Bull. Inst. Chem. Res., Kyoto Univ., Vol. 60, No. 2, 1982

Two Computer Codes for K- and L-Shell Ionization Cross Sections in the Plane-Wave Born Approximation

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Received March 30. 1982

Two computer codes for the K- and L-shell ionization cross sections by heavy charged-particle impact in the plane-wave Born approximation are presented. These codes are the modified versions of the computer code DEKY written by us. One of them, called DEKY2, calculates the relativistic cross sections based on the correction recently derived by Brandt and Lapicki and the corrections for the binding-energy and Coulomb-deflection effects are also included. The second code, DEKY3, includes the correction for polarization effect in addition to all the corrections mentioned above and is useful for intermediate- and high-velocity projectiles.

KEY WORDS: K- and L-shell ionization cross section/ Plane-wave Born approximation/

I. INTRODUCTION

It is well known that the inner-shell ionization process by heavy charged-particle bombardments can be described in the plane-wave Born approximation (PWBA).[1] The extensive amount of experimental data of K- and L-shell ionization cross sections for various projectiles on a variety of target elements have been reported and most of them are in satisfactory agreement with the PWBA calculations.

However, in the case of low-energy projectiles the measured cross sections are generally smaller than the theoretical predictions. This is due to two effects not included in the PWBA model; (1) the increase in the binding energy of the target electron due to penetration of the projectile into the inner-shell radius during collision and (2) the Coulomb deflection of the projectile in the field of the target nucleus. The corrections for these effects have been estimated by Basbas *et al.*[2] for K shell and by Brandt and Lapicki[3] for L shell, and their results are incorporated in the PWBA model. The modified PWBA theory has been successfully used to compare with the experimental data. Furthermore, for low-energy projectiles on heavy elements the electronic relativistic effect becomes important, while at intermediate and high velocities the polarization effect plays an important role.

There have been so for published several numerical tables for the PWBA calculations for K- and L-shell ionization cross sections,[4-8] and the theoretical cross section can be obtained from these tables by interpolation technique. Recently, Benka and Kopf[7] pointed out that the use of the exact limits of integration with respect to energy and

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momentum transfer considerably reduces the ionization cross section for low-energy protons. This fact means that the cross sections for low-energy projectiles do not show the universal behavior, but depend on the mass of the projectile. All the PWBA tables described above, except for that of Benka and Kopf, are the universal ones based on the approximate values of integration limits and can be used for low-energy projectiles only when the projectile mass is sufficiently large. On the other hand, the table of Benka and Kopf⁷⁾ is applicable only for protons. Considering these facts, it is useful to develope computer codes to calcuate the PWBA cross sections for arbitrary projectile with the exact values of integration limits as well as with the corrections for various effects described above.

For this purpose, we have written the computer code DEKY⁹⁾ for calculation of the PWBA cross sections for K- and L-shell ionization. The corrections for the binding-energy and Coulomb-deflection effects are included by the method of Brandt *et al.*²⁾³⁾ and the relativistic effect is taken into account through the method proposed by Merzbacher and Lewis.¹⁾ This code has been extensively used by us to estimate the theoretical cross sections these several years. However, the relativistic correction in this code is found to underpredict the K-shell ionization cross section for low-energy protons considerably,¹⁰⁾ and neglection of the polarization effect leads to underprediction of the cross section for intermediate- and high-energy projectiles.

Recently we have improved the orginal DEKY code⁹⁾ and developed two modified versions of the DEKY. The first one, called DEKY2, is used to calculate the relativistic K- and L-shell ionization cross sections. The relativistic effect is introduced by the method of Brandt and Lapicki.¹¹⁾ The second one, called DEKY3, includes the polarization effect in addition to all the corrections described above. The DEKY2 is suitable to calculate the cross sections for low-energy projectile, while the DEKY3 is useful for medium- and high-energy projectiles and especially for highly charged projectiles. Both computer codes are written for the FACOM M-200 computer in the Data Processing Center of Kyoto University and for the PDP-11/40 computer in the Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI). In the present paper, simple description of these computer codes is given and the results of the sample calculations for the codes, DEKY, DEKY2, and DEKY3, are presented and compared with each other.

II. THEORY

A. Ionization Cross Section

According to the PWBA theory,¹⁾ the s-shell ionization cross section is given by

$$\sigma_s(\theta_s,\ \eta_s)=\frac{8\pi Z_1^2}{Z_s^4\eta_s}f_s(\theta_s,\ \eta_s)a_0^2, \qquad (1)$$

where Z_1 is the charge of the projectile, Z_s is the effective nuclear charge of the s-shell electron in the target atom, and a_0 is the Bohr radius of the hydrogen.

For the projectile with the velocity v_1, the scaled projectile velocity parameter is defined as

$$\eta_s=\frac{1}{Z_s^2}(\hbar v_1/e^2)^2, \tag{2}$$

and the scaled target-electron binding energy is given by

$$\theta_s=I_s n^2/(Z_s^2 R_\infty), \tag{3}$$

where I_s is the measured ionization potential of the s-shell electron, R_∞ is the Rydberg energy, and n is the principal quantum number of the s shell. The effective nuclear charge is estimated from the Slater's recipe,[12] and taken to be $Z_K=Z_2-0.3$ for K shell and $Z_L=Z_2-4.15$ for L shell, where Z_2 is the atomic number of the target.

The function $f_s(\theta_s,\ \eta_s)$ is written as

$$f_s(\theta_s,\ \eta_s)=\int_{W_{\min}}^{W_{\max}} dW \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q^2}\,|F_{Ws}(Q)|^2, \tag{4}$$

where $Z_s Q^{1/2}/a_0$ is the momentum transfer and $WZ_s^2 R_\infty$ is the energy transfer. The minimum and maximum values of Q and W are given by[1,7]

$$Q_{\min}=(M_1/m)^2\eta_s\{1-[1-mW/(M_1\eta_s)]^{1/2}\}^2, \tag{5}$$
$$Q_{\max}=(M_1/m)^2\eta_s\{1+[1-mW/(M_1\eta_s)]^{1/2}\}^2, \tag{6}$$
$$W_{\min}=\theta_s/n^2, \tag{7}$$
$$W_{\max}=(M_1/m)\eta_s, \tag{8}$$

where M_1 is the mass of the projectile and "m" is that of the electron.

The form factor for K and L shells, $F_{Ws}(Q)$, can be written in the explicit form and is given in Refs. 4 and 5. If we use the approximate values for integration limits in Eqs. (5), (6), and (8), *i.e.*, $Q_{\min}=W^2/(4\eta_s)$ and $Q_{\max}=W_{\max}=\infty$, $f_s(\theta_s,\ \eta_s)$ is the function of only θ_s and η_s. In the present case, this function depends also on M_1.

B. Binding-Energy and Coulomb-Deflection Effects

The corrections for binding-energy and Coulomb-deflection effects are made in the manner similar to those of the DEKY code.[9] According to the perturbed-stationary-state theory developed by Basbas *et al.*,[2] the binding-energy factor by which the scaled binding energy is increased is expressed as

$$\varepsilon_s=1+2(Z_1/Z_s\theta_s)g_s(\xi_s), \tag{9}$$

where $\xi_s=2v_1/(\theta_s v_s)$, $v_s=Z_s v_0/n$, and $v_0=e^2/\hbar$ is the Bohr velocity. The function $g_s(\xi_s)$ is given in Refs. 2 and 3 and also in Ref. 9. The binding-energy effect is introduced by replacing θ_s in Eq. (1) by $\varepsilon_s\theta_s$.

The Coulomb-deflection effect is also taken into consideration through the method of Brandt *et al.*[2,3] The multiplicative Coulomb-deflection factor is written by

$$C_s=9E_{10}(\pi d q_0), \tag{10}$$

for K-and L_1-shell ionization and by

$$C_s=11E_{12}(\pi d q_0), \tag{11}$$

for L_2- and L_3-shell ionization. Here $\hbar q_0$ is the miminum momentum transfer for s-shell ionization, d is the one-half of the distance of closest approach in a head-on collision, and $E_n(x)$ is the exponential function of order n.

C Relativistic Effect

The relativistic effect is incorporated into the DEKY2 and DEKY3 codes through the method proposed by Brandt and Lapicki.$^{11)}$ They developed the relativistic correction in a manner similar to the way used for the binding-energy correction. Introducing a local relativistic electron mass, they averages it over all impact parameters with the weighting function determined from the impact-parameter-dependent ionization cross section. The relativistic correction factor thus obtained is given by

$$m_s^R(\xi_s)=(1+1.1\,y_s^2)^{1/2}+y_s, \tag{12}$$

where

$$y_{K,L_1}=0.40(Z_{K,L_1}/137)^2/(n\xi_{K,L_1}), \tag{13}$$

and

$$y_{L_2,L_3}=0.15(Z_{L_2,L_3}/137)^2/\xi_{L_2,L_3}, \tag{14}$$

The relativistic correction is made by replacing η_s by $m_s^R\eta_s$ in the nonrelativistic PWBA cross section formula.

D. Polarization Effect

For intermediate- or high-velocity projectiles, the PWBA cross sections corrected for the binding-energy and Coulomb-deflection effects underpredict the experimental data. This is known due to a Z_1^3-dependent term, which is asccribed to the polarization of bound states of the target electron by the projectile passing with large impact parameters. This polarization effect causes an increase in the energy transfer and is treated as a reduction in the binding energy of the target electron. The effect becomes larger with increasing Z_1.

In the DEKY3 code, this polarization effect is taken into account by the method of Basbas *et al.*$^{13)}$ Using the isotropic harmonic oscillator model of Hill and Merzbacher,$^{14)}$ they obtained the binding-polarization correction factor in the perturbed-stationary-state approach:

$$\zeta_s(\xi_s;\ c_s)=1+(2Z_1/Z_s\theta_s)[g_s(\xi_s;\ c_s)-h_s(\xi_s;\ c_s)], \tag{15}$$

where $g_s(\xi_s;\ c_s)$ is given by Eq. (19) in Ref. 11,

$$h_s(\xi_s;\ c_s)=(2n/\theta_s\xi_s^3)I(c_sn/\xi_s), \tag{16}$$

and $I(x)$ is obtained from Eq. (27) of Ref. 13. The factor c_s is taken to be 3/2 for K and L_1 shells and 5/4 for L_2 and L_3 shells. The correction for the polarization effect is incorporated into the PWBA model by replacing the binding-energy factor ε_s by the binding-polarization factor ζ_s.

III. DESCRIPTION OF THE PROGRAM

According to Sect. II the final experssion for the s-shell ionization cross section in the DEKY2 is given by

$$\sigma_s = C_s(\pi d q_0 \varepsilon_s)\, \sigma_s^{PWBA}(m_s^R \eta_s,\ \varepsilon_s \theta_s), \tag{17}$$

where $\sigma_s^{PWBA}(m_s^R \eta_s,\ \varepsilon_s \theta_s)$ is the s-shell ionization cross section in the PWBA, Eq, (1). In the case of the DEKY3, ε_s in Eq. (17) is replaced by ζ_s.

The DEKY2 code is designed to calculate the PWBA cross section corrected for the relativistic effect (PWBA-R), the PWBA-R modified for the binding-energy effect (PWBA-BR), and the PWBA-BR including the Coulomb-deflection effect (PWBA-BCR). On the other hand, the DEKY3 code calculates the PWBA-R, the PWBA-R modified for the binding-energy and polarization effects (PWBA-BPR), and the PWBA-BPR including the Coulomb-deflection effect (PWBA-BCPR).

The input data for two codes are the same as those for the DEKY code. The programs do not calculate the nonrelaivistic cross section, but other procedures and flow are similar to the DEKY. The output format is also the same as that of the DEKY, except that the value of m_s^R is printed out in addition to the parameters used in the DEKY.

IV. RESULTS OF SAMPLE CALCULATIONS

A test run has been made for the K-shell ionization cross section by 1-MeV protons on copper ($Z_2=29$). The K-shell binding-energy of copper atom is taken to be 8.979 keV.[15] The K-shell ionization cross sections including the binding-energy and Coulomb-deflection effects calculated by three codes are shown in Table 1 together with the parameters used for their evaluation and compared with each other.

In Fig. 1 the calculated K-shell ionization cross sections for protons on copper ($Z_2=$

Table 1. Comparison of the K-shell ionization cross sections and the parameters used for their evaluation, calculated by three computer codes. The calculations have been made for 1-MeV protons on copper. The cross sections are expressed in units of barn.

	DEKY		DEKY2	DEKY3
	Nonrelativistic	Relativistic		
θ_K	0.802	0.791	0.802	0.802
η_K	0.0486	0.0486	0.0486	0.0486
m_K^R	——[a]	——[a]	1.032	1.032
ξ_K	0.550	0.558	0.559	0.559
$g_K(\xi_K)$	0.750	0.746	0.745	0.625[b]
ε_K	1.065	1.066	1.065	1.054[c]
$f_K(m_K^R\eta_K,\ \varepsilon_K\theta_K)$	7.23×10^{-4}	7.82×10^{-4}	8.16×10^{-4}	8.66×10^{-4}[c]
$\sigma_K^{PWBA-BR}$[b]	15.4	16.7	16.9	17.9[c]
$C_K(\pi d q_0 \varepsilon_K)$	0.926	0.926	0.926	0.926[c]
σ_K[b]	14.3	15.5	15.6	16.6[c]

[a] Corresponding to $m_K^R=1$.

[b] $g_K(\xi_K;\ 3/2)-h_K(\xi_K,\ 3/2)$.

[c] The factor ε_K is replaced by ζ_K.

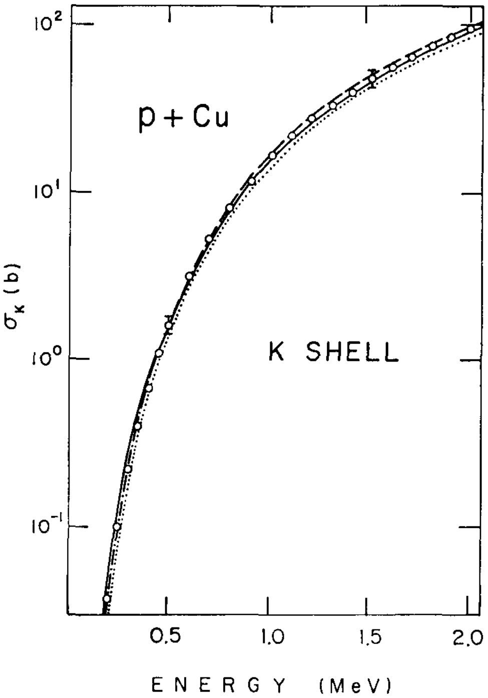

Fig. 1. Comparison of the calculated values of the K-shell ionization cross sections for protons on copper with the experimental values. The curves represent the values calculated by: ··················DEKY (Nonrelativistic, PWBA-BC) ; — • — • —DEKY (Relativistic, PWBA-BCR) ; ———— DEKY2 (PWBA-BCR) ; — — — — DEKY3 (PWBA-BCPR). The experimental data are taken from Lopes *et al.* (Ref. 16).

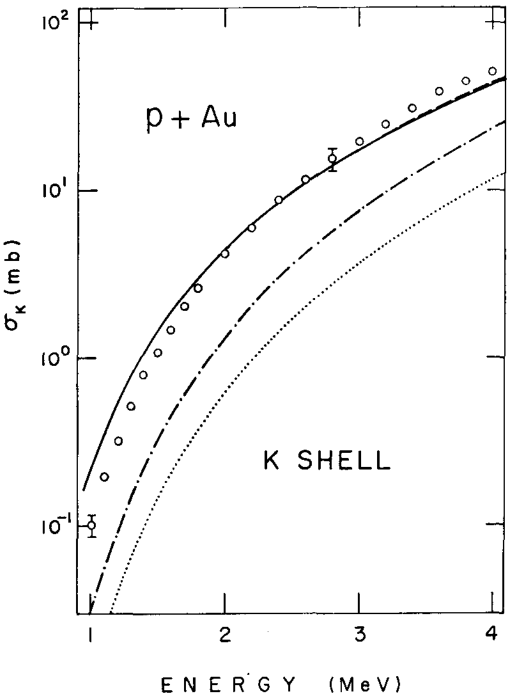

Fig. 2. Same as Fig. 1, but for protons on gold. The experimental data are from Kamiya *et al.* (Ref. 17).

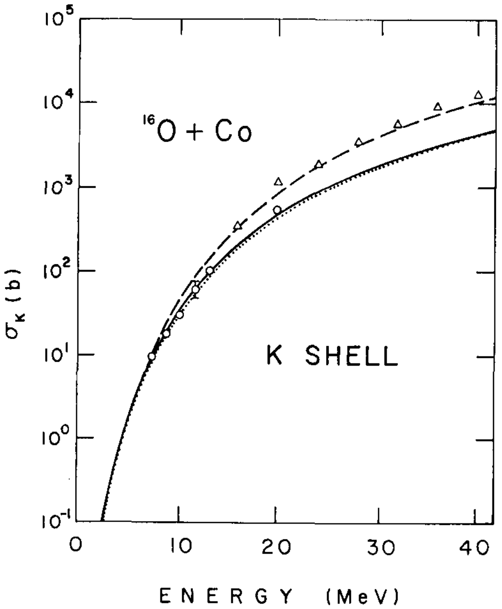

Fig. 3. Same as Fig. 1, but for ^{18}O ions on cobalt. The experimental data are taken from Knaf *et al.* (○) (Ref. 18) and Chaturvedi *et al.* (△) (Ref. 19). Two PWBA-BCR cross sections in the DEKY and DEKY2 cannot be distinguished with each other in the figure.

29) are compared with the experimental data of Lopes *et l.*[16] Similar comparison of the theoretical values with the experimental K-shell ionzation cross sections is made in Fig. 2 for protons on gold ($Z_2=79$). The experimental values are taken from Kamiya *et al.*[17] In the case of heavy-ion impact, the polarization effect becomes important. Figure 3 shows such an example for the K-shell ionization cross sections by ^{16}O-ion impact on cobalt ($Z_2=27$). The experimental results are obtained from Knaf *et al.*[18] and Chaturvedi *et al.*[19]

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