

# XRF PEAK DECONVOLUTION USING PEAK RATIOS REFINED BY FUNDAMENTAL PARAMETERS

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Fixed ratio Gaussian peak group model is frequently used for deconvolution of multi-element XRF spectrum. However, the intra-element peak ratios are not constants and changed for different samples because of matrix effects in the absorption of both irradiating and fluorescence X-rays. Errors in intra-element peak ratios causes errors in separation of the elements of heavily overlapping XRF peaks. In order to overcome the problem, we have produced peak deconvolution software that uses intra-element peak ratios calculated based on the fundamental parameter (FP) method. The results on various samples are compared with conventional fixed-ratio peak deconvolution.

The calculation is iterative sequences of fixed intra-element peak intensity ratio Gaussian peak fitting, composition calculation using FP method and intra-element peak ratios determinations using FP method. The initial values of intra-element peak ratios are obtained from pure element samples and stored in a table. XRF intensity of each element is calculated using fixed-ratio Gaussian fitting. The model of XRF peaks is

$$\sum_{z,l} (P_z \cdot R_{z,l} \cdot G(E - E_{z,l}, W(E_{z,l})))$$

where  $G(E, W)$  is Gaussian function,  $E_{z,l}$  is peak energy,  $W(E)$  is FWHM at energy  $E$ ,  $P_z$  is the height of the main peak of the element and  $R_{z,l}$  is the intra-element peak height ratios. For the peak fitting,  $P_z$  is the fitting parameter and all others are fixed. After obtaining peak intensities, the concentrations of elements are calculated using FP method. Based on the concentrations calculated, peak intensity ratios  $R_{z,l}$  are calculated using FP method. Using 'refined' peak ratios, the second round of peak fitting and concentration calculation are done. The results are compared with the previous round. If the differences are small enough, the process is ended. If not, the process proceeds to the next round.

The figure (a) shows the fitting result of Cu-Zn alloy based on the intra-element peak ratios of pure Cu and Zn samples. Since there is Cu-K absorption edge at the energy between Zn-K $\alpha$  and Zn-K $\beta$ . Therefore, Zn-K $\beta$  is strongly absorbed by Cu atoms and there is large error in fitting in Zn-K $\beta$  region. The figure (b) shows the result of the method discussed in this report. By refining the Zn K $\beta$ /K $\alpha$  ratio taking the absorption in consideration, the fitting is better than the conventional method.

