Definition of the Detection Limit in Energy-dispersive Spectrometry

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Energy-dispersive and wavelength-dispersive spectrometry (EDS, WDS) is not only used for the analysis of major and minor elements but also for trace element analysis. For these trace elements the detection limit needs to be known in order to decide whether an element is present or not in a specimen. There are several different definitions. An often used definition of the spectral detection limit is defined by the lowest peak intensity of a line I that can be detected with a certain confidence level which is defined by the counting error σ_b of the background intensity B [1], fig. 1. The counting error is given by $\sigma_b = B^{1/2}$. Normally, a 3σ criterion is chosen, which means that $I > 3B^{1/2}$. When a calibration sample for this trace element is available then smallest concentration that can be detected in a specimen can be calculated.

When WDS peak-background measurements are done then the interpolated background intensity at the peak energy is subtracted and the criterion for the detection limit can easily be applied.

For EDS the intensity of the central channel of the peak to be analyzed can be used in the same way. But this means that information from the neighboring channels is not taken into account. Instead the peak intensity and background intensity in a certain region of interest (ROI) can be used. In order to find the optimum detection limit the chosen ROI should not be too wide or too small and should depend on the full-width-half-maximum (FWHM) of the peak.

There are already general discussions in the 70s about the optimum ROIs in EDS for given peak heights above the background [2]. However, there are still a lot of different definitions in use today. A constant ROI for a certain peak, as proposed in [3], will lead to a detection limit which is independent from the FWHM and will not benefit from spectra with good energy resolution. Also, generally using the "number of peak counts" and the "background counts under the peak" without the definition of a ROI, as mentioned in [4], is not accurate enough.
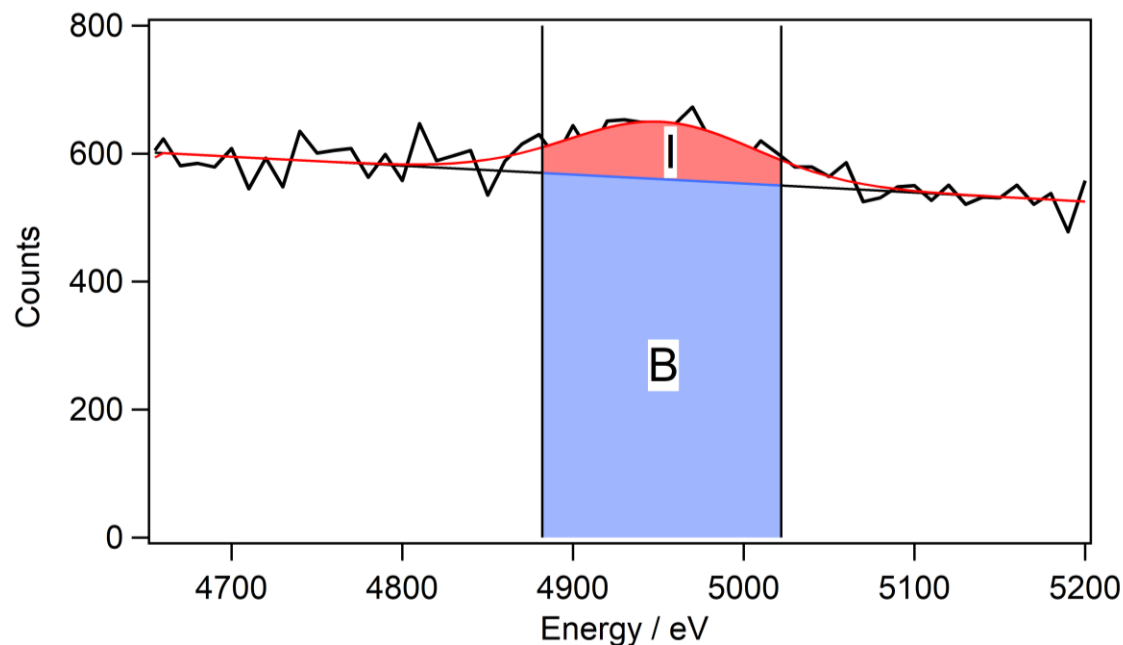

Figure 1. Spectrum with peak intensity (I) and background intensity (B) in a certain ROI.

References

[1] DB Williams, DB Carter, "Transmission electron microscopy", Springer, New York, (2009)

[2] MA Short, X-ray Spectrum. 5 (1976), p. 169

[3] T Ernst et al, X-Ray Spectrom. 43 (2014), p. 13

[4] J Goldstein et al, "Scanning Electron Microscopy and X-ray Microanalysis", Springer, New York, (2018)