Bull. Inst. Chem. Res., Kyoto Univ., Vol.68, No. 2, 1990

Review

K-Shell Ionization of Atoms by Mesons

Takeshi Mukoyama*, Harumi Kaji+, and Kenji Yoshihara*

Received June 22, 1990

The K-shell ionization cross sections by negatively- and positively-charged muons and pions have been calculated in the plane-wave Born approximation. The corrections for the electronic relativistic effect, the Coulomb-deflection effect, the binding-energy effect, and the polarization effect are taken into account. The dependence of the K-shell ionization cross sections on the sign of the projectile is studied and experimental possibilities for ionization processes by meson impact are discussed.

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

1. INTRODUCTION

The inner-shell ionization by heavy charged-particle impact has been studied extensively as a basic process in atomic physics as well as an important process in applications for solid-state physics, astrophysics, plasma physics, and chemistry. It is well known that the experimental inner-shell ionization cross sections for high-energy projectiles are in good agreement with the theoretical calculations within the framework of the first-order Born approximation, such as the plane-wave Born approximation (PWBA)[1] and semiclassical approximation (SCA)[2]. In this case, the ionization cross section is proportional to Z_1^2, where Z_1 is the projectile charge.

However, for low-energy projectiles the Coulomb deflection of the projectile in the field of the target nucleus plays an important role. In addition, the distrotion in the binding energy of the target electrons due to penetration of the projectile into the inner-shell radius during ion-atom collision should be taken into consideration for low-velocity projectiles, while at intermediate and high velocities the polarization effect of the target electron orbital by the projectile becomes important. Owing to these effects the inner-shell ionization cross sections deviate from the simple Z_1^2 scaling law predicted by the first-order theory. Various theoretical models including these effects have been developed and used to explain the experimental results.

Recently, the first experimental study on the inner-shell ionization process by

---

* 向山　毅：Laboratory of Nuclear Radiation, Institute for Chemical Research, Kyoto University, Uji, Kyoto

+ 鍛冶東海：Department of Chemistry, Faculty of Sciences, Tohoku University, Aoba, Aramaki, Sendai

* 吉原賢二：Department of Chemistry, Faculty of Sciences, Tohoku University, Aoba, Aramaki, Sendai

heavy antiparticle impact has been performed by Andersen *et al.*[3,4] at the CERN low-energy antiproton ring (LEAR). This kind of experiment is very useful to provide additional insight into the dynamics of atomic inner-shell ionization processes. In particular, it is interesting to study the dependence of the inner-shell ionization cross sections on the sign of the projectile charge.

For positively-charged projectiles, the presence of the projectile increases the binding energy of the target electron and this binding-energy effect decreases the ionization cross section. On the other hand, the energy distortion effect by the projectile of negative charge works as the anti-binding effect and causes the larger cross section. The second difference is due to the change in the Rutherford trajectory of the projectile. The positive projectile is deflected by the repulsive Coulomb potential of the target and the Coulomb-deflection effect reduces the ionization cross section, while the cross section is enhanced by the Coulomb trajectory due to the attractive potential for the negative projectile. At high projectile velocities, the polarization effect of the target electron orbital by the positively-charged projectile increases the ionization cross section, but the polarization effect for the negative projectile becomes repulsive, decreasing the cross section.

The theoretical calculations of the K-shell ionization cross sections by antiprotons have been made by the use of various theoretical models; the modified PWBA[5], the SCA with Rutherford trajectory[6,7], the coupled-channels method[8-11], the classical trajectory Monte Carlo (CTMC) technique[11-13], and the continuum-distorted-wave method[14-16]. The calculated total K-shell ionization cross sections and K-ionization probabilities as a function of impact parameter have been compared with the corresponding values for proton impact.

The experimental studies on the ratio of K-shell ionization cross sections by particle and antiparticle impact have been performed by low-energy electrons and positrons[18-20]. The large discrepancy between electron and positron impact ionization has been observed at low energies and the measured cross section ratios are in agreement with the theoretical calculation based on the Rutherford trajectory[21]. This fact indicates that for electron and positron impact the Coulomb-deflection effect plays a dominant role in the ionization process because of their small rest mass.

On the other hand, there have been reported no experimental results for the difference in the single K-shell ionization cross sections by heavy positive and negative projectiles. Although Andersen *et al.*[3,4] found the large difference in the ratios of double to single ionization cross sections of He atoms by protons and antiprotons, their single K-shell ionization cross sections for both projectiles are in agreement within the experimental error.

Considering these facts, it is interesting to measure the K-shell ionization cross sections by other particles and the corresponding antiparticles, such as muons ($\mu^{\pm}$) and pions ($\pi^{\pm}$). These mesons are considered to be more favorable projectiles than the electron and the proton to study the dependence of the ionization cross sections on the sign of the projectile charge in the following reasons. First, since their rest mass is smaller than the mass of the proton, the Coulomb-deflection effect at the same projectile velocity is expected to be larger. Second, the first-order Born cross sections for particles and antiparticles show the Z_1^2 scaling law, while the scattering process of the positron (Bhabha scattering) is different from that of the electron (Mϕller scattering). Third, the charge exchange channel, which should be taken into consideration for proton impact, can be neglected.

In contrast to the case of proton or heavier ion impact, the theoretical calculations for inner-shell ionization cross sections by meson impact are scarce. Martir *et al.*[8] estimated the K-shell ionization cross sections for positive and negative muons on copper in the energy region between 1 and 2 MeV/amu. They showed that the Coulomb-deflection effect on the cross sections is quite large in comparison with the results for proton and antiproton imapct. Cohen[22] used the CTMC method and calculated the ionization and capture cross sections for negative muons on hydrogen atoms in the energy range from 3 eV to 150 keV. To the authors' knowledge, there is no theoretical calculations for pions in low-energy region.

It is the purpose of the present work to estimate the K-shell ionization cross sections by positive and negative mesons and to stimulate experiments by the use of these particles. For this purpose, we use the modified version of the DEKY code[23,24] and calculate the K-shell ionization cross sections in the PWBA theory corrected for the electronic relativistic effect, the Coulomb-deflection effect, the binding-energy effect, and the polarization effect.

2. THEORETICAL MODEL

The theoretical model in the present work is, in principle, same as that used for protons and antiprotons by Brandt and Basbas[5]. In PWBA theory[1], the K-shell ionization cross section is given by

$$\sigma_K^{\mathrm{PWBA}}(\theta,\ \eta)=\frac{8\pi Z_1^2}{Z_{2K}^4\eta}f(\theta,\ \eta)a_0^2 \tag{1}$$

where $Z_{2K}=Z_2-0.3$ is the effective nuclear charge of the target K-shell electron, Z_2 is the atomic number of the target, and a_0 is the Bohr radius of hydrogen.

The scaled projectile velocity η and the scaled K-shell binding energy θ are defined as

$$\eta=\frac{1}{Z_{2K}^2}\ (\hbar v_1/e^2) \tag{2}$$

$$\theta=I_K/(Z_{2K}^2R_\infty) \tag{3}$$

where v_1 is the projectile velocity, I_K is the measured K-shell ionization potential, and R_∞ is the Rydberg energy.

The function $f(\theta,\ \eta)$ is written by

$$f(\theta,\ \eta)=\int_{W_{min}}^{W_{max}}dW\int_{Q_{min}}^{Q_{max}}\frac{dQ}{Q^2}\ |\ F_W(Q)\ |^2 \tag{4}$$

Here $Z_{2K}Q^{1/2}/a_0$ is the momentum transfer and $WZ_{2K}^2R_\infty$ is the energy transfer during collision. The minimum and maximum values of Q are given by

$$Q_{min}=(M_1/m)^2\eta \left\{ 1-[1-mW/(M_1\eta)]^{1/2}\right\}^2 \tag{5}$$

$$Q_{max}=(M_1/m)^2\eta \left\{ 1+[1-mW/(M_1\eta)]^{1/2}\right\}^2 \tag{6}$$

where M_1 is the mass of the projectile and m is the rest mass of the electron. The minimum and maximum values of W are $W_{min}=\theta$ and $W_{max}=(W_1/m)\eta$. The form factor $F_W(Q)$ is given in Ref. 1.

The distortion of the energy state of the target electron by the projectile is taken into account through the so-called binding-evergy correction developed by Basbas *et al.*[25] Following the perturbed-stationary-state (PSS) approach, the binding-energy factor is given by

$$\varepsilon=1+(2Z_1/Z_{2k}\theta)\ g(\xi) \tag{7}$$

where $\xi=2v_1/(\theta v_2)$, $v_2=Z_{2K}v_0$, and $v_0=e^2/\hbar$ is the Bohr velocity. The function $g(\xi)$ is defined in Refs. 23 and 25.

Basbas *et al.*[26] introduced the correction for the polarization effect in the similar manner. The combined binding-polarization correction factor in the PSS approach is expressed as[26]

$$\zeta=1+(2Z_1/Z_{2k}\theta)\ [g(\xi)-h(c,\ \xi)] \tag{8}$$

where $h(c, \xi)$ is given by

$$h(c,\ \xi)=(2/\theta\xi^3)\ I(c/\xi) \tag{9}$$

Here c is taken as 3/2 for K shell and $I(x)$ is obtained from Eq. (27) in Ref. 26. The correction for the binding-energy and polarization effects can be made by replacing θ in Eq. (1) by $\zeta\theta$.

The electronic relativistic effect is incorporated in the PWBA theory through the method of Brandt and Lapicki[27]. The relativistic correction is performed by multiplying the factor m^R to η in Eq. (1). The relativistic correction factor is given by

$$m^R=(1+1.1y^2{}_K)^{1/2}+y_K \tag{10}$$

where

$$y_K=0.40(Z_{2K}/137)^2/\xi \tag{11}$$

Basbas *et al.*[25] proposed a multiplicative correction factor for the Coulomb-deflection effect. The factor $C_K(x)$ is expressed as a function of the parameter $x=2\pi dq_0\zeta/z_K(1+z_K)$, where d is the one-half of the distance of closest approach in a head-on collision, $\hbar q_0$ is the minimum momentum transfer in ionization, and z_K is the parameter for the energy-loss correction. The function $C_K(x)$ is given by

$$C_K(x)=9\int_1^{T_M}\frac{e^{\pm xt}}{t^{10}}\,dt \tag{12}$$

where T_M is the maximum energy transfer to the K-shell electron, the plus and minus signs correspond to the antiparticle and the particle respectively. The parameter for the energy-loss effect is written by[28]

$$z_K=(1-\xi\Delta_K)^{1/2} \tag{13}$$

where Δ_K is the energy loss divided by the kinetic energy of the projectile in the center-of-mass system.

The integrand in Eq. (12) decreases rapidly with increasing x. By this reason, Eq. (12) for particle reduces to

$$C_K(x)=9\int_1^{T_M}\frac{e^{-xt}}{t^{10}}\,dt\simeq 9E_{10}(x) \tag{14}$$

where $E_{10}(x)$ is the exponential integral of order 10. On the other hand, the numerical integration is employed for the case of antiparticles. In practice, the integration is terminated before the integrand reaches its minimum, as pointed out in Ref. 5.

Including all the corrections described above, the final expression for the K-shell ionization cross section is written by

$$\sigma_K=C_K[2\pi dq_0\xi/z_K(1+z_K)]\,\sigma_K^{\mathrm{PWBA}}(\xi\theta,\ m^R\eta) \tag{15}$$

This model is same as that used in the DEKY code[24], except for the energy-loss effect in the Coulomb-deflection factor, and can be called the Coulomb-deflection-corrected PSS theory with relativistic correction (CPSSR). For antiparticles, the ionization cross section is obtained by simply changing the sign of the projectile charge and calculating the Coulomb-deflection factor directly from Eq. (12).

Although the present method is almost same as the widely-used ECPSSR theory[28], it should be noted that in the ECPSSR the integration limits in Eq. (4) are approximated as $Q_{min}=W^2/(4\eta)$ and $Q_{max}=W_{max}=\infty$, and then the energy-loss effect is taken into account by the correction factor. On the other hand, in our computer code the integration in Eq. (4) is performed with exact integration limits and the energy-loss effect is automatically included correctly.

3. RESULTS AND DISCUSSION

In order to test our computer code, the new version of DEKY, we calculated the K-shell ionization cross sections for protons to antiprotons on aluminum. The ratios of the cross sections for antiprotons and protons with and without, the Coulomb-deflection effect are in good agreement with the results of Brandt and Basbas[5]. It is quite natural because our model is practically same as theirs.

For positive and negative muons, the only available data are the K-shell ionization cross sections of copper atoms by the coupled-channels (CC) calculations of Martir *et al.*[8] In Fig. 1, the present results are plotted as a function of projectile energy and compared with the CC results. The present values are expressed as the ratio to the PWBA ones with the relativistic correction. The solid curves represent the CPSSR, while the dashed curves indicate the results without the Coulomb-deflection effect, the PSSR. On the other hand, the CC results are divided by the SCA values with straight-line path. The dotted curves show the CC results with straight line path and the dash-dotted curves to those for Rutherford trajectory. It is clear that the present

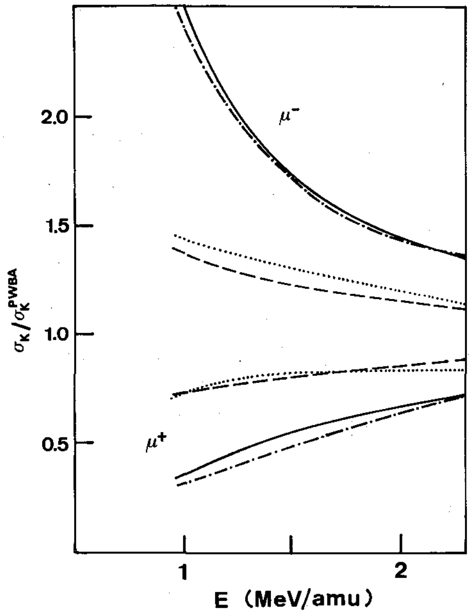

Fig. 1. Copper K-shell ionization cross sections by muons as a function of projectile energy. The cross sections are expressed as the ratios to the first-order Born cross section. The solid curves represent the CPSSR, while the dashed curves indicate the PSSR. The CC results with Coulomb trajectory are shown by the dot-dashed curves and the CC with straight-line path by the dotted curves (Ref. 8).

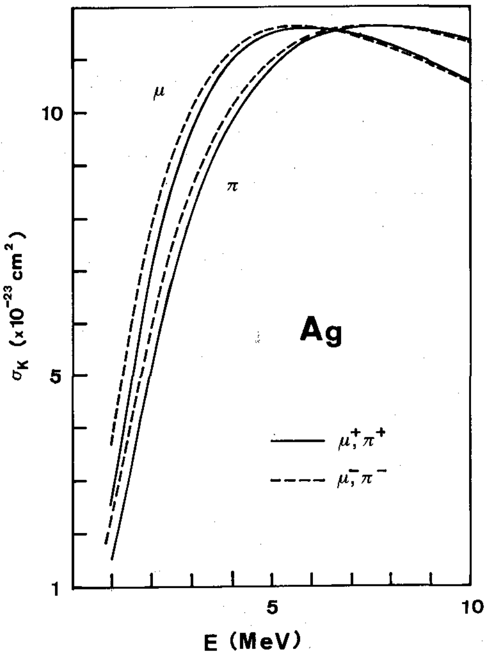

Fig. 2. Silver K-shell ionization cross sections by muons and pions as a function of projectile energy.

results agree well with the CC values with and without the Coulomb-defection effect.

In Fig. 1, the PSSR cross sections for negative muons are above the PWBA ones because of decrease in the binding energy, i. e. the anti-binding effect, while the corresponding cross sections for positive muons are below the PWBA values due to the binding-energy effect. The Coulomb-deflection effect is quite large in this energy region and the large difference in the CPSSR cross sections between positive and negative muons is expected. However, at present it would be difficult to obtain muon beams with energy as low as a few hundred keV.

Figure 2 shows the K-shell ionization cross sections for muons and pions on silver in the energy range from 1 to 10 MeV. In Fig. 3, the cross sections for 1-20-MeV muons and pions on gold are plotted as a function of energy. For low-energy region, the cross sections for negatively-charged projectiles are larger than those for positive particles because of the Coulomb-deflection and binding-energy effects. However, at high energies the values for negative muons and pions become slightly larger than those for positive mesons. This fact can be explained as follows. The Coulomb-deflection effect is negligibly small in high-energy region and the polarization effect becomes important. This effect increases the cross sections for positive charge and decreases those for negative particles.

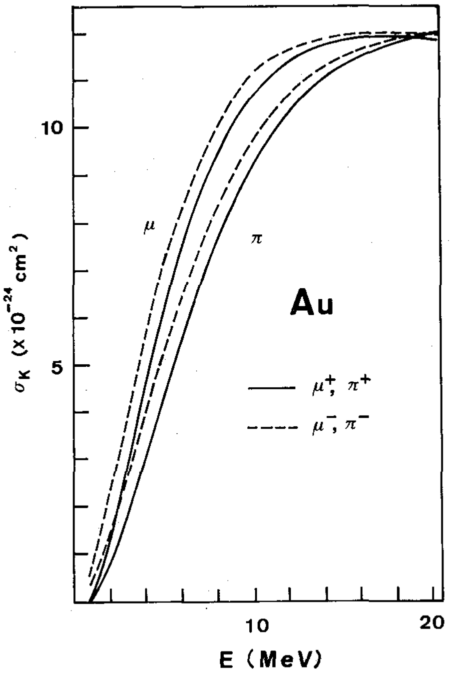

Fig. 3. Gold K-shell ionization cross sections by muons and pions as a function of projectile energy.

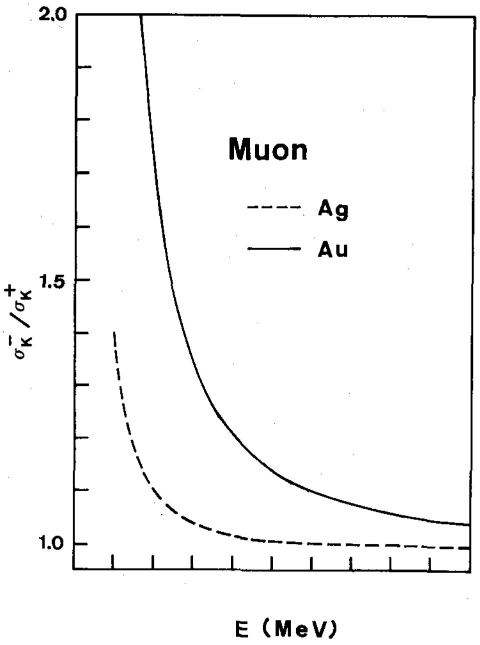

Fig. 4. K-shell ionization cross section ratios for negative and positive muons on silver and gold as a function of projectile energy.

In Fig. 4, we present the ratios of the K-shell ionization cross sections for negative and positive muons on Ag and Au. The ratios for pions are slightly lower because of smaller Coulomb-deflection effect, but almost same as the values for muons.

From Figs. 2 and 3, it can be seen that the order of magnitude of the K-shell ionization cross sections by muons and pions is 10^{-22} cm^2 for Ag in the energy range from 1 to 10 MeV and 10^{-24} cm^2 for Au. Elsener[29] pointed out that the quality of negative muon beams is still not sufficient for atomic collision experiments. However, in near future the experimental studies on the K-shell ionization cross sections by muons and pions will be possible. If we assume that the experimental error in the ratios of ionization cross sections for antiparticle and particles is 10%, the projectile energy should be less than 2 MeV for Ag and 6 MeV for Au, as shown in Fig. 4.

It has been demonstrated by Paul[30] that the ECPSSR theory overpredicts the experimental K-shell ionization cross sections for low-energy region. This discrepancy probably comes from deficiencies in the corrections for the Coulomb-deflection effect and the binding-energy effect. The electronic relativistic effect is also overestimated for heavy elements in low-energy region[31]. Nevertheless, the present results provide a useful benchmark values for more elaborate theoretical models of the K-shell ionization process by muons and pions.

REFERENCES

(1) E. Merzbacher and H. Lewis, "Handbuch der Physik," Vol. 34, ed. by D. Flügge, Springer-Verlag, Berlin, (1958), p. 116.

(2) J. Bang and J. M. Hansteen, *Kgl. Dansk. Vidensk. Selsk. Mat. Fys. Medd.*, **31**, No. 13 (1959).

(3) L. H. Andersen, P. Hvelplund, H. Knudsen, S. P. Møller, K. Elsener, K. G. Rensfelt, and E. Uggerhøj, *Phys. Rev. Lett.*, **57**, 2147 (1986).

(4) L. H. Andersen, P. Hvelplund, H. Knudsen, S. P. Møller, A. H. Sørensen, K. Elsener, K. G. Rensfelt, and E. Uggerhøj, *Phys. Rev. A*, **36**, 3612 (1987).

(5) W. Brandt and G. Basbas, *Phys. Rev. A*, **27**, 578 (1983); **28**, 3142 (E) (1983).

(6) P. A. Amundsen, *J. Phys. B*, **10**, 2177 (1977).

(7) D. Trautmann, F. Rösel, and G. Bauer, *Nucl. Instr. and Meth.*, **214**, 21 (1983).

(8) M. H. Martir, A. L. Ford, J. F. Reading, and R. L. Becker, *J. Phys. B*, **15**, 1729 (1982).

(9) G. Mehler, B. Müller, W. Greiner, and G. Soff, *Phys. Rev. A*, **36**, 1454 (1987).

(10) A. Müller-Groeling and G. Soff, *Z. Phys. D*, **9**, 223 (1988).

(11) A. M. Ermolaev, *Hyperfine Interactions*, **44**, 375 (1988).

(12) R. E. Olson, *Phys. Rev. A*, **36**, 1519 (1987).

(13) D. R. Schultz, *Phys. Rev. A*, **40**, 2330 (1989).

(14) P. D. Fainstein, V. H. Ponce, and R. D. Rivarola, *Phys. Rev. A*, **36**, 3639 (1987).

(15) P. D. Fainstein, V. H. Ponce, and R. D. Rivarola, *J. Phys. B*, **21**, 2989 (1988).

(16) P. D. Fainstein, V. H. Ponce, and R. D. Rivarola, *Phys. Rev. A*, **40**, 2828 (1989).

(17) P. D. Fainstein, V. H. Ponce, and R. D. Rivarola, *J. Phys. B*, **22**, L559 (1989).

(18) S. Ito, S. Shimuzu, T. Kawaratani, and K. Kubota, *Phys. Rev. A*, **22**, 407 (1980). Old works are cited therein.

(19) P. J. Schultz and J. L. Campbell, *Phys. Lett. A*, **112**, 316 (1985).

(20) F. Ebel, W. Faust, C. Hahn, M. Rückert, H. Schneider, A. Singe, and I. Tobehn, *Phys. Lett. A*, **140**, 114 (1989).

(21) G. Hock, "Proc. XIth ICPEAC, Kyoto, 1979," ed. by K. Takayamagi and N. Oda, North-Holland, Amsterdam, (1979), p. 974.

(22) J. S. Cohen, *Phys. Rev. A*, **27**, 167 (1983).

(23) T. Mukoyama and L. Sarkadi, *Bull. Inst. Chem. Res., Kyoto Univ.*, **58**, 60 (1980).

(24) T. Mukoyama and L. Sarkadi, *Bull. Inst. Chem. Res., Kyoto Univ.*, **60**, 67 (1982).

(25) G. Basbas, W. Brandt, and R. Laubert, *Phys. Rev. A*, **7**, 983 (1973).

(26) G. Basbas, W. Brandt, and R. Laubert, *Phys. Rev. A*, **17**, 1655 (1978).

(27) W. Brandt and G. Lapicki, *Phys. Rev. A*, **20**, 465 (1979).

(28) W. Brandt and G. Lapicki, *Phys. Rev. A*, **23**, 1717 (1981).

(29) K. Elsener, *Comm. At. Mol. Phys.*, **22**, 263 (1989).

(30) H. Paul, *Nucl. Instr. and Meth.*, **192**, 11 (1982).

(31) T. Mukoyama and L. Sarkadi, *Phys. Rev. A*, **28**, 1303 (1983).