Target-atom Inner-shell Vacancy Distributions Created in Collisions with Heavy Ion Projectiles

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K-shell vacancy production in collisions by fast heavy-ion projectiles is typically accompanied by the creation of multiple vacancies in the L and higher shells of the target atoms. The distributions of these *original* vacancy configurations provide information about the collision dynamics. Their properties may be deduced from the associated K x-ray or Auger electron spectra by taking into account the fast vacancy rearrangement processes occurring between the time of the collision and the time of x-ray or electron emission. However, this task is a very formidable one, and so far only analyses which take into account a limited number of rearrangement transitions and/or a lim number of decay channels have been attempted.

In the our previous report on this subject [1] we described a more general, yet conceptually more justified and mathematically more straightforward method of approach to this problem. There we demonstrated how the method can be applied to the analysis of K x-ray spectra measured both with a wavelength-dispersive spectrometer and with an energy-dispersive detector. In this report we focus on the details of the description of electronic configuration distributions of target atoms produced in collisions with fast heavy ions and the results of calculations.

In the model that was developed for this purpose, the first problem was to find a way to describe the relatively complex original electronic configuration distribution by a single variable parameter. This was necessary in order to ensure a unique solution to the problem. To accomplish this task, it was assumed (1) that the original population distribution of vacancies in the L shell is binomial, so that it can be characterized by the average ionization probability per electron p_L^o, (2) that the distribution of L electrons over the L subshells (L_1, L_2, and L_3) is statistical, (3) that the original average number of L electrons n_L and the original average number of M electrons n_M are related according to the universal scaling formula of Sulik et al. [2], (4) that the distribution of M electrons over the M subshells (M_1, M_2, M_3, M_4, and M_5) is statistical, and (5) that the N shell and the shells above it are empty at all times. However, the assumption (4) proved to be inadequate and had to be modified, as will be discussed in the text that follows.

The results of the calculations were required to match measured values of quantities that can be determined from the K x-ray spectra with good accuracy. These include (a) the relative intensities of the

Kαsatellite peaks, (b) the overall intensity of Kβ satellites relative to that of Kα satellites, and (c) the energy shifts of Kαsatellite peaks from the diagram-line value. However, it was found that not all of these requirements could be met within the framework of the statistical model outlined above.

In particular, in the measurements with 10 MeV/u projectiles colliding with stationary Cu targets, the measured values of the overall intensity of Kβ satellites relative to those of Kα satellites ($R_{\beta\alpha}$) were found to be consistently higher than the single-vacancy atom value of 0.137 and generally increased as a function of the projectile atomic number Z_1 (at least for low values of Z_1). On the other hand, the model calculations predicted values lower than 0.137 that decreased as a function of Z_1, as shown in Figure 1a. Clearly, the experimental results suggest that the populations of 3p orbitals relative to 2p orbitals in the target atom increase as a consequence of multiple ionization in heavy ion collisions. Indeed, much better agreement with experiment was obtained when the statistical model described above was modified by assuming that the 3p orbital is preferentially populated during the decay sequence. This new model was named PP3p, where PP stands for "preferentially populated". The results of the calculations using the PP3p model are also shown in Figure 1a.

Measured average energy shifts from the diagram-line value per L vacancy for each Kα satellite peak are compared with those predicted by the statistical model and the PP3p model in Figure 1b. It appears that the statistical model reproduces the experimental energy shifts somewhat better than the PP3p model. However, neither model is capable of completely reconciling the large number of 3p electrons required to explain the high experimental $R_{\beta\alpha}$ values and the small number of M electrons required to explain the rather large measured energy shifts. The PP3p model provides for the most effective increase in the $R_{\beta\alpha}$ values with the given (small) number of M electrons at the time of collision. In addition, the discrepancy between themeasured energy shifts and those calculated using the PP3p model is small compared to the discrepancy between the measured $R_{\beta\alpha}$ values and those calculated using the statistical model. On the other hand, it is possible that the results of the Dirac-Fock calculations used to determine the energy shifts from the number of M electrons are not adequate. For all these reasons it was decided to adopt the PP3p model in the calculations. The apparent preferential population of the 3p orbital may be caused by an effective state-selective combination of electronic excitations and de-excitations or by selective interatomic transitions to the valence band, which were not taken into account.

The PP3p model was recently applied to calculate the average Kα and Kβ fluorescence

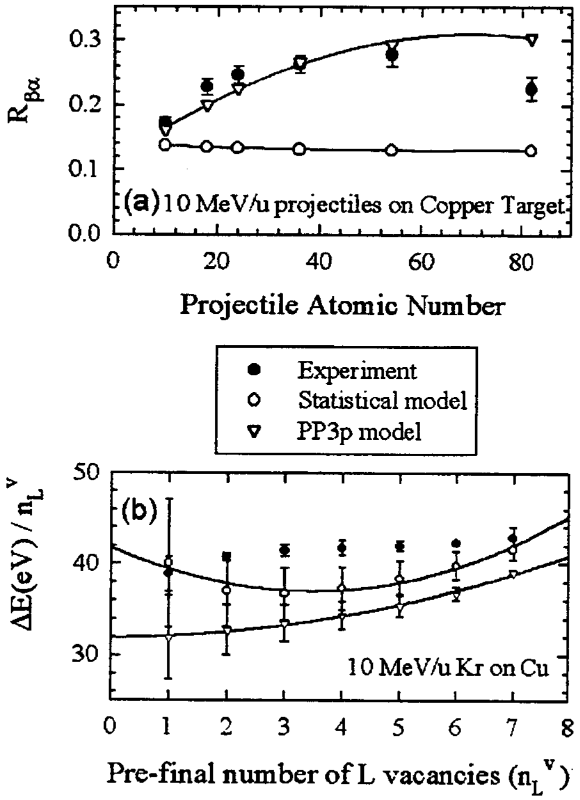

Figure 1. (a) Comparison between measured and calculated values of the overall intensity of Kβ satellites relative to that of Kα satellites $R_{\beta\alpha}$ as a function of projectile atomic number. (b) Comparison between measured and calculated values of the energy shifts of Kα satellite peaks from the diagram-line value per L vacancy as a function of the number of L vacancies n_L^v present in that (pre-final) state.

yields for aluminum target atoms under bombardment by 10 MeV/u projectiles. Again, the calculations were based on a set experimentally determined values. The results are shown in Figure 2 as a function of the parameter $p_L^{K\alpha}$, defined as the average number of L electrons just before the Kα x-ray emission divided by 8.

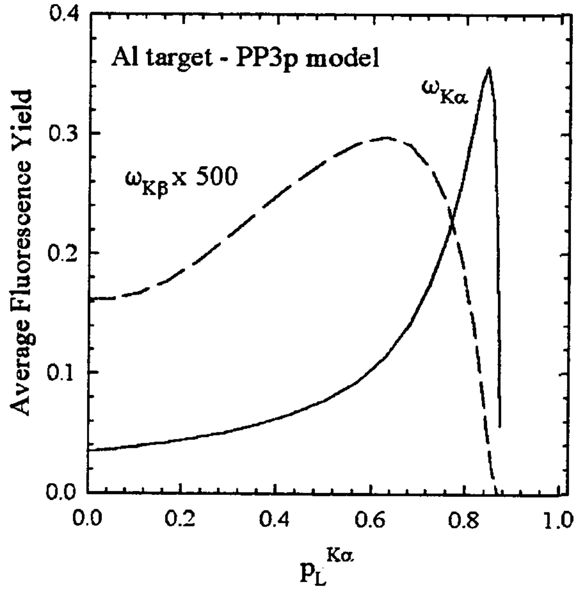

Figure 2. Calculated average fluorescence yield to be used to convert Kα and Kβ x-ray production cross sections to K vacancy-production cross sections for Al atoms as a function of the parameter $p_L^{K\alpha}$.

References

[1] V. Horvat, R.L. Watson, and J.M. Blackadar, Progress in Research, 1998-1999, Cyclotron Institute, TAMU, p. IV-11.

[2] B. Sulik, I. Kádár, S. Ricz, D. Varga, J. Végh, G. Hock, and D. Berényi, Nucl. Instrum. Methods **B28** (1987) 509.

K-shell Ionization by Secondary Electrons

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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

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