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Electronic relativistic effects on K-shell ionization by low-energy protons

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K-shell ionization cross sections by low-energy proton impact have been calculated in the relativistic plane-wave Born approximation, taking into account the effects of binding-energy increase and Coulomb deflection. The calculated values are compared with the recent experimental cross sections of Zander and Andrews. It is found that the use of Dirac wave functions for target electrons improves agreement with the experimental results, but the theoretical predictions are still systematically higher at the lower proton energies.

I. INTRODUCTION

It is well known that at low projectile energies the plane-wave Born approximation (PWBA)[1] overpredicts the inner-shell ionization cross sections by charged-particle impact. A modification of the PWBA has been made by Basbas *et el.*[2] They developed the perturbed-stationary-state (PSS) theory, and the effects of Coulomb deflection of projectiles and of increased binding energy of the target electrons according to the PSS are incorporated into the PWBA (CPSS). Both of these effects reduce the ionization cross sections for low-energy projectiles, and a satisfactory agreement between experimental data and the CPSS has been observed for a variety of projectiles and target elements. However, with decreasing projectile energies the relativistic effects for target electrons become increasingly important even for targets with small atomic numbers.

Recently, Zander and Andrews[3] investigated the K-shell ionization of Ti, Fe, Ni, and Zn by 60–150-keV protons. The measured K-shell ionization cross sections were compared with the theoretical predictions calculated from the CPSS including a correction factor for electronic relativistic effects[4] (CPSSR). They found that the CPSSR systematically overpredicts the experimental results for low-energy protons and the discrepancy becomes larger at the lower energies. For their lowest energy region the theoretical predictions are about eight times larger than the experimental values. They claimed that this large discrepancy may be partially due to the approximate relativistic correction and also due to the approximation made in the lower limit of the momentum transfer.

Considering the large correction factor for the relativistic effects, as large as 2.62 for 100-keV protons on Zn, it is worthwhile to calculate the K-shell ionization cross sections by low-energy proton impact by the use of relativistic wave functions for target electrons and to test the PWBA model for low-energy projectiles.

We have already studied electronic relativistic effects in K-shell ionization by charged-particle impact on targets with large atomic numbers.[5] The ionization cross sections have been calculated in the PWBA, using Dirac wave functions for the target electrons and the corrections for Coulomb-deflection and binding-energy effects have been taken into account (RPWBA-BC). In the present work, we extend this model and calculate the K-shell ionization cross sections for low-energy proton impact. The calculated results are compared with the experimental data of Zander and Andrews.[3]

II. THEORETICAL MODEL

The theoretical model used in the present work is the same as that described in detail earlier,[5] except that the exact values of the limits of the momentum transfer are used instead of the approximate ones.

In the PWBA, the differential cross section for ejection of the K-shell electron with the kinetic energy E_f is written by[1]

$$\frac{d\sigma}{dE_f} = 8\pi\alpha^2 Z_1^2 \frac{M_1}{E_1} \int_{q_{\min}}^{q_{\max}} \frac{dq}{q^3} |F_{if}(q)|^2 , \tag{1}$$

where q is the momentum transfer, $F_{if}(q)$ is the form factor, α is the fine-structure constant, and Z_1, M_1, and E_1 are the charge, mass, and kinetic energy of the projectile, respectively. Throughout the present work, the rational units ($\hbar = m_e = c = 1$) are used.

The lower and upper limits of the momentum transfer corresponding to the energy transfer W are given by

$$q_{\min}^2 = 2M_1E_1[1-(1-W/E_1)^{1/2}]^2, \quad (2)$$

$$q_{\max}^2 = 2M_1E_1[1+(1-W/E_1)^{1/2}]^2. \quad (3)$$

The analytical expressions of the form factor for Dirac wave functions are calculated following the method of Jamnik and Zupančič[6] and given in Ref. 5. The screening effects are taken into account as usual in the PWBA through the inner- and outer-screening method.[5] The total K-shell ionization cross section σ_K is evaluated by integrating Eq. (1) over E_f.

The correction for the binding-energy effect is made in a manner similar to the method of Basbas *et al.*[2] by replacing the screening number θ_K by $\epsilon\theta_K$, where ϵ is the binding-energy factor estimated with the Dirac wave functions.

The effect of Coulomb deflection is also taken into account through the method proposed by Basbas *et el.*[2] The K-shell ionization cross section modified for the Coulomb-deflection effect is given by

$$\sigma_K = 9E_{10}(\pi d q_0)\,\sigma_K^{PWBA}, \quad (4)$$

where σ_K^{PWBA} is the K-shell ionization cross section in the PWBA, $E_{10}(x)$ is the exponential integral of order 10, q_0 is the minimum momentum transfer, and d is one-half of the distance of closest approach in a head-on collision.

III. RESULTS AND DISCUSSION

In order to compare the calculated results with the experimental data, it is convenient to introduce the function

$$F(\eta_K/\epsilon^2\theta_K^2) = \sigma_K\epsilon\theta_K/[\sigma_0 9E_{10}(\pi d q_0\epsilon)], \quad (5)$$

where η_K is the scaled velocity of the projectile, $\sigma_0 = 8\pi a_0^2 Z_1^2/Z_{2K}^4$, a_0 is the first Bohr radius of hydrogen, and Z_{2K} is the screened nuclear charge of the target. This function has a universal behavior for the CPSS, but for the RPWBA-BC it depends on the target atomic number Z_2.

The solid curve in Fig. 1 represents the theoretical values of the function $F(\eta_K/\epsilon^2\theta_K^2)$ for Fe calculated from the RPWBA-BC. At the fixed value of $\eta_K/\epsilon^2\theta_K^2$, the values for Zn are about 10% larger than those for Fe, while the values for Ti are about 10% smaller. This weak Z_2 dependence of the function is supported by the nearly universal nature of the experimental data. The experimental values were estimated from the K-shell x-ray production cross sections measured by Zander and Andrews.[3] These cross sections were converted to the K-shell ionization cross sections σ_K by the use of the K-shell fluorescence yields taken from the table of Krause.[7]

It can be seen from the figure that the large

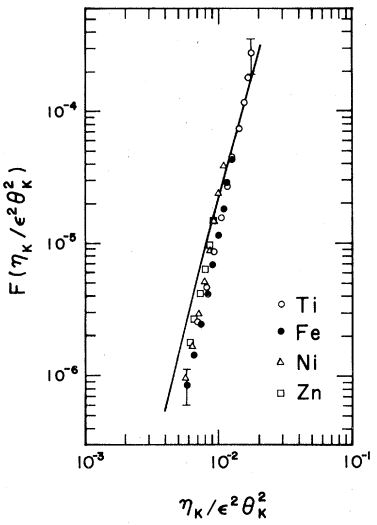

FIG. 1. Comparison of theoretical and experimental values of the function $F(\eta_K/\epsilon^2\theta_K^2)$. The solid curve represents the RPWBA-BC calculations for Fe. The experimental values are taken from Ref. 3.

discrepancy between theory and experiment observed by Zander and Andrews is ascribed to their overestimation of relativistic effects and the use of Dirac wave functions considerably improves agreement with the experimental data. However, for $\eta_K/\epsilon^2\theta_K^2 < 10^{-2}$ the theoretical predictions are still systematically higher than the experimental values and the discrepancy becomes larger with decreasing $\eta_K/\epsilon^2\theta_K^2$. In the case of 70-keV proton bombardment on Fe, corresponding to the lowest $\eta_K/\epsilon^2\theta_K^2$ value in the measurements of Zander and Andrews, the theoretical value is three times larger than the experimental one. A similar trend has also been observed by Shima[8] for lower-energy protons on the lower-Z_2 elements.

It is clear that the electronic relativistic effects partially account for the discrepancy between theory and experiment, but there still remain quantitative disagreements. Another possible origin of the discrepancy is the choice of electronic wave functions. In the present work, we used the relativistic hydrogenic (Dirac) wave functions. More realistic wave functions, such as Hartree-Fock wave functions, may improve agreement with experiment in the low-energy region.

This effect has been nonrelativistically studied by two groups, but their conclusions are confusing. For protons on Al Basbas *et al.*[2] showed that the Hartree-Slater wave functions give larger K-shell ionization cross sections than the

hydrogenic wave functions for the energy region $\eta_K/\theta_K^2 < 0.02$, though for higher energies the difference between the cross sections calculated with the two wave functions is negligibly small. If we assume a similar trend in the relativistic case, the discrepancy becomes enhanced by the use of self-consistent-field wave functions.

On the other hand, Ford *et al.*[9] indicated that the Hartree-Fock wave functions yield lower K-shell ionization cross sections than the hydrogenic ones. In the case of 750-keV proton impact on Al ($\eta_K/\theta_K^2 = 0.36$), the cross section obtained with the Hartree-Fock wave functions is about 20% smaller than that with the hydrogenic wave functions and reduction increases with decreasing proton energy. They also showed that inclusion of the second Born effect further reduces the cross sections. For 500-keV protons on Ti ($\eta_K/\theta_K^2 = 0.07$), the second-order cross section calculated with the Hartree-Fock wave functions is about half of the value with the hydrogenic wave functions. If these results can be extended to the lower-energy region, the disagreement with theory and experiment may be resolved. However, no calculations have been made in the low-energy region, and the behavior of the Hartree-Fock cross sections in the energy region studied in the present work is not clear.

Recently, Anholt *et al.*[10] pointed out that the discrepancy is reduced if we take into consideration energy loss of the projectiles in the targets due to ionization. This may be one of possible explanations for the discrepancy, but there are also other possibilities, such as breakdown of the PWBA in the low-energy region, and insufficiencies of the corrections for Coulomb-deflection and binding-energy effects.

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