K-shell Ionization by Secondary Electrons

V. Horvat, R.L. Watson, and J.M. Blackadar

The method developed previously [1] for calculating the K-shell ionization probability for Cu target atoms bombarded by secondary electrons produced in collisions with 10 MeV/u beams of Kr, Xe and Bi has been improved in several areas. This has resulted in better agreement between the results of calculations and measurements. In addition, the previously reported discrepancy by about a factor of 7 was traced down to the erroneously omitted factor of 2π (~ 6.28).

The calculations are based on the following scenario. A heavy-ion projectile travels inside the target gradually losing its energy with negligible angular straggling. (a) At some depth z inside the target the projectile collides with a target-atom electron. The electron emerges from the collision as a binary encounter (BE) electron with kinetic energy E_e, traveling in the direction defined by the polar angle θ and the azimuthal angle φ. The y axis is chosen to be in the upward direction. (b) The BE electron gradually loses its energy in soft collisions with other target electrons and nuclei and at some point it ionizes a target-atom K-shell electron. It is assumed that the range of the BE electron is small compared to the diameter of the target and the target-to-detector distance, but not necessarily small compared to the target thickness. (c) The K vacancy produced in the collision decays via the emission of a secondary Kα x ray, which is subsequently detected. The number of detected target-atom Kα x rays per beam particle $N_{det}(K\alpha)/N_p$ is then equal to

$$\frac{N_{\rm det}(K\alpha)}{N_{\rm p}} = \int dz\, P_c(z) \int dE_e \int d(\cos\theta) \int d\varphi\, P_b(z, E_e, \theta, \varphi)\, P_a(z, E_e, \theta, \varphi)\ , \qquad (1)$$

where P_a, P_b and P_c, respectively, are the probabilities for the events (a), (b), and (c) described above. The probability P_a is given by the following expression:

$$P_a(z, E_e, \theta, \varphi) = \frac{N_A\, \rho_2\, D}{A_2}\ \frac{d^2\sigma_{BE}(z, E_e, \theta, \varphi)}{dE_e d\Omega}\ , \qquad (2)$$

where

$$\frac{d^2\sigma_{BE}}{dE_e d\Omega} = \sum_{i=1}^{Z_2} \frac{Z_1^{\,2} e^4}{(4\pi\varepsilon_o)^2}\ \frac{s\, J(p_z)\, \sqrt{E_e\, E_{CM}}}{8(E_{CM} + E_B^{\ i})^{5/2} \sqrt{t}\ (\sqrt{E_{CM}} + \sqrt{E_e}\cos\theta - \sqrt{t})^2} \qquad (3)$$

is the doubly differential cross section for the production of BE electrons in collisions between projectile nuclei and target-atom electrons in the laboratory-frame, calculated in the impulse approximation. It was derived by transforming the corresponding expression [2] from the center-of-mass frame. In the equations above, $d\Omega = d(\cos\theta)d\varphi$ is the differential emission solid angle and

$$E_{CM} = E_e + t - 2\sqrt{E_e t}\cos\theta \qquad (4)$$

is the electron kinetic energy in the center-of-mass frame. The quantities $t = m_e w^2 / 2$ and $s = m_e w$ are usually referred to as the cusp energy and cusp momentum, respectively, where m_e is the electron mass and

$$w = \frac{V(z)}{1 - N_A m_e / A_1} \qquad (5)$$

is the velocity of the center-of-mass. Here V(z) is the projectile velocity in the laboratory frame at depth z inside the target, while N_A is Avogadro's number. The projectile and target-atom molar masses are A_1 and A_2, respectively, D is the maximum target depth (effective thickness), and ρ_2 is the target density. The quantity E_B in Eq. (3) is the binding energy of the ejected target electron, while Z_1 and Z_2 are the projectile and target atomic numbers, respectively. In the calculations, the dependence of projectile velocity on depth inside the target was calculated using the method of Ziegler [3].

The z-component of the target electron momentum is given by

$$p_z = s\,[1 - \sqrt{(E_{CM} + E_B^i)/t}\,], \qquad (6)$$

while its distribution (Compton profile) is defined in terms of the bound electron's wave function ψ in momentum space as

$$J(p_z) = \int\int |\psi(p)|^2 dp_x dp_y \,. \qquad (7)$$

The function $J(p_z)$ is symmetric about $p_z = 0$. Moreover, since the target atoms are randomly oriented, its variance is equal to one third of the average value of $|\mathbf{p}|^2$, so that

$$\sigma_J^2 = 2\, m_e\, E_B^i / 3 \,. \qquad (8)$$

For the purpose of this work, $J(p_z)$ was approximated by a Gaussian having centroid equal to zero and standard deviation equal to σ_J.

The probability P_b is given by the following expression:

$$P_b(z, E_e, \theta, \varphi) = \frac{N_A\, \rho_2\, R_{eff}(z, E_e, \theta, \varphi)}{A_2}\, \sigma_e^{eff}(E_e)\,, \qquad (9)$$

in which R_{eff} is the effective range inside the target of the BE electrons emitted at depth z with kinetic energy E_e in the direction defined by the angles θ and φ before their energy drops below the threshold energy $E_o = 8.98$ keV [4] for target-atom K-shell ionization. The quantity σ_e^{eff} is the effective cross section for K-shell ionization of target atoms by these electrons.

The effective electron range R_{eff} is related to the nominal range R, which in turn is related to the stopping power. The stopping power was calculated using the relativistic Bethe formula with the Bloch correction [5] and then fit with a function

$$S(E) = E^{1-n} / (nA) . \qquad (10)$$

R was then obtained in the form

$$R = A [E^n - E_o^n]. \qquad (11)$$

The best fit values of the parameters A (multiplied by ρ_2) and n (for E in keV) were found to be 5.510 $\mu g/cm^2$ and 1.765, respectively.

If a BE electron remains inside the target while its kinetic energy is above the threshold energy for target-atom K-shell ionization, its effective range R_{eff} is equal to its nominal range R. If, on the other hand, the BE electron leaves the target with kinetic energy greater than the threshold energy for target-atom K-shell ionization, its effective range will be equal to its actual path length inside the target, which is smaller than its nominal range. The effect of target thickness on the effective range of electrons was taken into account by assuming a straight-line path of the BE electrons. In this case, following simple geometrical arguments, it can be shown that electrons emitted at depth z towards the target back surface in the direction specified by the polar angle ϑ and the azimuthal angle φ travel the distance

$$r_B = (D - z) / (\cos\vartheta + \sin\vartheta \sin\varphi) \qquad (12)$$

before they leave the target, assuming that the target is tilted 45° (relative to the projectile direction) about the x axis and that the back surface of the target is facing up. It is also implied that $\sin\varphi > -\cot\vartheta$ (for emission in the direction of the target back surface). Similar considerations involving the target front surface lead to the expression for the distance traveled ;

$$r_F = - z / (\cos\vartheta + \sin\vartheta \sin\varphi) , \qquad (13)$$

where it is implied that $\sin\varphi < -\cot\vartheta$. The effective range of the BE electrons is then equal to

$$R_{eff} = \min (R, r) , \qquad (14)$$

where r is equal to r_B or r_F, whichever applies for the given values of ϑ and φ. Finite target thickness effects were found to be important. They reduce the calculated number of secondary Cu Kα x rays per beam particle by as much as 46 % at D values as large as 1 mg/cm^2, compared to the calculations in which finite target thickness effects are not taken into account.

The cross section σ_e^{eff} is the average value of the cross section for Cu K-shell ionization by electron impact and includes contributions (with the appropriate statistical weights) from electrons having energies at the time of impact between their initial energy and zero. It was discussed in full detail in the previous report [1].

Finally, $P_c(z)$ is given by the expression

$$P_c(z) = \omega\, \varepsilon \exp(-\mu z) , \qquad (15)$$

where ω is the target-atom fluorescence yield for Kα x rays, ε is the detection probability, and μ is the x-ray attenuation coefficient for Cu Kα x rays in the Cu target.

BE electrons can be produced also by the elastic scattering of projectile electrons from target nuclei. However, the relative contribution from this process to secondary Cu Kα x ray production is expected to be small. According to Shima [6], the average number of electrons n_e attached to 10 MeV/u Kr, Xe, and Bi projectiles in copper is 4.2, 8.8, and 18.3, respectively, which is significantly less than the number of target electrons per atom ($Z_2 = 29$). Furthermore, the nuclear charges of the projectiles (36, 54, and 83), are larger than the nuclear charge of copper. Therefore, keeping in mind that the doubly differential cross section for BE electron production scales with square of the nuclear charge, it follows that the contribution of projectile electron elastic scattering from target nuclei is smaller than the contribution of target electron elastic scattering from projectile nuclei by a factor of $Z_2 n_e/Z_1^2$, which is only 8 % for Bi projectiles. The contribution from projectile electrons is further reduced as a consequence of the following: (a) on average, the projectile electrons are more tightly bound than the target electrons and hence, their scattering cross sections are smaller, and (b) the scattered projectile electrons have lower average energies than the scattered target electrons and hence, the fraction of high-energy BE electrons is smaller.

The intensity of Auger electrons emitted by the projectiles is expected to be very small. This is because (a) at 10 MeV/u the projectiles are highly stripped inside the target, so that the number of possible Auger transitions is limited, and (b) Auger yields are small for heavy ions. Furthermore, Auger electrons emitted from target atoms have energies that are normally below the threshold for K-shell ionization of other target atoms.

Calculated contributions from Kα x-ray production by BE electrons to the Kα diagram line peaks in Cu x-ray spectra, as a function of target thickness are compared with the measured values [7] in Figure 1. It is evident that the calculations agree rather well with the measurements both in terms of the dependence on target thickness and projectile atomic number. It should be noted that the calculated values scale with the square of the projectile atomic number.

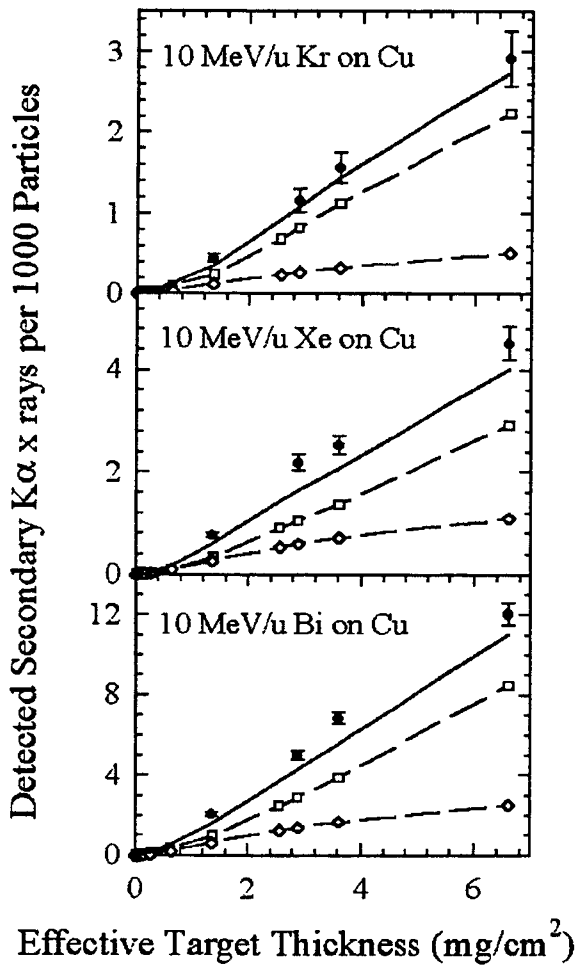

Figure 1. Number of detected secondary Cu Kα x rays as a function of target thickness in collisions with 10-MeV/u Kr, Xe, and Bi projectiles. The experimental data are represented by filled circles, while squares connected by dashed lines show the calculated contribution from fluorescence by secondary x rays. Calculated contributions from binary encounter electrons are represented by diamonds connected by dashed lines. The sum of the x-ray fluorescence and binary encounter electron contributions is shown by solid lines.

References

[1] V. Horvat, R.L. Watson, and J.M. Blackadar, Progress in Research, 1998-1999, Cyclotron Institute, TAMU, p. IV-8.

[2] D.H. Lee, P. Richard, T.J.M. Zouros, J.M. Sanders, J.L. Shinpaugh, and H. Hidimi, Phys. Rev. A **41**, 4816 (1990).

[3] J. F. Ziegler, program SRIM version as of January 11, 1996 (private communication).

[4] C.M. Lederer and V.S. Shirley, *Table of Isotopes*, 7th ed., (Wiley-Interscience, New York, 1978).

[5] F. Bloch, Z. Phys. **81**, 363 (1933); D.H. Jakubassa-Amudsen and H. Rothard, Phys. Rev. A **60**, 385 (1999).

[6] K. Shima, T. Ishihara, and T. Mikumo, Nucl. Instrum. Methods **200**, 605 (1982).

[7] R.L. Watson, J.M. Blackadar, and V. Horvat, Phys. Rev. A60 (1999) 2959.