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In typical close collisions with heavy-ion projectiles, multiple inner-shell vacancies are created in target atoms. Various decay processes that occur before K x-ray emission can considerably alter the original L-shell vacancy distribution. The original vacancy distribution, which carries information about the collision dynamics, may be deduced from the measured x-ray or electron spectra if these rearrangement processes are taken into account. However, this task is generally a very formidable one. In contrast to the existing partial methods of approach to this problem, a more general yet conceptually more justified and mathematically more straightforward method has been developed and is described here.

In the high-resolution spectra of K x rays, emitted when a Cu target is irradiated with a beam of heavy ions, it is possible to resolve four groups with up to eight peaks each, corresponding to single-electron x-ray transitions from 2p and 3p orbitals into the 1s orbital in the presence of spectator vacancies. The groups involve the  $K\alpha$  transitions (from the 2p orbital) and the  $K\beta$  transitions (from the 3p orbital) into the 1s orbital having a single vacancy (satellite transitions) or a double vacancy (hypersatellite transitions). The peaks in a group correspond to transitions in the presence of different numbers of vacancies in the L shell (up to seven for  $K\alpha$  transitions and up to eight for  $K\beta$  transitions). The peaks due to transitions involving a given fixed number of K and L vacancies and different numbers of M vacancies cannot be resolved because of their

small energy separation compared to the natural line width. Therefore, spectator vacancies in the M shell only affect the widths of the resolved peaks and their positions. For the sake of simplicity, we neglect the hypersatellite transitions and study only target atoms with a single vacancy in the K shell at the time of collision. Inclusion of atoms with a double K-shell vacancy at the time of collision is possible, but it is not likely to significantly affect the results.

The calculations start with an assumed assumption of the initial vacancy distribution in the target atom at the time of collision. The evolution of this distribution is then followed along all decay branches that end when no further decays are allowed except those that result in the filling of the K vacancy. An inventory list of the resulting K x-ray transitions provides the information necessary to calculate the quantities that can be determined from the measured spectra. These include the intensity distribution of  $K\alpha$  satellite peaks, their overall intensity relative to that of the  $K\beta$  peaks, and the average number of M vacancies associated with each one of them. As a bonus, the ratio of the total number of K x rays and the initial number of atoms with a K vacancy can be calculated. This ratio is equal to the average fluorescence yield and can be directly used for conversion between the K x-ray production and K vacancy production cross sections. After comparison with the measured spectrum is made, the assumed initial vacancy distribution in the target atom at the time of

collision is modified and the calculations are repeated until satisfactory agreement between the calculated and the measured spectral features is reached. The whole procedure can be automated, and once all the data files are prepared, the results for each case can be obtained within a few minutes of run time on a personal computer with a 120-MHz Pentium processor.

The intensities of the  $K\alpha$  and  $K\beta$  satellite peaks (corrected for detector efficiency and x-ray absorption) generally follow a binomial distribution as a function of the associated number of target-atom L-shell vacancies. This distribution is described by a single parameter  $p_L$  representing its average value and standard deviation. The same applies to the distribution of the number of L-shell vacancies created in the collisions. However, the value of  $p_L$  in this case is different because of L-shell vacancy rearrangement prior to K x-ray emission. The  $p_L$  value that characterizes the original L-vacancy distribution (at the time of collision) can be determined in the calculations. The two values of  $p_L$  are compared in Figure 1 for a Cu target.

The calculated average values of the fluorescence yield to be used for conversion between the  $K\alpha$  x-ray production and K vacancy-production cross sections are shown in Figure 2 as a function of the  $p_L$  value describing the Cu target-atom L-vacancy distribution at the time of  $K\alpha$  x-ray emission.

The calculations require the knowledge of the values of radiative and non-radiative transition rates for the most probable excited configurations of Cu atoms having single K vacancies. However, these values are currently not available. Therefore, they were derived from the rates for

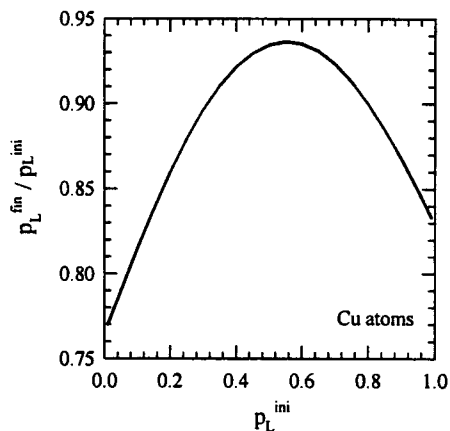


Figure 1. Comparison between the value of  $p_L$  describing the Cu target-atom L-vacancy distribution created in the collision with heavy ions ( $p_L^{ini}$ ) and the corresponding value at the time of K x-ray emission ( $p_L^{fin}$ ).

single-vacancy atoms [1, 2] by applying the commonly used scaling procedure of Larkins [3].

In applying the scaling procedure it was necessary to exclude Coster-Kronig transitions

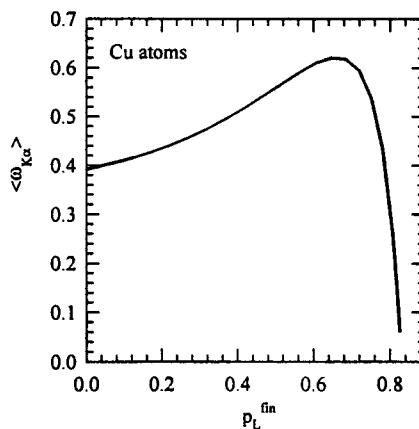


Figure 2. Calculated average fluorescence yield to be used for conversion between the  $K\alpha$  x-ray production and K vacancy-production cross sections in Cu atoms as a function of the  $p_L$  value describing the L-vacancy distribution at the time of  $K\alpha$  x-ray emission.

that are not energetically allowed. Extensive multiconfigurational Dirac-Fock calculations [4] were performed to identify these configurations.

Another set of multiconfigurational Dirac-Fock calculations was performed to determine the average transition energy of each  $K\alpha$  satellite peak from the associated average number of M electrons  $\langle n_M(n_L) \rangle$  predicted by the calculations. For each  $K\alpha$  satellite peak these calculations were performed for all configurations having the appropriate number of L vacancies  $n_L$ , separately for  $L_3 \rightarrow K$  and  $L_2 \rightarrow K$  transitions. The number of M vacancies, which had to be an integer in the Dirac-Fock calculations, was set equal to the integer value of  $\langle n_M(n_L) \rangle$  and then to the integer value of  $\langle n_M(n_L) \rangle$  plus one, so that the desired results could be obtained by interpolation.

The largest number of configurations in a single calculation was 2683, corresponding to  $n_L = 5$  and  $n_M = 9$ .

### References

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