

Quantification of the reduction of uncertainties due to the calibration with standards by X-Ray Fluorescence (XRF) and Particle-Induced X-Ray Emission (PIXE)

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Abstract

Calibration with standards is usually the first step for determining the elemental concentrations of a sample in XRF and PIXE. The first advantage of this calibration over the standardless analysis is the cancellation out of several instrumental and fundamental parameters which can bring uncertainties. The second advantage is the reduction of the uncertainties due to the parameters involved in the so-called matrix effects, like the mass absorption coefficients; the photoelectric and proton cross sections; the X-ray and the proton energies from the sources; and the proton stopping power. In this work we present the calculation of this reduction simulating uncertainties in these last parameters and propagating them in several kinds of calibrations, like the calibration with thin films, pure thick elements and reference samples. This analysis is applied to some theoretical representative samples and the comparison between PIXE and XRF for these calibrations is discussed. The results show that in XRF the uncertainties due to the mass absorption coefficients play a major role in the propagation than other parameters and can be overcome only using a calibration with similar standards, while in PIXE the uncertainties due to the proton cross section play the major role which can be overcome using calibration with thin film standards and improved with pure thick elements or similar reference samples. The propagation of uncertainties due to the excitation sources and also some systematic errors are also discussed.

Keywords: XRF, PIXE, Calibration, X-Ray spectrometry