Where Compton Matters

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In the classical approach of the fundamental parameter (FP) method, the count rates of the analytical lines are extracted from the observed spectrum by peak fitting or deconvolution and by subtracting the background, which is determined by numerical procedures. The quantification of an unknown sample is performed in an iterative procedure where those measured count rates are compared with computed X-ray fluorescence intensities, calculated with analytical equations.

Modern FP-based quantification is not limited to the calculation of primary and secondary fluorescence count rates. The analytical calculation includs all effects in the detection path up to the detector and electronic response. Nowadays the modeling/computation no longer produces a set of fluorescence intensities but a calculated spectrum, which can be directly compared to the measured one. The advantage of this approach is the reduction of empirical assumptions, as e.g. a purely numerical background model can be insufficient for trace element analysis. The challenge is to include effects influencing the measured spectrum background that have been neglected in the classical approach. We present two of them in this work:

- **Compton scattering after XRF in the sample**: While secondary fluorescence is a well-known second order effect, which is included in most FP-libraries, double interaction processes including scattering effects are usually not considered. However, inelastic scattering of fluorescence radiation inside the sample can add a significant low energy wing to the XRF line, which could be misinterpreted as an overlapping fluorescence peak. Thus, in selected samples, the quantification of minor or trace elements is hampered, if this effect is neglected.
- **Compton escape artifact**: Spectra with substantial count rates in the energy range above 30 keV show a significant increase of the low energy background. This artifact is caused by inelastic scattering of incident photons in the detector crystal and the subsequent escape of the scattered radiation and is well-known in gamma-ray detectors.
  The high energy photons which cause this effect can only be eliminated from the spectrum at the cost of measured fluorescence intensity of most elements. Therefore, for a reliable quantification it is necessary to model the effect thoroughly.

These effects are two modules included in a novel FP quantification routine for commercial XRF and micro-XRF spectrometers.