SIMULATIONS OF POLYCAPILLARY-BASED WAVELENGTH DISPERSIVEX-RAY FLAT-CRYSTAL SPECTROMETER

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The polycapillary x-ray optics is widely used in x-ray fluorescence applications. Polycapillary x-ray lenses can collect a radiation emitted from a small source into a large solid angle and therefore they have a strong impact on the development of x-ray fluorescence analysis by improving the detection limits. Increasing demands for developing new and complementary x-ray methods to be used for various applications are presently focused on high-resolution and high-sensitivity x-ray fluorescence techniques combined with a narrow, down to the sub-micrometer range, x-ray beam excitation. For this reason, a new polycapillary based flat-crystal x-ray wavelength dispersive spectrometer (WDS) [1] have been implemented for the x-ray micro-fluorescence analysis applications at the ESRF ID21 beamline.

The factors affecting transmission of x-rays through a polycapillary optics include its shape, size, surface roughness, x-ray source – polycapillary geometry and x-ray energy and polycapillary optical properties. In order to predict the focusing properties and energy resolution of the polycapillary-based wavelength dispersive x-ray spectrometer, the Monte-Carlo simulation software was created. The calculations of x-ray transmission through the polycapillary exploit the phenomenon of total external reflection of x-rays by a surface below a critical angle, including the multiple reflections. In this simulations the quasi-parallel x-ray beam formed by a policapillary is directed onto a flat crystal at an angle θ, where the photons are diffracted according to the Bragg formula, and finally they are recorded by a detector placed at the angle 2θ. The simulation software has been written using C++ compiler, which gives a possibility to predict the transmission, spectrometer resolution and x-ray fluorescence spectrum.

The developed WDS spectrometer was applied to study the trace elements in speleothems (stalactite, cave pearl) from the Paradise Cave (central Poland) (see Fig. 1).

The Monte-Carlo simulations predict reasonable well the main characteristic of the polycapillary-based WDS spectrometer, which was tested experimentally (see Fig.2). The developed high-resolution WDS spectrometer was found to be well suited for the measurements of trace elements in geological samples (speleothems).

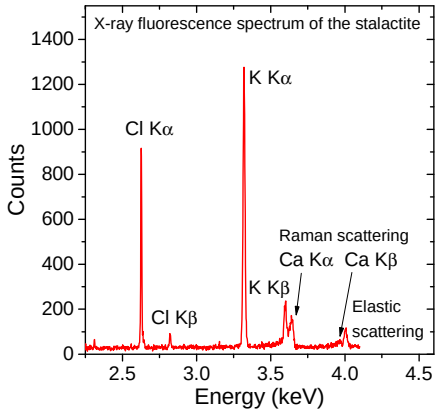

Figure 1. X-ray fluorescence spectrum recorded for stalactite sample measured with WDS spectrometer.

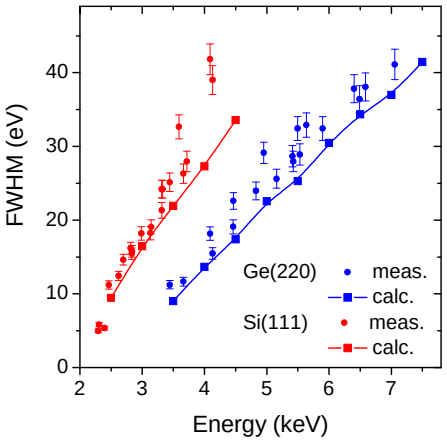

Figure 2. Energy resolution of the spectrometer with a Si(111) (in red) and Ge(220) (in blue) crystals: measured (circles) and calculated with the Monte-Carlo simulations (squares).

References

[1] J. Szlachetko, *et al.*, "Wavelength-dispersive spectrometer for x-ray micro-fluorescence analysis at the X-ray Microscopy beamline ID21 (ESRF)", *J. Synchrotr. Rad.* **17** (2010) 400–408.