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Development of a standardless miniature XRF system for the analysis of actinides: coupling MC modelling and fundamental parameters

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1. Introduction

X-ray fluorescence (XRF) is a powerful quantitative and qualitative analytical tool for elemental analysis; it is suitable for solid, liquid and powdered samples, and for a wide range of elements. It is non-destructive, requires little sample preparation and short measurement time.

In this work a standardless XRF setup with two measurement channels intended to actinide analysis is presented.

2. Miniature X-ray fluorescence system

The miniature XRF system includes two channels: the first one presents the classical XRF, the second channel contains additionally optical element located between the sample holder and the detector: the highly oriented pyrolytic graphite (HOPG) monochromator (Figure 1)

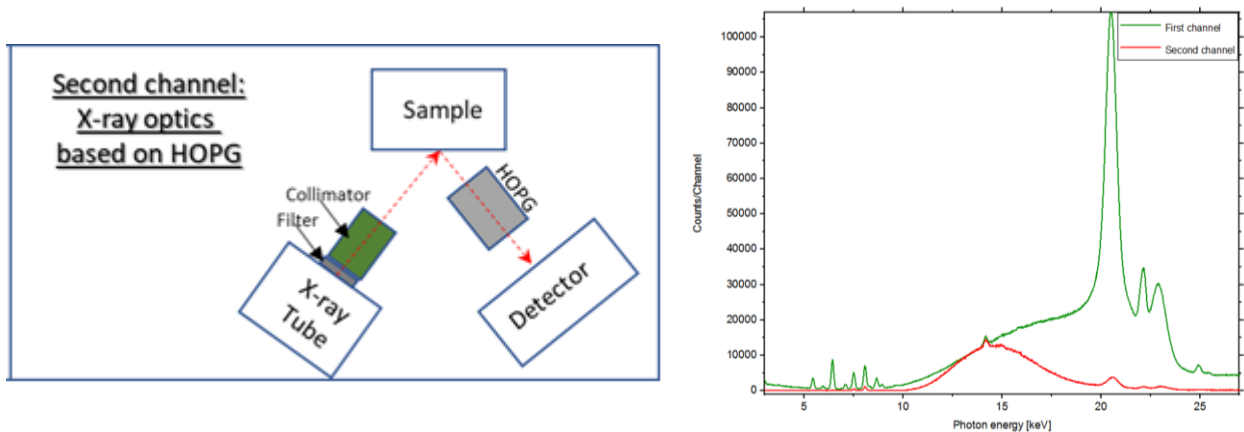


Figure 1. Monochromator based channel of the miniature XRF setup for spectrum analysis (left); comparison of measured spectra of the same sample measured with both channels (right).

HOPG can be used as a very efficient focusing and monochromatizing device [1, 2], allowing to focalize in a desired energy range (Figure 1), increase the intensity, and minimize undesirable spectrum parts.

It is possible to quantify the spectrum obtained from a sample with the classical XRF channel using fundamental parameters software [3]. The FP express the theoretical intensity/concentration relationship and requires the correct description of the setup. Since, the second channel has built-in optical element, which modifies the fluorescence intensity, it does not allow to quantify the spectrum using the FP algorithm. A solution consists in modeling of the transfer function of the monochromator (the function that represents the relationship between the input and output of the optical element) and include it in the FP algorithm.

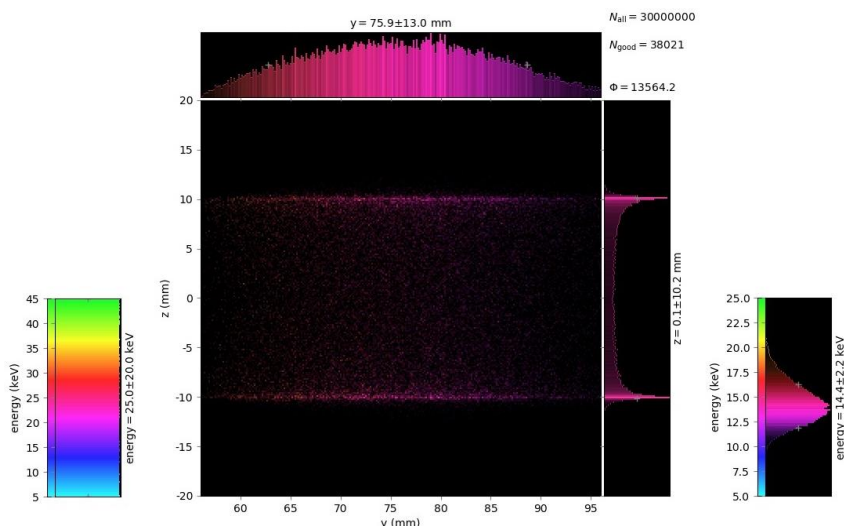


Figure 2. Simulation results of the diffraction of x-rays by cylindrical HOPG monochromator with x-ray tracing (XRT) package: a polychromatic source spectrum implemented before the monochromator (left); multiple-reflection processes in HOPG cylinder (center); obtained spectrum after passing through the monochromator (right).

3. Simulation of the XRF system

The modelization of the optical element of the setup is performed with x-ray tracing (XRT) package [5]. The XRT allows to modelize only the multiple-reflection processes realized in cylindrical HOPG monochromator rather than all physical interactions in XRF setup. The mosaic structure of a presented HOPG crystal was successfully implemented in the code. Simulation results are illustrated in the Figure 2. In order to simulate the whole setup, it is necessary to obtain

the input source for the HOPG monochromator. This can be performed with the Monte Carlo (MC) simulation code of electron and photon transport [4]. Previously, it was verified that the simulated results of the classical XRF channel with the MC simulation code are in a good agreement with experimental results. The combination of both simulation code results permits to modelize the optical-based channel of the setup.

A good agreement between simulation results and experimental data enables to obtain a transfer function of monochromator and include it in the fundamental parameters algorithm, allowing to quantify the results obtained with the specific XRF system. Furthermore, using the simulation codes mentioned above, the mini XRF setup could be modified in order to improve the performance.

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