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Electronic Relativistic Effects in K-Shell Ionization by Charged-Particle Impact

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The K-shell ionization cross sections by heavy charged-particle impact are evaluated in the plane-wave Born approximation, using relativistic Dirac functions for the atomic electrons. The effect of binding-energy increase due to the projectile is estimated by the use of relativistic wave functions for K-shell electron and the Coulomb-deflection effect is also taken into account. Numerical results are compared with the corresponding values of the nonrelativistic plane-wave Born approximation and the relativistic semiclassical approximation as well as the experimental data.

KEY WORDS: Relativistic PWBA / Binding-energy effect / Coulomb-deflection effect /

I. INTRODUCTION

Inner-shell ionization by charged-particle impact has long been the interesting subject in the field of atomic physics. In recent years, however, this field has received special attention mainly due to progress in experimental techniques. The amount of experimental results has increased and extensive studies on theoretical treatments have also been made.[1~3] When incident energy of the projectile is high, it is believed that the direct Coulomb interaction between the projectile and the atomic electron in the target plays a dominant role. There have been developed three theoretical models for direct Coulomb ionization: Binary-encounter approximation (BEA),[4] semiclassical approximation (SCA),[5] and plane-wave Born approximation (PWBA).[6]

In all the approximations mentioned above, the target electrons are usually described by nonrelativistic hydrogenic wave functions. When the incident energy is not so high, it is possible to treat projectiles nonrelativistically, but for atomic numbers higher than 50, the use of nonrelativistic wave functions for target atom underestimates the ionization cross section considerably. The electronic relativistic effects for K shell were first studied by Jamnik and Zupančič[7] in PWBA. Using relativistic (Dirac) wave functions for target electrons, they showed that the relativistic effects increase the cross section substantially for targets with high atomic numbers. Similar calculations for L shell have been performed by Choi.[8] In the case of BEA, Hansen[9] took relativistic effects into account by using the relativistic mass-velocity relation for the atomic electron. Bergen group[10,11] has

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developed the relativistic SCA theory (RSCA) by the use of relativistic hydrogenic wave functions for target electrons. Their results indicate that relativistic effects become increasingly important with decreasing projectile energies, and that the relativistic cross section is 30% higher than the nonrelativistic one even for atomic number as low as 29 (Cu) for the projectile energy of 0.2 MeV/amu.

For ionization by slower projectiles, other effects become important. First, the deflection effect of the projectile in the nuclear Coulomb field will no longer be negligible. This means that it is not valid to approximate the projectile as a plane wave[6] or a straight line.[5] Second, for heavier projectiles the increase in the binding energy of the target electron due to penetration of the projectile in the field of the target atom should be taken into consideration. Basbas *et al.*[12] used the perturbed-stationary-state theory[13] and introduced the modifications to the PWBA for Coulomb-deflection and increased binding-energy effects. The modified PWBA theory has been successfully employed to interpretate the experimental data. However, it should be noted that this theory is nonrelativistic. At low projectile energies and for high target atomic numbers, the relativistic effects are expected to be important.

In the case of RSCA, Amundsen[11] included the Coulomb-deflection effect in his calculations as a correction factor, but not binding-energy effect. Recently, Pauli *et al.*[14] have developed the RSCA theory in hyperbolic path. They corrected their results for binding-energy increase by the use of the correction factor derived by Basbas *et al.*[12]

On the other hand, there has been reported no relativistic PWBA theory (RPWBA) including binding-energy and Coulomb-deflection effects. The calculated values of Jamnik and Zupančič in RPWBA for proton impact on Pb are systematically larger than the experimental results in low-energy region. This fact indicates that these effects are important for heavy elements for low-energy projectiles.

The aim of the present work is to calculate the K-shell ionization cross section in RPWBA with binding-energy and Coulomb-deflection effects, and to compare with the experimental data as well as the results of the RSCA calculations.

II. RELATIVISTIC PLANE-WAVE BORN APPROXIMATION

A. Cross Section

In PWBA, the differential cross section for ejection of K-shell electron by the projectile is written by[2,6]

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E_f}=\frac{8\pi}{\hbar^2}Z_1^2e^4\frac{M_1}{E_1}\int_{q_{\min}}^{q_{\max}}\frac{\mathrm{d}q}{q^3}|F_{if}(q)|^2, \tag{1}$$

where E_f is the kinetic energy of the ejected electron, $\hbar \boldsymbol{q}$ is the momentum transferred to the K-shell electron, and Z_1, M_1, and E_1 are the charge, mass, and kinetic energy of the projectile, respectively. The form factor $F_{if}(q)$ is defined as

$$F_{if}(q)=\int e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\psi_f^*(\boldsymbol{r})\psi_i(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}. \tag{2}$$

Here $\psi_i(\boldsymbol{r})$ and $\psi_f(\boldsymbol{r})$ are the electron wave functions for the initial and final states.

When the energy ΔE lost by the projectile in the collision is small compared with the incident energy E_1, the minimum value of q can be approximated as

$$q^2_{\min} \simeq (\Delta E)^2 M_1/(2\hbar^2 E_1)[1+\Delta E/(2E_1)]. \tag{3}$$

On the other hand, we may in most cases set $q_{\max}=\infty$ without appreciable error.

For the wave functions of the electrons, we use the solution of the Dirac equation in the Coulomb field

$$\phi^\mu_\kappa = \begin{pmatrix} g_\kappa(r) & \chi^\mu_\kappa(\Omega) \\ \mathrm{i}f_\kappa(r) & \chi^\mu_{-\kappa}(\Omega) \end{pmatrix}, \qquad \kappa=\pm 1,\ \pm 2,\cdots\cdots \tag{4}$$

where $\chi^\mu_\kappa(\Omega)$ is the spin-angular wave function, and μ is the z component of the angular momentum j, $\kappa=\mp(j+1/2)$ for $j=l\pm 1/2$, and l is the orbital angular momentum.

Integrating the square of Eq. (2) over angular variables, summing over the final magnetic quantum numbers, and averaging over the initial magnetic quantum numbers, we obtain

$$|F_{if}(q)|^2 = \sum_{\kappa_f} |\kappa_f| \{\int j_l(qr)[f_{\kappa_i} f^*_{\kappa_f} + g_{\kappa_i} g^*_{\kappa_f}] r^2 \mathrm{d}r\}^2, \tag{5}$$

where κ_i and κ_f are the κ quantum numbers in the initial and final electronic states, and $j_l(x)$ is the spherical Bessel function of order l.

B. Calculation of Form Factor

The relativistic hydrogenic radial wave functions, $f_\kappa(r)$ and $g_\kappa(r)$, for the discrete and continuum states are given in the text book of Rose.[15] The wave functions for final continuum states are normalized per unit energy interval. In the case of K-shell electron, $\kappa_i=-1$. With these wave functions, the radial integral in Eq. (5)

$$I = \int j_l(qr)[f_{-1} f^*_{\kappa_f} + g_{-1}\ g^*_{\kappa_f}] r^2 \mathrm{d}r, \tag{6}$$

can be calculated by following the method of Jamnik and Zupančič.[7]

The final result is

$$I = Aq^{-(\gamma+\gamma'+1)} S(\zeta/q), \tag{7}$$

where $\zeta=\alpha Z_2$, $\gamma=[\kappa^2-\zeta^2]^{1/2}$, Z_2 is the atomic number of the target, α is the fine structure constant, and the primed quantities refer to the final state. The factor A is

$$A = \frac{\pi^{1/2}\Gamma(2a)}{2^{l+1}} D_i D_f, \tag{8}$$

where

$$D_i = (2\zeta)^{\gamma+1/2}/[2\Gamma(2\gamma+1)]^{1/2},$$

and $a=(\gamma+\gamma'+l+1)/2$. The factor D_f depends on whether the final state is discrete or continuous.

For the discrete final state with principal quantum number n,

$$D_f = [\Gamma(2\gamma'+n'+1)/\{(n'!)\zeta/\lambda(\zeta/\lambda-\kappa)\}]^{1/2}(2\lambda)^{\gamma'+1/2}/[2\Gamma(2\gamma'+1)],$$

with
$$n' = n-|\kappa|,$$
$$W = [1+\zeta^2/(n'+\gamma')^2]^{-1/2},$$
$$\lambda = (1-W^2)^{1/2},$$

and for the continuum final state,

$$D_f=\frac{2^{\gamma'-1}}{\Gamma(2\gamma'+1)}(m_0/\pi)^{1/2}p^{\gamma'-1/2}\exp(\pi y/2)\,|\Gamma(\gamma'+iy)|,$$

with

$$W=(E_f+m_0c^2)/m_0c^2,$$
$$p=(W^2-1)^{1/2},$$
$$y=\zeta W/p.$$

On the other hand,

$$S(x)=F\sum_m P_m(-1)^m x^{2m}+G\sum_m Q_m(-1)^m x^{2m+1}, \tag{9}$$

where

$$P_m=\frac{(a)_m(b)_m}{(c)_m m!}p_m, \qquad Q_m=\frac{(a+1/2)_m(b+1/2)_m}{(c+1)_m m!}q_m,$$
$$b=(\gamma+\gamma'-l)/2, \qquad c=1/2,$$

and $(a)_m$ is a Pochammer symbol.

The quantities p_m and q_m are

$$p_m=[s(\zeta/\lambda-\kappa)F(-2m,\ -n';\ 2\gamma'+1\ ;\ u)$$
$$\qquad -tn'F(-2m,\ -n'+1\ ;\ 2\gamma'+1\ ;\ u)]\,v^{2m},$$
$$q_m=[s(\zeta/\lambda-\kappa)F(-2m-1,\ -n'\ ;\ 2\gamma'+1\ ;\ u)$$
$$\qquad -tn'F(-2m-1,\ -n'+1\ ;\ 2\gamma'+1\ ;u)]\,v^{2m+1},$$
$$s=[(1+\gamma)(1+W)]^{1/2}+[(1-\gamma)(1-W)]^{1/2},$$
$$t=[(1+\gamma)(1+W)]^{1/2}-[(1-\gamma)(1-W)]^{1/2},$$
$$u=2\lambda/(\lambda+\zeta), \qquad v=(\lambda+\zeta)/\zeta,$$

for the discrete final state, and

$$p_m=2\ \mathrm{Re}\{F(-2m,\ \gamma'+1+iy\ ;\ 2\gamma'+1\ ;\ u)\,v^{2m}X\},$$
$$q_m=2\ \mathrm{Re}\{F(-2m-1,\ \gamma'+1+iy\ ;\ 2\gamma'+1\ ;\ u)\,v^{2m+1}X\},$$
$$u=2ip/(\zeta+ip), \qquad v=(\zeta+ip)/\zeta,$$
$$X=\{[(W+1)(1+\gamma)]^{1/2}-i[(W-1)(1-\gamma)]^{1/2}\}(\gamma'+iy)\exp(i\eta),$$
$$\exp(2i\eta)=-(\kappa-iy/W)/(\gamma'+iy),$$

for the continuum final state. Here $F(a,\ b\ ;\ c\ ;\ x)$ is the Gauss-type hypergeometric function.

C. Screening Effects and Energy Integration

The screening effects are taken into account as usual in PWBA. First, the effective nuclear charge Z_{eff} is used to take account of inner screening. For this purpose, the Slater screening constant[16] is used and the nuclear charge in the electron wave functions is replaced by $Z_{eff}=Z_2-0.3$. Second, the outer screening effect is introduced by adding a constant term V/e due to the presence of outer electrons to the Coulomb potential $Z_{eff}e/r$. The energy V is determined as the difference between the observed ionization energy of the K-shell electron and the "ideal" binding energy estimated from the hydrogenic model for effective nuclear charge Z_{eff}. Hock[17] pointed out that in the vicinity of the K-shell radius the atomic potential thus obtained is a good approximation to the relativistic self-consistent-field potential calculated by Carlson *et al.*[18] Using this potential, the outer screening effect is taken into account by replacing the kinetic energy of the electron E_f by the effective value $E_f - V$.

The total K-shell ionization cross section σ_K is evaluated by integrating Eq. (1) over the energy of the ejected electron:

$$\sigma_K = \int_0^\infty \frac{d\sigma}{dE_f} dE_f. \tag{10}$$

For energies with $E_f < V$, the effective energy $E_f - V$ becomes negative. In this case, it is assumed that the electron transfers to the distrete state, in which n' is non-integer and a continuum variable. In order to integrate over these states with respect to W, the square of the radial integral, [Eq. (6)], should be multiplied by

$$\frac{dn'}{dW} = [(n'+\gamma')/W]^3/\zeta^2. \tag{11}$$

Thus the square of the from factor is integrated over q according to Eq. (1) and then the ionization cross section is calculated from integration over E_f [Eq. (10)].

III. BINDING-ENERGY FACTOR AND COULOMB DEFLECTION

A. Binding-Energy Factor

When the projectile penetrate deeply within the K shell of the target atom during collision, the target K-shell electrons become more tightly bound to the nucleus due to the presence of the projectile. The increased binding reduces the K-shell ionization probability. This effect for K-shell electron was first estimated by Basbas *et al.*[12] non-relativistically by the use of hydrogenic wave functions. Using the nonrelativistic differential ionization cross section for K shell derived by Bang and Hansteen,[5] they showed in the perturbed-stationary-state approximation[13] that the binding-energy effect can be taken into account by replacing the screening number θ_K by $\varepsilon\theta_K$ in the PWBA theory. Here the screening number θ_K is defined as the ratio of the observed K-shell binding energy to the "ideal" ionization energy in the absence of outer-shell electrons. The binding-energy factor ε is given by

$$\varepsilon = 1 + \langle \Delta E_K \rangle / E_K, \tag{12}$$

where E_K is the observed K-shell binding energy, and $\langle \Delta E_K \rangle$ is the average change in K-shell binding energy during collision.

In the first-order perturbation theory, the change in binding energy is given by

$$\Delta E_K = \int \psi_K^*(\boldsymbol{r}) \frac{Z_1 e^2}{|\boldsymbol{R}-\boldsymbol{r}|} \psi_K(\boldsymbol{r})\, d\boldsymbol{r}, \tag{13}$$

where $\psi_K(\boldsymbol{r})$ is the unpertubed wave function for K-shell electron, $\boldsymbol{R}$ is the coordinate of the projectile, and $\boldsymbol{r}$ is that of the K-shell electron.

For K-shell electron we use relativistic wave function given in Eq. (4). Using a multipole expansion of $1/|\boldsymbol{R}-\boldsymbol{r}|$, and choosing z axis along $\boldsymbol{R}$, we can perform easily integration over angular variables. Then Eq. (13) simplifies to

$$\Delta E_K = Z_1 e^2 [\int_0^R \{g^2_{-1} + f^2_{-1}\} r^2 dr/R + \int_R^\infty \{g^2_{-1} + f^2_{-1}\} r dr], \tag{14}$$

where $R \equiv |\boldsymbol{R}|$. Inserting the radial wave functions in Ref. (15) into Eq. (14), we obtain

$$\Delta E_K = \frac{Z_1 e^2}{\Gamma(2\gamma+1)} \frac{1}{R} [\gamma(2\gamma+1,\ 2R/a_{2K}) + \frac{2R}{a_{2K}} \Gamma(2\gamma,\ 2R/a_{2K})], \tag{15}$$

where $a_{2K} = Z_{2K}/a_0$, $Z_{2K} = Z_2 - 0.3$, and a_0 is the Bohr radius. The two functions $\gamma(a, x)$ and $\Gamma(a, x)$ are the incomplete gamma functions defined as follows:

$$\gamma(a,\ x) = \int_0^x \exp(-t)\, t^{a-1} dt,$$

and

$$\Gamma(a,\ x) = \int_x^\infty \exp(-t)\, t^{a-1} dt.$$

Following Basbas *et al.*,[12] we assume that the projectile is described in a straight-line trajectory with an impact parameter b and R can be approximated by b. Then we obtain in units of Ry

$$\Delta E_K = \frac{Z_1 Z_{2K}}{\Gamma(2\gamma+1)} \frac{2}{y} [\gamma(2\gamma+1,\ 2y) + 2y\Gamma(2\gamma,\ 2y)], \tag{16}$$

with $y = b/a_{2K}$. This expression is equivalent to that derived by Amundsen,[19] and in the limit of $\gamma = 1$ reduces to the nonrelativistic expression obtained by Basbas *et al.*[12]

In Fig. 1, the quantity $\Delta E_K/(Z_1 Z_{2K})$ is plotted against the impact parameter for $Z_2 =$ 50, 79, and 92. For comparison, the nonrelativistic result is also plotted. It should be noted that the relativistic results depend on the target atomic number Z_2. The relativistic effects become pronounced with increasing Z_2 and with decreasing b.

The average value of ΔE_K is defined as

$$\langle \Delta E_K \rangle = \int_0^\infty \Delta E_K(y) \left(\frac{d\sigma_K}{dE_f}\right)_b y dy \Big/ \int_0^\infty \left(\frac{d\sigma_K}{dE_f}\right)_b y dy, \tag{17}$$

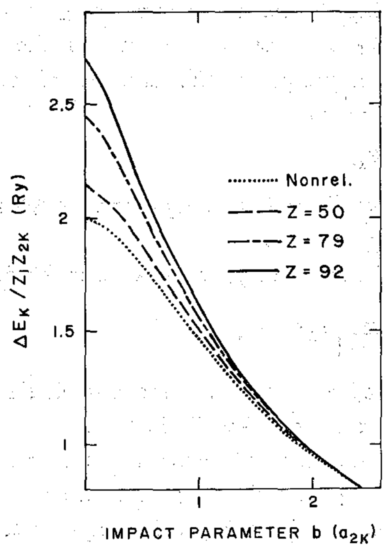

Fig. 1. Increase in scaled binding energy of K-shell electron as a function of impact parameter in units of K-shell radius.

where $(d\sigma_K/dE_f)_b$ is the K-shell ionization cross section with the impact parameter b. The leading term of this cross section has been derived by Bang and Hansteen[5] as

$$\left(\frac{d\sigma_K}{dE_f}\right)_b=\frac{C}{2\pi}q^{-8}(bq)^4K_2^2(bq), \tag{18}$$

where C is a constant, $K_2(x)$ is the modified Bessel function of order 2, $q=(E_f+E_K)/\hbar v_1$ is the minimum momentum transfer, and v_1 is the velocity of the projectile.

Using Eq. (18) and introducing the new parameters, $q_0=E_K/\hbar v_1$, $x=bq_0$, and $\xi=(a_{2K}q_0)^{-1}$, Eq. (17) can be written as

$$\langle\Delta E_K\rangle=2Z_1g(\xi)E_K/(Z_{2K}\theta_K), \tag{19}$$

where

$$g(\xi)=\frac{5}{2^5}\frac{Z^2_{2K}E_H}{\Gamma(2\gamma+1)}\frac{\theta_K}{\xi E_K}\int_0^\infty[\gamma(2\gamma+1,\ 2\xi x)+2\xi x\Gamma(2\gamma,\ 2\xi x)]x^4K_2^2(x)\,dx, \tag{20}$$

and E_H is the Rydberg unit.

From Eqs. (12) and (19),

$$\varepsilon=1+2Z_1g(\xi)/(Z_{2K}\theta_K). \tag{21}$$

B. Nuclear Coulomb Deflection

In SCA, Bang and Hansteen[5] calculated K-shell ionization cross section for the projectile moving on the classical hyperbolic path in the Coulomb field of the target nucleus. They showed that the ionization cross section can be approximated from that on the straight-line path by multiplying a correction factor. Integrating the differential cross section of Bang and Hansteen with respect to the energy transfer and using some approximations, Basbas *et al.*[12] derived the modified PWBA cross section including the Coulomb-deflection effect:

$$\sigma_K=9E_{10}(\pi dq_0)\sigma_K^{PWBA}, \tag{22}$$

where σ_K^{PWBA} is the K-shell ionization cross section in PWBA. The function $E_{10}(x)$ is the exponential integral of order 10;

$$E_{10}(x)=\int_1^\infty t^{-10}\exp(-xt)\,dt. \tag{23}$$

The argument in the exponential integral is expressed as

$$\pi dq_0=\frac{1}{2}\pi Z_1(m_0/M)\theta_K^{-2}(\eta_K/\theta_K^2)^{-3/2}, \tag{24}$$

where $\eta_K=(\theta_K/2)^2\xi$, $\hbar q_0$ is the minimum momentum transfer, d is the one-half of the distance of closest approach in head-on collision, and M is the reduced mass of the projectile and the target.

Equation (22) has been successfully used to explain the experimental data for projectiles in low-energy region where the Coulomb-deflection effect is important. However, it should be noted that the calculation of Bang and Hansteen in hyperbolic trajectory includes only the monopole term ($l=0$). Therefore, the validity of Eq. (22) is limited to monopole transition and the Coulomb-deflection effect is only partially taken into account by this procedure.

Recently, the Coulomb-deflection effect in the K-shell ionization has been studied extensively within the framework of SCA by Kocbach,[20] Amundsen,[21] and Pauli and Trautmann.[22] According to Pauli and Trautmann,[22] the contribution from the monopole term is dominant for the ejected electrons in low-energy region and for this region the correction for Coulomb deflection by the method of Bang and Hansteen[5] yields roughly the same results as the SCA in hyperbolic path. This fact indicates that for the integrated K-shell ionization cross section σ_K, in which the main contribution comes from the electrons ejected in the low-energy region, Eq. (22) is a good approximation to the cross section in hyperbolic path. In the present work, the Coulomb-deflection effect is taken into account by Eq. (22).

IV. RESULTS AND DISCUSSION

The K-shell ionization cross sections have been computed from Eq. (10) by numerical integration. All the calculations in the present work have been performed on the FACOM M-190 computer of the Data Processing Center of Kyoto University. In general, numerical accuracy is better than 5%.

In Fig. 2, relativistic and nonrelativistic cross sections for protons on Au are plotted together with experimental results. Theoretical predictions are calculated according to the PWBA, the PWBA modified for binding-energy and Coulomb-deflection effects (PWBA-BC), the PWBA-BC corrected for relativistic effects (PWBA-BCR), the relativistic PWBA (RPWBA), and the RPWBA modified for binding-energy and Coulomb-deflection effects

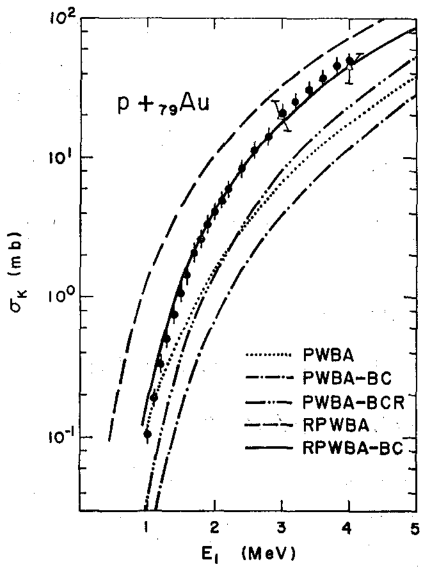

Fig. 2. K-shell ionization cross section for gold bombarded by protons as a function of incident energy. The theoretical predictions: The PWBA, the PWBA modified for binding-energy and Coulomb-deflection effects (PWBA-BC), the PWBA-BC corrected for relativistic effect (PWBA-BCR), the relativistic PWBA (RPWBA) and the RPWBA modified for binding-energy and Coulomb-deflection effects (RPWBA-BC). The experimental points: (●) Kamiya *et al.* (Ref. 23) and (△) Waltner *et al.* (Ref. 24).

(RPWBA-BC). In the case of PWBA-BCR, the relativistic corrections were incorporated through the usual method of Merzbacher and Lewis.[6] They proposed that the relativistic effects can be approximately taken into account in the PWBA by replacing the screening number $\theta_K = I_K/I_{NR}$ by

$$\theta_K = 1-(I_R-I_K)/I_{NR}, \tag{25}$$

where I_K is the measured K-shell ionization energy, I_{NR} is the ionization energy estimated by the nonrelativistic hydrogenic model, and I_R that by the relativistic hydrogenic model.

The comparison between the PWBA and the RPWBA curves indicates that the relativistic effects significantly increase the K-shell ionization cross section. The reason for this increase is ascribed to the increase in the electron density near the target nucleus caused by the relativistic effects, as already pointed out by Jamnik and Zupančič.[7] There is a serious discrepancy between the experimental data and the PWBA values. With the modification for binding-energy and Coulomb-deflection effects, this discrepancy is enhanced and the nonrelativistic PWBA theory (PWBA-BC) remarkably underpredicts the experiment. The relativistic correction by the use of Eq. (25) can improve this situation to some extent, but there still remains a large discrepancy between theory and experiment. This fact suggests that the procedure to include relativistic effects [Eq. (25)] is too crude. On the other hand, the RPWBA overpredicts the experimental results as expected from the results of Jamnik and Zupančič for Pb.[7]

It is clear from the figure that by introducing the modification for binding-energy and Coulomb-deflection effects into the RPWBA (RPWBA-BC), we obtain a satisfactory agreement with the experimental data. For proton bombardment on this element, two

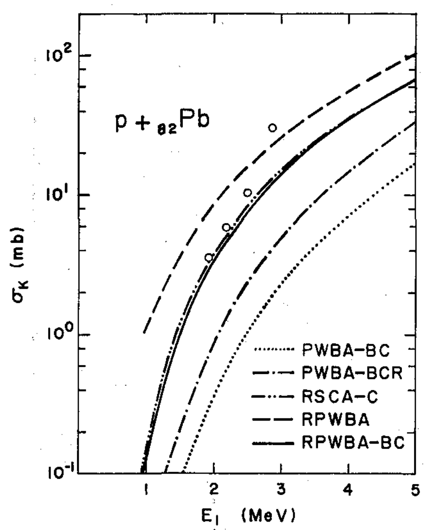

Fig. 3. K-shell ionization cross section for lead bombarded by protons as a function of incident energy. The theoretical predictions: The PWBA-BC the PWBA-BCR, the relativistic SCA modified for Coulomb deflection (RSCA-C), the RPWBA, and the RPWBA-BC. The experimental points are taken from Lewis *et al.* (Ref. 25).

RSCA calculations have been reported; the RSCA modified for Coulomb deflection by Amundsen,[11] and the RSCA including binding-energy and Coulomb-deflection effects by Kamiya *et al.*[23] Both results are in agreement with the present RPWBA-BC curve.

Figure 3 shows nonrelativistic and relativistic cross sections for protons on Pb, together with relevant experimental data. The RPWBA values are in good agreement with the results calculated by Jamnik and Zupančič.[7] The RSCA modified for Coulomb deflection (RSCA-C), calculated by Amundsen,[11] yields almost the same results as the RPWBA-BC. Considering numerical accuracy, 5%, of calculations, we can say that both theories are in good agreement with each other. It should be noted that the RSCA-C does not include the effect of binding-energy increase. For protons in the energy region concerned, this effect is not so large because of small projectile charge. It is also interesting to note that the Coulomb-deflection effect in the RSCA-C[11] was estimated by using a tangential path and introducing an effective projectile velocity.[20]

It can be seen from the figure that the similar conclusion to the case of Au is drawn for Pb. The PWBA-BCR is not enough to predict the experiment and the RPWBA-BC curve fits very well to the experimental data at low proton energies. At 2.88 MeV the experimental value is larger than the values expected by the RPWBA-BC and the RSCA-C. It is hoped to perform further experimental studies in this energy region.

In Fig. 4, the calculated cross sections for α particles on Pb are compared with the experimental values of Dost *et al.*[26] Both the PWBA-BC and the PWBA-BCR considerably underpredict the K-shell ionization cross sections in this case. Pauli *et al.*[14] calculated the RSCA cross sections in hyperbolic path, which are systematically 10% higher than the experimental values. When the correction for binding-energy increase

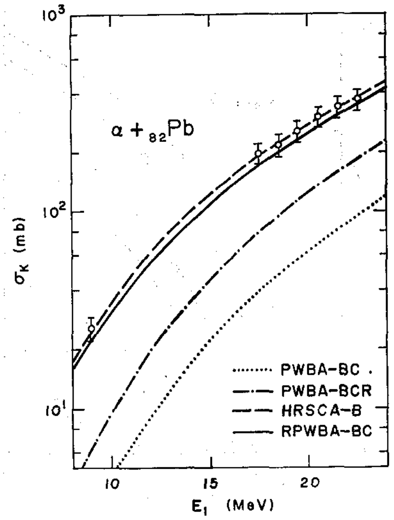

Fig. 4. K-shell ionization cross section for lead bombarded by α particles as a function of incident energy. The theoretical predictions: The PWBA-BC, the PWBA-BCR, the relativistic SCA in hyperbolic path modified for binding-energy effect (HRSCA-B), and the RPWBA-BC. The experimental points are taken from Dost *et al.* (Ref. 26).

is introduced by the method of Basbas *et al.*,[12] the theoretical values (HRSCA-B) are in excellent agreement with the experimental ones. The present RPWBA-BC values are slightly smaller than the experimental ones, but agree well with them within the experimental errors.

V. CONCLUSION

We have calculated the K-shell ionization cross section by charged-particle impact in the relativistic PWBA modified for the binding-energy and Coulomb-deflection effects. A satisfactory agreement between the calculated results and the experimental data has been found for heavy elements. The relativistic SCA including binding-energy and Coulomb-deflection effects leads to practically the same results. This comes from the equivalence of the PWBA and the SCA for total ionization cross sections.[2,27] On the other hand, the relativistic correction frequently used in the PWBA (PWBA-BCR) underpredicts the cross section considerably.

In order to study the electronic relativistic effects in more detail, further comparison between theory and experiment is needed. However, the number of experiments on the K-shell ionization cross section for heavy elements at low bombarding energies is small because of experimental difficulty due to smallness of ionization cross sections. Especially, there is no experiment for heavy projectiles, such as carbon, nitrogen, and oxygen ions, on targets with high atomic numbers. This kind of experiments, if performed, are very interesting because the electronic relativistic effect on the binding-energy increase is expected to be large.

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