HIGH SPEED MATRIX AND SECONDARY FLUORESCENCE CORRECTIONS BASED ON MONTE-CARLO CALCULATIONS

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Due to recent advances in modeling of x-ray intensities (including secondary fluorescence) of both bulk and boundary conditions, Monte Carlo simulations of electron solid interactions can provide quantitative estimates of these effects for specific compositions. By utilizing these intensity calculations for ranges of binary compositions combined with the hyperbolic relationship, first described by Ziebold and Ogilvie, high precision matrix corrections can be achieved in seconds, even for complex matrices.

We are systematically calculating intensities for 11 binary compositional pairs from 1 to 99 weight percent for all emitters and absorbers for the main emission lines (Kα, Kβ, Lα, Lβ, Mα and Mβ) at beam energies from 1 to 50 keV and fitting the results to the alpha expression as proposed by Mark Rivers at UC Berkeley where C is the weight fraction and K is the intensity k-ratio:

$$\alpha = (C/K - C)/(1 - C)$$

As described by Armstrong, fitting this expression to a three coefficient polynomial, one can handle cases of extreme absorption and fluorescence. For complex matrices the alpha factors are combined as a beta factor using the expression here:

$$\beta_B = \sum_1^{n_A} \left(\alpha_{1(B,A)} + C_A * \alpha_{2(B,A)} + C_A^2 * \alpha_{3(B,A)}\right) * C_A$$

Where $\alpha_1, \alpha_2, \alpha_3$ are the polynomial fit coefficients and C is the concentration of the absorbing element. For secondary fluorescence from boundary corrections, the approach is to subtract from the measured k-ratio (K_{raw}), the difference between the calculated boundary (K_{AB}) and bulk (K_A) intensity k-ratios obtained from binary Monte-Carlo simulations using the expression:

$$K_{corr} = K_{raw} - (K_{AB} - K_A)$$

An example of the variation in the difference between K_{AB} and K_A is shown below for the Fe-Ni binary. Note that because the same Monte-Carlo dataset is used for both the boundary and bulk conditions, random errors in the Monte-Carlo calculation are minimized during the correction.