Systematics of *Kα* X-Ray Satellite Peak Centroids

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Gaussian widths of the satellite peaks were the subject of a systematic analysis of the spectra of *K*α x rays, as described in the preceding report [1]. Presented here is an extension of this analysis that focuses on the systematics of the satellite peak centroids. The study was restricted to satellite peaks whose centroids were determined in a least squares fitting procedure without any constraints.

For each target, independently determined centroids of the satellite peaks were plotted as a function of their associated numbers of spectator *L* vacancies (*i*) and the apparent average number of *L* vacancies (n_L) present in the target atom at the time of *K* x-ray emission [2]. In order to reduce the error due to uncertainties in the energy calibrations, the satellite peak centroids were determined relative to the centroid of the corresponding *K*α diagram peak. In Fig. 1, the satellite shifts as a function of n_L are shown for a Cu target. The data indicate that, for a given value of *i*, the satellite shifts are linear functions of n_L.

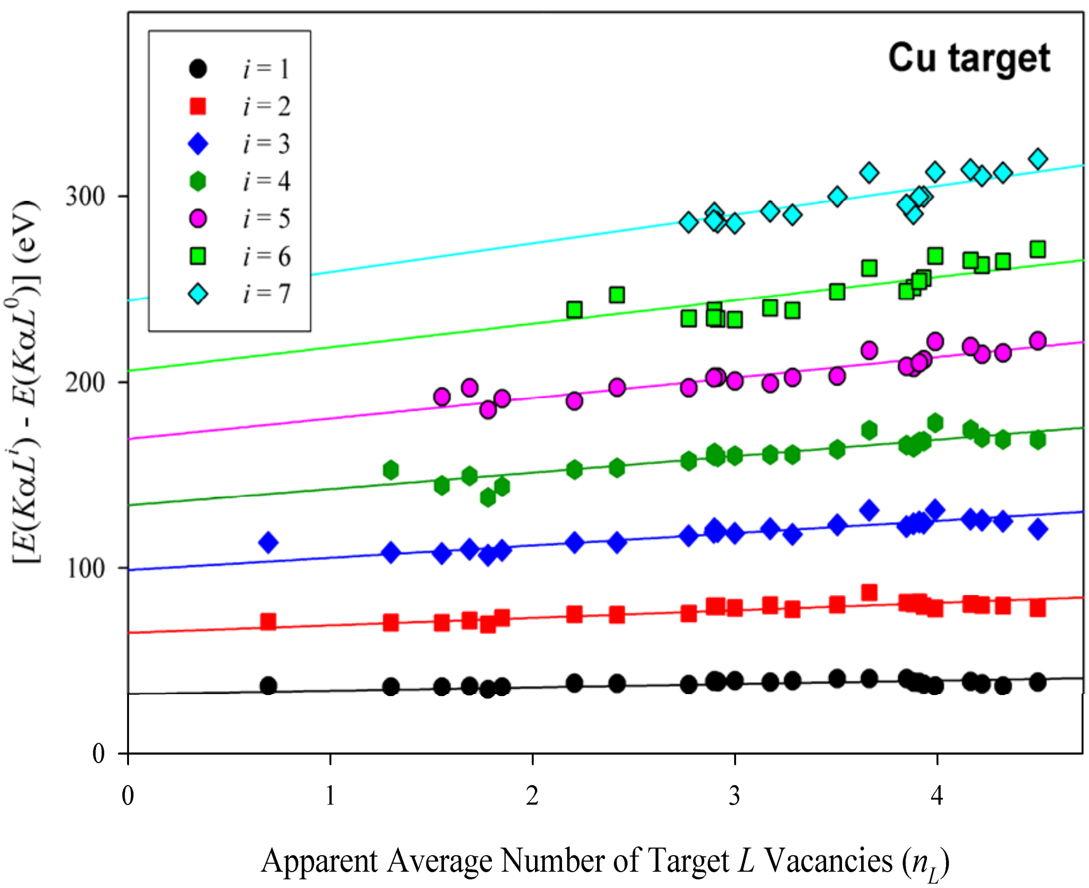

Figure 1. Cu *K*α satellite peak centroid shifts as a function of the associated number of *L* vacancies (*i*) and the apparent average number of target *L* vacancies (n_L).

As n_L approaches zero, it seems reasonable to expect that the degree of outer-shell ionization approaches to zero as well. Consequently, the satellite shifts for $n_L = 0$ can be predicted by atomic structure calculations. This was accomplished using the multiconfigurational Dirac-Fock code of Desclaux [3]. The results were then used as the ordinate intercepts of the straight lines shown in Fig. 1, while their slopes were determined from the available data using linear regression. The slope of each one of the seven straight lines in Fig. 1 can be interpreted as the excess shift ΔE^i divided by n_L, where ΔE^i is the difference between the actual shift of a $K\alpha$ satellite peak corresponding to i spectator L vacancies and its corresponding value at $n_L = 0$.

A similar analysis was also applied to the data obtained for six other targets. This resulted in a set of 49 values of ΔE^i / n_L, each corresponding to a different target and a different value of i. They are plotted in Fig. 2 as a function of i and as a function of the target atomic number (Z_2).

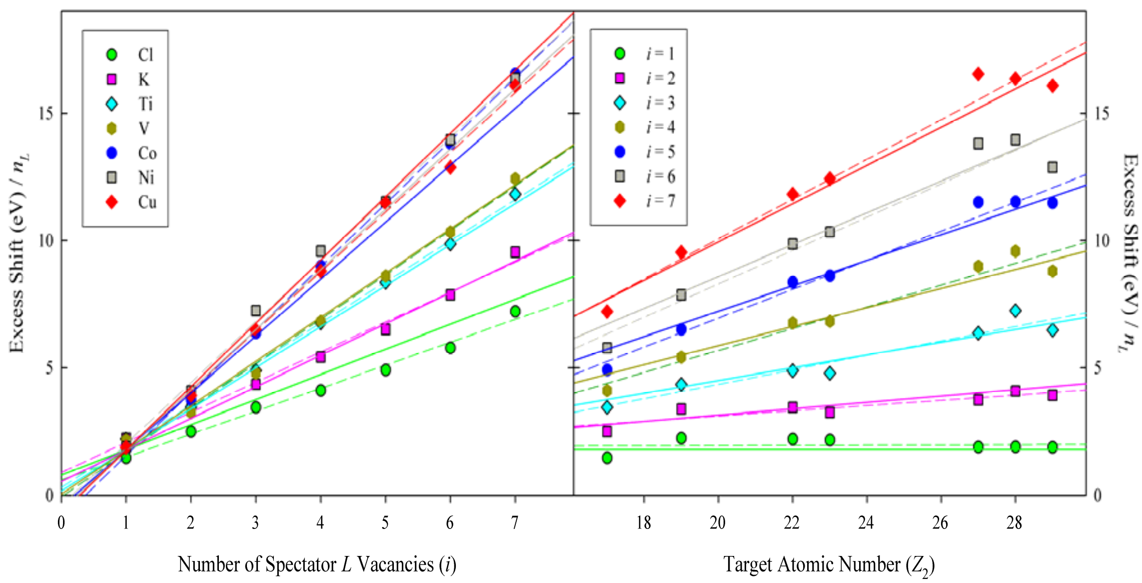

Figure 2. Excess shift of $K\alpha$ satellite peaks divided by the apparent average number of L vacancies (n_L) as a function of the associated number of spectator L vacancies (i) and the target atomic number (Z_2).

Based on the trends observed in the two graphs of Fig. 2, it was found that with reasonable accuracy ΔE^i / n_L can be parameterized as

$$\Delta E^i (Z_2) / n_L = (i - 1)\,(Z_2 - b_1) / 8 + b_2 \,, \tag{1}$$

where a_1, and b_2 are constants. Their best-fit values were found to be

$$b_1 = 9.11 \pm 0.28 \qquad b_2 = 1.79 \pm 0.12 \,. \tag{2}$$

The dashed lines in Fig. 2 represent the results of linear regression applied to each individual set of data points with the given value of i or Z_2, while the solid lines represent the predictions based on eq.(1) and eq.(2).

In summary, based on a large number of measurements and a large variety of projectile, target, and collision energy combinations, a comprehensive analysis was undertaken in order to study the systematics of the spectra of $K\alpha$ x rays. The main result is a set of semi-empirical formulas that can be used to predict the shape of the spectrum with reasonable accuracy. The apparent average number of L vacancies present at the time of K x-ray emission (n_L) can be estimated using the formula given in ref.[2]. Then, eq.(1) and eq.(2) can be used to estimate the satellite peak centroids. Finally, eq.(1) and eq.(2) of ref.[1] can be used to estimate the Gaussian widths of the satellite peaks. The remaining parameter that needs to be estimated is the instrumental resolution. Additionally, for a complete description of the structure of Kα x-ray spectra, the contributions to the diagram peaks due to secondary ionization need to be calculated. Examples of calculations were presented in ref.[4] and ref.[5]. These results are expected to apply to any collision system involving a solid target with atomic number Z_2 = 17-29, a projectile with atomic number Z_1 = 6-83, and energy between 2.5 and 25 MeV/amu.

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[2] V. Horvat *et al.*, *Progress in Research*, Cyclotron Institute, Texas A&M University (2004-2005), p. IV-9.

[3] J. P. Desclaux, Comp. Phys. Commun. **9**, 31 (1975).

[4] R. L. Watson, J. M. Blackadar and V. Horvat, Phys. Rev. A **60**, 2959 (1999).

[5] V. Horvat and R. L. Watson, J. Phys. B **34**, 777 (2001).