

FUNDAMENTAL PARAMETER DETERMINATION FOR IMPROVED XRF QUANTIFICATION IN THE SOFT X-RAY RANGE

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Fundamental Parameter (FP) based X-Ray Fluorescence (XRF) analysis offers the advantage of extrapolating beyond calibration curves which are frequently used in many fields of application. In the field of micro- and nanoscaled material characterizations, FP based XRF is indispensable for a reliable quantification, because appropriate reference samples are typically not available. Here, the modeling of the sample system, of the experimental setup and of the physical interactions related to the x-ray emission processes ensures a more accurate quantification. Furthermore a complete reference-free [1] quantification became feasible when calibrated instrumentation could be employed.

The reliability of the FP methods depends strongly on the uncertainty of the available FP data, part of which is still debatable, in particular in the soft-x-ray regime. During the last three decades only few experiments were performed in order to determine FP values employing state-of-the-art instrumentation.

The high brilliance provided at synchrotron radiation facilities and the high-resolution of state-of-the-art wavelength-dispersive spectrometers allows for more detailed studies of the interaction of x-rays with matter. Employing a calibrated high-resolution spectrometer allow for the quantitative access to the cross sections of these interactions. In the field of XRF analysis these are the atomic FP. The most important FP are transition probabilities, fluorescence yields, photo-electric cross sections and Coster-Kronig factors.

In PTB's laboratory at the electron storage ring BESSY II a calibrated wavelength-dispersive spectrometer was used to measure FP by performing pure photon-in-photon-out experiments. In order to improve the reliability of XRF analysis we determined all FP needed for the quantitative description of the L fluorescence emission of selected transition metals such as Ni by means of high-resolution X-ray Emission Spectrometry [2]. In addition to an improved reliability of the FP databases, this kind of studies has the potential to increase our knowledge about the interaction of X-ray radiation and matter, e.g. regarding satellite emissions, cascade effects and chemical state effects on the fluorescence cross sections.

References

[1] B. Beckhoff, *J. Anal. At. Spectrom.*, **23**, 845 (2008)

[2] M. Müller, B. Beckhoff, R. Fliegauf, and B. Kanngießer, *Phys. Rev. A*, **79**, 032503 (2009).