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

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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

Most of XRF devices all over the world use FP (fundamental parameters) algorithm that is a standardless approach. But for a singular device, such as the CBA XRF spectrometer focused on the analysis of actinide XL-lines by using a graphite monochromator, the use of FP algorithm is not possible as mentioned in [1], and a semi-empirical approach is still in use. This algorithm necessitates the preparation of many standards and a calibration process which is time consuming. A similar miniaturized XRF device has been developed. This system is a prototype dedicated to R&D experiments. The main goal of this new device is to be focused on standardless approach for quantitative XRF analysis.

2. Miniature X-ray fluorescence system

Miniature XRF system contains two channels for sample analysis. The first channel contains a classical XRF, including the X-ray tube, the sample and the silicon drift detector (SDD). Quantitative analysis of fluorescence spectra of this channel will be carried out with the data analysis tool PyMCA (Python multichannel analyser) [2], and/or the Amptek's XRS-FP software [3], which takes into account all attenuation processes. Both software are based on the fundamental parameter (FP) approach. The FP approach is based on theoretical equation, which helps calculating theoretical net X-ray intensities emitted by each element from a specimen of known composition. FP take into account the geometry, the x-ray tube, the shape of primary beam, all attenuators, and the detector efficiency. Also, it requires an accurate description of sample matrix. FP use a database, which include all the required parameters to calculate absorption coefficients, fluorescence yields, jump factors, line energies, etc.

The second channel includes X-ray tube, sample, a highly oriented pyrolytic graphite (HOPG) monochromator and a SDD. The operating principles of the second channel is the same as for the spectrometer in CBA.

The key part of both devices, spectrometer in CBA and miniature XRF, is HOPG. It is a mosaic crystal consisting of a large number of small nearly perfect crystallites. Diffraction of the incident X-ray on the crystalline structure obey the Bragg's law. The random distribution of scattering planes of the crystal helps x-rays of the same energy, emitted by a point source, to always find a crystal plane at the correct Bragg angle, and to be refocused on a single point at the image plane (Figure 1).

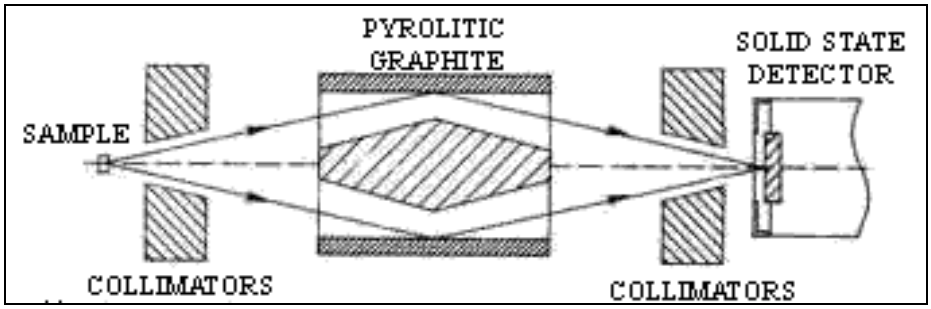

Figure 1. Focusing properties of HOPG monochromator.

A monochromator could be used as a very efficient focusing and monochromatizing device owing to its excellent integral reflectivity [4]. For both devices it is applied as a path band filter in order to cut off unnecessary information as Compton and Rayleigh scattering and to focus on the energy range of interest.

The concentration of the main actinides of interest (U, Np, Pu, Am, and Cm) can be determined by XRF using a device built specifically for these actinides analyses via their L-line X-ray between 12 and 17 keV. Setting up the monochromator at certain distance between the sample and the detector, it is possible to reach required energies.

For the second channel beforehand the use of FP algorithm needs to adequately characterize the monochromator.

3. Monte Carlo simulation

The second channel will be simulated using the Monte Carlo simulation software McXtrace [5], a package for simulating X-ray optics (not allowed by other Monte Carlo simulation software as Geant4, PENELOPE), beamlines and experiments. The modeling step of the system with monochromator is the most difficult task. Indeed, it is very important to describe the crystalline structure of the inside surface of HOPG, the geometry and position of it. All geometrical aspects and all interaction processes should be taken into account during the simulation.

The goal is, to simulate the different processes for the monochromator and after that to study how to integrate this simulation for fundamental parameters algorithm. In other words to apply XRF analysis coupling fundamental parameters (FP) approach with Monte Carlo simulation and avoid any calibration step.

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