

Modeling XRF intensities for portable/handheld analyzers using Fundamental Parameters Approach

A.G. Karydas^{1,4}, D. Sokaras², M. Drozdenko³, V. Kantarelou⁴, R. Padilla-Alvarez¹, A. Markowicz¹

¹Nuclear Spectrometry and Applications Laboratory, International Atomic Energy Agency (IAEA), IAEA Laboratories, A-2444, Seibersdorf, Austria, A.Karydas@iaea.org

²Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

³Institute of Applied Physics, National Academy of Sciences of Ukraine, Sumy, Ukraine

⁴Institute of Nuclear Physics, NCSR Demokritos, 15310, Athens, Greece

XRF analyzers based on low power x-ray tube excitation (few Watts-50 Watts), developed either as commercial instruments or customized in-house for specific applications, have nowadays reached a remarkable level of analytical performance. The miniaturization and subsequent optimization of the geometrical configuration of the instrumental/hardware components together with a wide selection of operational parameters (high voltage, current, type of filter, vacuum/He atmosphere) allowed improving the elemental sensitivities, the detection limits and to shorten the measuring times. The utilization of portable/handheld XRF analyzers in various applications rapidly expands from simple in-situ screening investigations to more demanding analyses including quantification. Inter-laboratory exercises have demonstrated the potential for further improvement of the results by means of Fundamental Parameters (FP) and Compton correction based analytical methodologies. However, the role of FP remains still to be further explored and validated in quantitative routines applied in portable/handheld XRF spectrometers.

This contribution presents the results of modeling XRF intensities for pure elements/compounds produced by different portable/handheld XRF spectrometers. A methodology based on X-ray FP is described and possible uncertainties are discussed including their contribution to the simulated results. The enhancement of the fluorescence intensities as a result of second order processes such as secondary fluorescence, photoelectron excitation and cascade effect is estimated for specific matrices. The results of the present work can be used to assess whether and to which extent theoretical modeling can simulate efficiently and accurately portable/handheld XRF intensities and to identify potential pitfalls that require further investigation and development. The introduction/validation of FP approaches in portable/handheld XRF spectrometers will improve robustness of the analysis, but also would provide a universal method to be applied for quantification in a wide range of analytical applications.