from the shell α . In addition, ϵ_1 , ϵ_2 and ϵ_n denote the first, the second, and the n -th ionization energies.

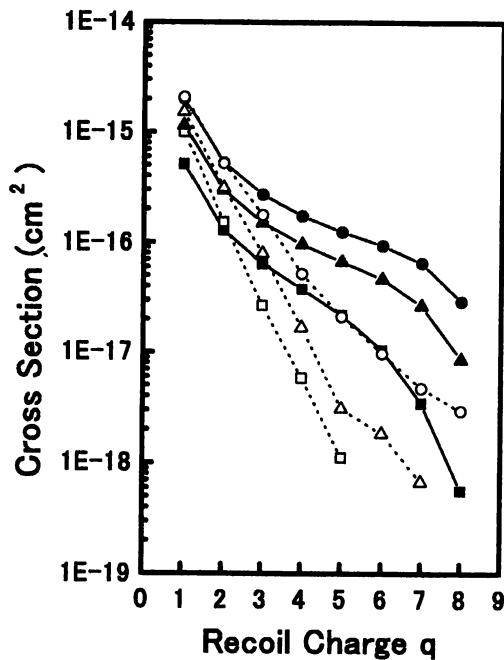


FIG. 1. The multiple ionization cross sections of a Ar atom by the 1.05 MeV/amu Ar^{Z_1+} ($Z_1=4,6,8$) impact. The ionization energies for the atomic states are used[18]. The solid symbols connected by solid lines show the theoretical results. The open symbols connected by dashed lines show, respectively the experimental data[7]. The squares, triangles and circles show the cases, respectively where the incident charges are 4, 6, and 8.

The C is the normalization constant. Figure 2 shows the multiple ionization cross sections calculated by using the successive ionization model. Here, the experimental data and the symbols are the same as in fig.1. The ionization energies used here are shown in ref.[19]. Figure 3 shows the multiple ionization cross sections of Ne atom with 1.05 MeV/amu Ar^{Z_1+} ($Z_1=4,6,8$) impact[9]. These are the same the symbols as in fig.1. Figure 4 is the multiple ionization cross sections of Ar atom by the 2 MeV C^{3+} impact together with the data[10]. The solid squares connected by the solid lines and the open squares connected by the dashed lines show the theoretical results and the experimental data, respectively.

4. Conclusion

In this paper, the multiple ionization process of Ne, and Ar atoms collided bombarded by fast charged particle faster than the Bohr velocity was studied on the basis of a new theoretical formula. Using the derived theoretical formula, we calculated the multiple ionization cross sections with the two kinds of the IEM. The numerical results show good agreement with the data both on the recoil-charge dependence and on the incident-charge dependence. The IEM with the use of the successive ionization energies, depending on the residual charge state, gives better results than the IEM with the use of binding energies of neutral atoms. It means that the multiple ionization will take place in the one-by-one process, and the residual electron system will be successively in the transient ground states.

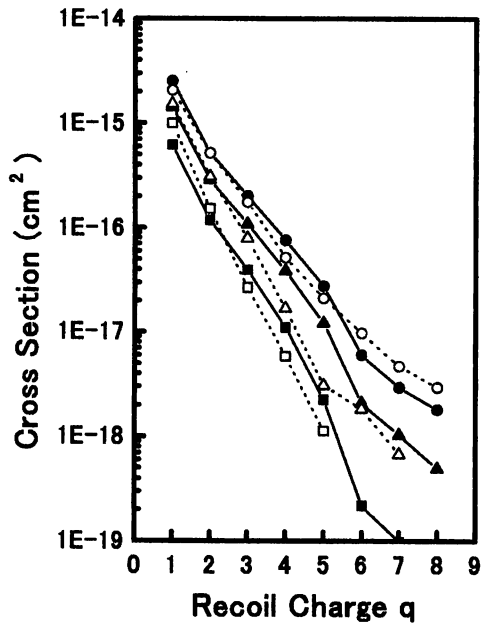


FIG. 2. The multiple ionization cross sections of Ar atom by the 1.05 MeV/amu Ar^{Z_1+} ($Z_1=4,6,8$) impact[7]. The symbols are the same as in fig. 1.

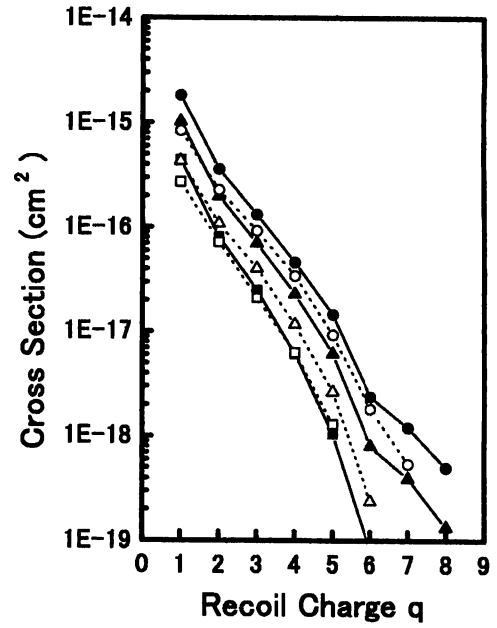


FIG. 3. The multiple ionization cross sections of Ne atom by the 1.05 MeV/amu Ar^{Z_1+} ($Z_1=4,6,8$) impact[9]. The symbols are the same as in fig. 1.

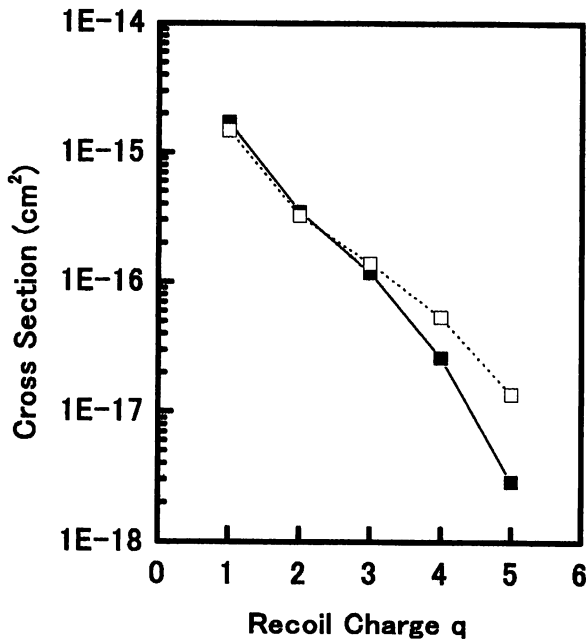


FIG. 4. The multiple ionization cross sections of Ar atom by the 2 MeV C^{3+} impact. The solid squares connected by solid and open squares connected by dashed lines show the calculation results and the experimental data[10], respectively.

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