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Physical Modeling of the Background of XRF Spectra

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X-ray fluorescence (XRF) analysis is a well established non-destructive analytical technique for the determination of the element concentration in bulk and layered specimens, providing limits of detection considerably lower than for the case of excitation with electrons. For quantitative XRF the net peak areas are the main input information for the quantification routines. For this purpose, an accurate subtraction of the spectral background is of decisive importance. Popular XRF quantification software packages rely on spectral background reconstruction by pure mathematical or empirical means.

The spectral background of energy dispersive (ED)-XRF spectra is determined mainly by the ED spectrometer properties and by X-ray scattering in the specimen. Especially for specimens having a low average atomic number the background of the XRF spectra is in fact defined by scattering. The aim of this work is to describe the X-ray scattering by means of a relative simple physical model. In order to verify the model, accurate measurements on reference materials have been performed with a well-known photon excitation source (X-ray tube spectrum) [1], a calibrated ED spectrometer and under a well-known geometry in a SEM (Scanning Electron Microscope) [2].

The calculation of an X-ray tube spectrum was performed by means of a procedure based on measurements of photon generation yields with calibrated SEM/EDS instrumentation [1].

Elastic (Rayleigh) and inelastic (Compton) scattering is calculated from the well-known Thomson and Klein-Nishina formulae corrected for: scattering anisotropy [3], atomic (bound) electrons [3], and relative pre-collision motion electron-photon, *i.e.* "Compton broadening" [4]. The resulting total scatter spectrum is multiplied with the spectrometer efficiency and eventually convoluted with the spectrometer response functions, so that the model can be verified with metrological measurements.

The agreement between calculation and measurement for specimens containing elements of mid atomic number is fairly well over a large energy range, s. Fig. 1 for pure Al as a scatter body. For matrices of low atomic number, the agreement becomes unsatisfactory in the low-energy range, s. Fig. 2 for PMMA. Work on further improvements is in progress, *e.g.* Monte-Carlo simulations to elucidate the effect of multiple scattering, or manual fitting by means of background regions of interests (ROIs).

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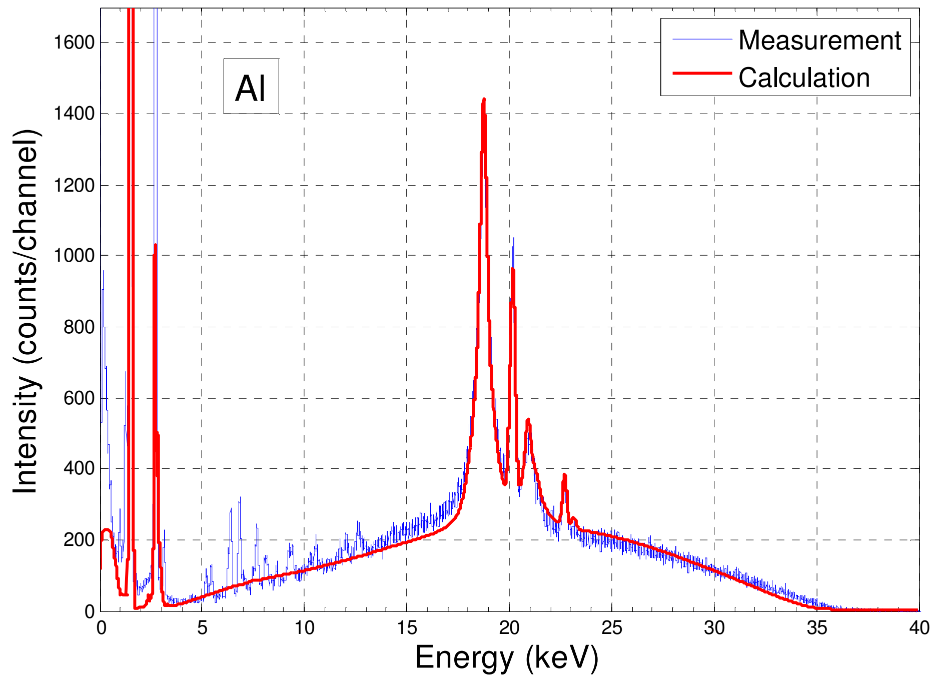

FIG. 1. X-ray scatter spectra of Al calculated as absolute intensity distribution (red) and measured (blue); excitation: 40 kV Rh anode voltage; scatter angle: 155°.

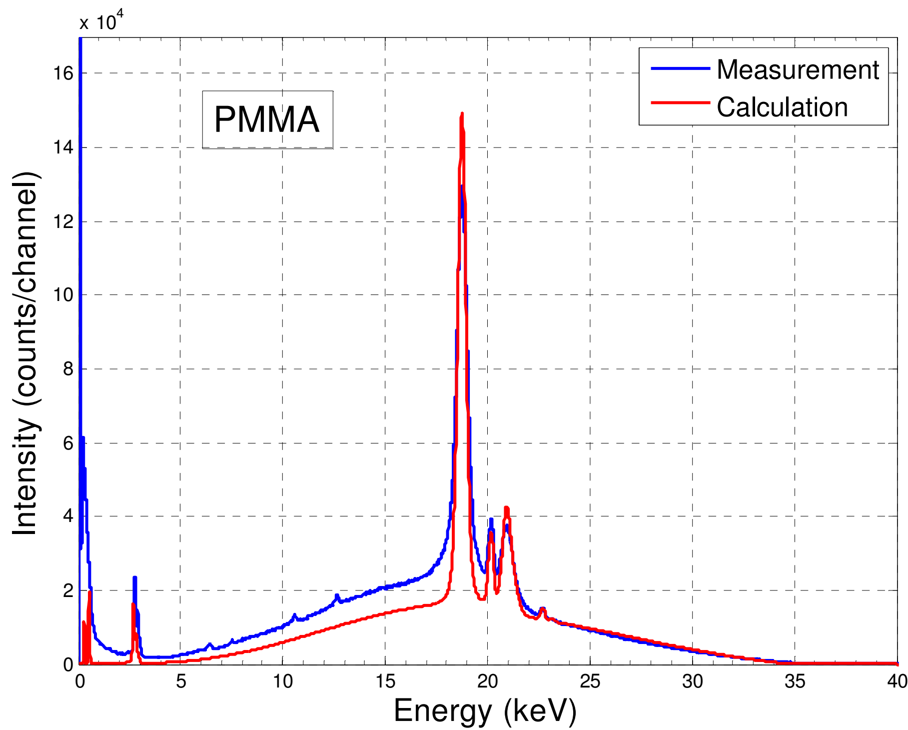

FIG. 2. X-ray scatter spectra of PMMA calculated as absolute intensity distribution (red) and measured (blue); excitation: 40 kV Rh anode voltage; scatter angle: 155.

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