Polarization Effect of Orbital Electrons in High-Energy Impact

I. 12 Polarization Effect of Orbital Electrons in High-Energy Impact

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Inner shell ionizations by bombardments with heavy charged particles have been extensively studied during this decade. Brandt and Basbas[1] have measured the projectile-charge dependence of inner-shell-ionization cross section and found the coulomb deflection effect in a low-energy region and the binding energy effect in an intermediate energy region. Recently[2], we have measured the projectile-charge dependence of Al K-shell ionization by the bombardment with protons and ^{3}He ions over the energy range of 3-20 MeV/amu and observed the polarization effect of Al K-orbital electrons. The experimental result, however does not agree well with the theory of Reading and Binstock[3] based on the Glauber approximation and a more precise theoretical treatment is desirable. In this report, the theory of polarization effect will be developed on the basis of ionization mechanism and compared with the experimental results of Al K-shell ionizations.

In conformity with the Glauber approximation, a scattered initial wave function is expressed by,

$$\psi_i = e^{i\vec{K}\cdot\vec{R}}\,\psi_{1s}(\vec{r})S(\vec{R},\vec{r}) \qquad \text{.....................(1)}$$

where $\psi_{1s}(\vec{r})$ is the wave function of 1s-state electron and $\vec{K}$ is the wave number of the projectile. The function $S(\vec{R},\vec{r})$ is to be derived from

$$i\hbar v\frac{\partial}{\partial z}S(\vec{R},\vec{r}) = (\tilde{H}_e - \frac{Z_1e^2}{|\vec{R}-\vec{r}|})S(\vec{R},\vec{r}) \qquad \text{.....................(2)}$$

with

$$\tilde{H}_e = -\frac{\hbar^2\nabla_r^2}{2m_e} + \frac{\hbar^2}{m_ea_s}\frac{\partial}{\partial r} \equiv \tilde{FT} + \tilde{BT} \text{ and } a_s = \frac{a_0}{Z},$$

where $\vec{R}$ and $\vec{r}$ are the position vectors for, respectively, the projectile and the electron with respect to the target-atomic nucleus, Z_1 is the atomic number of projectile, a_0 is the Bohr radius, Z_s is the effective nuclear charge, m_e is the electron rest mass, v is the velocity of projectile, and $\tilde{FT}$ and $\tilde{BT}$ are called, respectively, the freely recoiling term and the binding term.

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The solution of Eq. (2) is approximately given by

$$S(\vec{R},\vec{r}) = e^{-i\tilde{H}_e Z/\hbar v} e^{\frac{i}{\hbar v}\int_{-\infty}^{Z} V_I dz'} \qquad \text{.....................(3)}$$

with

$$V_I = e^{i\tilde{H}_e Z/\hbar v} \frac{-Z_1 e^2}{|\vec{R}-\vec{r}|} e^{-i\tilde{H}_e Z/\hbar v} ,$$

though the integral equation Eq. (3) can not be directly evaluated. According to Binstock and Reading, if the exchage term $[\frac{iz}{\hbar v}\tilde{FT}, \frac{iz}{\hbar v}\tilde{BT}]$ is negligible in comparison with $\frac{iz}{\hbar v}\tilde{FT}$ and $\frac{iz}{\hbar v}\tilde{BT}$, eq. (3) can be solved, and the exchange term is expressed by

$$[\frac{iz}{\hbar v}\tilde{FT}, \frac{iz}{\hbar v}\tilde{BT}] = \varepsilon(r)\frac{iz}{\hbar v}\tilde{FT}' . \qquad \text{.....................(4)}$$

Here,

$$\varepsilon(r) = -2i\frac{v_0}{v}\frac{z}{r} , \qquad \text{.....................(5)}$$

$$\tilde{FT}' = \tilde{FT} + \frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right) , \qquad \text{.....................(6)}$$

and v_0 is the average velocity of orbital electrons. If we assume that

$$\frac{v_0}{v} < 1 , \qquad \text{.....................(7)}$$

and

$$\frac{z}{r} < 1 , \qquad \text{.....................(8)}$$

the exchange term can be neglected. The condition Eq. (7) is satisfied in the present case. The effective value of Z is estimated from the uncertainty principle to be

$$Z \simeq 1/q ,$$

where q is the transfer momentum of the projectile. So that, Eq. (8) becomes $qr > 1$, which means a close collision.[4] The Binstock and Reading approximation should therefore be applicable to a close collision and the contribution of the polarization effect to the ionization cross section can be given by

$$\delta\sigma_c(Z_1) = \frac{8\pi a_0^2}{Z_s^4}\frac{Z_1^2}{\eta_K}\int_{W_{min}}^{\infty}\frac{dW}{W}\int_{Q_{min}}^{\infty}\frac{dQ}{Q} F_K^{cc}(W,Q)\int_0^1 dx' F(c(1-x'^2)^{1/2}), \qquad \text{.......(9)}$$

where η_K, W_{min} and Q_{min} should be referred to Merzbacher and Lewis.[5] The function $F_K^{cc}(W,Q)$ is the generalized oscillator strength of the K-shell for close collisions. The term $F(c(1-x'^2)^{1/2})$ is estimated using the function $S(\vec{R},\vec{r})$ and has been defined in Ref. 3. Values of the cross section ratio R calculated from Eq. (9) are shown with a solid line in Fig. 1, where R is defined as the ratio between the ionization cross sections divided by the square of the projectile charge Z_i for two kinds of projectiles of same velocity — $R \equiv Z_2^2\sigma(Z_1)/Z_1^2\sigma(Z_2)$ with $Z_1 > Z_2$. It is seen in Fig. 1 that the agreement with the experiment is improved than that of Binstock and Reading shown with the dot curve.

As was mentioned above, the Glauber approximation is not applicable to the calculation of the polarization effect in distant collision ($qr < 1$), whereas the distant-collision theory of Hill and Merzbacher[6] is applicable. Using the theory of Hill and Merzbacher, the contribution of the polarization effect is distant collisions is estimated to be

$$\delta\sigma_D(Z_1) = \frac{6\pi^2 a_0^2}{Z_5^5} \frac{Z_1^3}{(\eta_K)^{\frac{5}{2}}} (\ell n(\frac{4\eta_K}{\theta_K}) - 1.6) \ , \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(10)$$

where θ_K is the screening constant defind by Merzbacher and Lewis. Values of R calculated from Eq. (10) are shown with the dot and dashed curve in Fig. 1.

As the result, the inner-shell ionization cross section for high-energy impact can be expressed by

$$\sigma^i(Z_1) = \sigma_{PWBA}(Z_1) + \delta\sigma_D(Z_1) + \delta\sigma_C(Z_1) \ , \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(11)$$

where σ_{PWBA} is the ionization cross section given by Merzbacher and Lewis. The predictions from Eq. (11) are compared with the experiments in Fig. 2, where the agreement is quite satisfactory. It is thus found that the polarization effects in distant collisions and in close collisions cancel out each other in the high-energy region.

References

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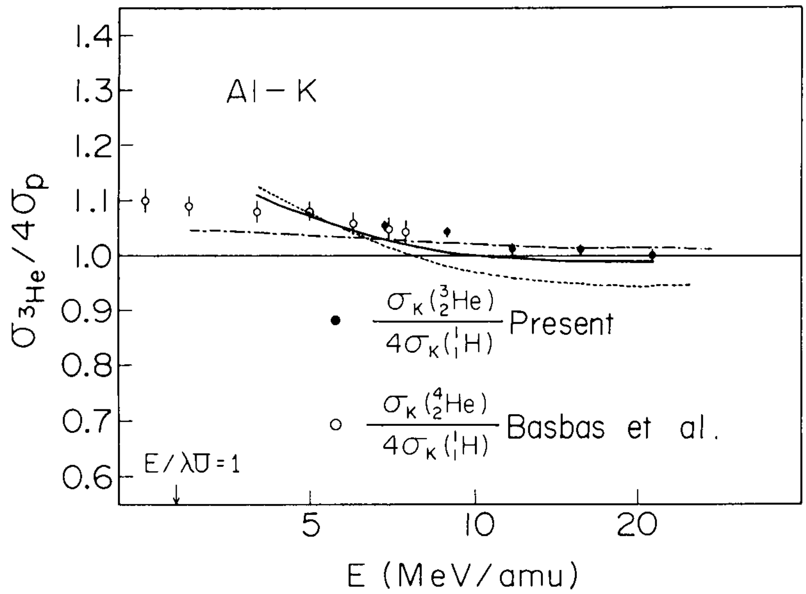

Fig. 1. The experimental results on Al K-shell ionizations are compared with the theoretical predictions. The dotted curve shows the result of calculation by Binstock and Reading. The solid and the dot and dashed curves show those from Eq. (9) and from Eq. (10), respectively.

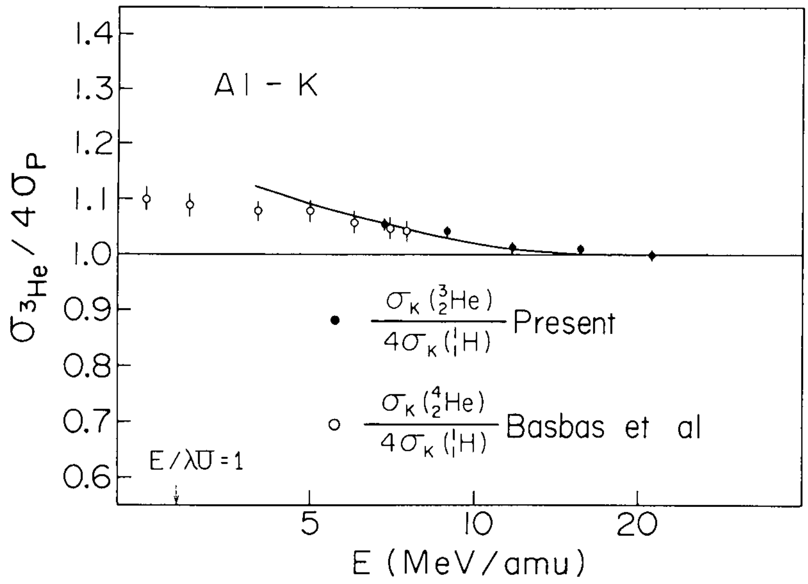

Fig. 2. Comparison between the experimental results and the calculation using the Glauber approximation combined with the distant-collision theory of Hill and Merzbacher.