Integrating spectrum analysis and fundamental parameter quantification

W. Malzer, R. Tagle, M. Haschke
Bruker AXS Microanalysis GmbH

Among the methods of quantification for XRF, the fundamental parameter method is the most flexible one, because it does not depend on reference materials. In particular for micro-XRF analysis, this flexibility is of importance, as the composition might change significantly within the investigation of one sample. Fundamental parameter quantification usually is carried out in two steps. With the first step, the spectrum deconvolution, net-intensities of the fluorescence lines are extracted. The second step is the actual quantification. With the net-intensities as input, the composition of the sample is iteratively calculated relying on the Sherman equation.

We will present a new approach, which integrates both steps. It also follows an iterative scheme, but within each cycle the spectrum is computed and fitted including all matrix effects.
Compared to the classical algorithm, the new scheme has some advantages. Strong absorption edges are treated correctly. Also, it is more robust in the case of critical peak overlapping of K-lines with L-lines, because the entire set of L-lines is used for the quantification.

For micro-XRF using a polycapillary lens, the influence of the optic to the excitation spectrum has to be considered. We solve this problem with a mathematical model for the transmission of the lens.

The quantification is extended by an advanced estimation of the uncertainties. Besides the counting statistics, uncertainties of the fundamental parameters and uncertainties in the modelling of the detector response are taken into consideration.

The poster will focus on the results of extensive tests with more than hundred certified reference materials. The tests had been performed with direct excitation using a collimator as well as with a micro-XRF spectrometer with polycapillary lens.