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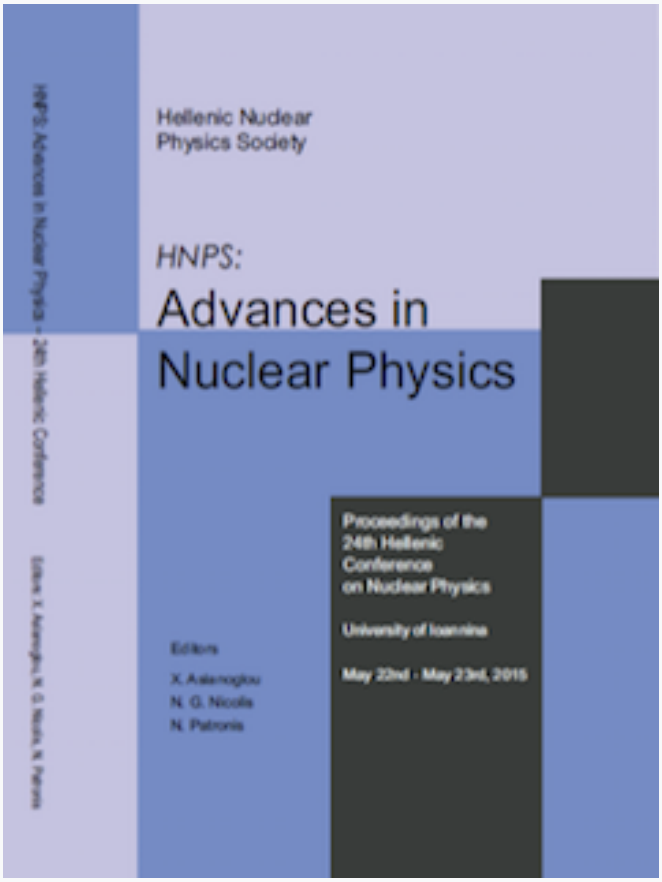

RICOCHET: A quick-and-dirty approach to analyze μ-XRF synchrotron data using open-source utilities

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RICOCHET: A quick-and-dirty approach to analyze μ-XRF synchrotron data using open-source utilities

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Abstract A semi-automated procedure based on open-source utilities was designed and built to analyze spectra collected at a synchrotron accelerator using the μ-XRF technique. The software (RICOCHET) has a fast, efficient and user-friendly design aimed at performing online analysis. A few examples of its application using recent μ-XRF data from the SUL-X beamline at ANKA Synchrotron Facility (KIT) are presented.

Keywords synchrotron, microbeam, μ-XRF, open source

INTRODUCTION

Synchrotron accelerators of the 3rd and 4th generation have tremendously boosted the quality and quantity of spectroscopic data. One of the most important analytical techniques applied at synchrotrons is X-Ray Fluorescence, based on ultra-bright, micro-focused beams of X-rays impinging the material under study (in short μ-XRF). The micro-focusing allows for detailed study of tiny sectors on a larger surface area, stimulating the emission of characteristic X-ray radiation from multiple chemical elements. Online analysis of the information is typically required to assess the results and plan the next steps in the experiment. In the majority of cases, the analysis is carried out using proprietary software packages (e.g. Igor Pro) or requiring customized procedures that have to run offline.

The necessity to analyze large μ-XRF data sets in almost-live time in a fast, efficient and user-friendly way resulted in adopting standard open-source tools available on Linux and OSX platforms to create RICOCHET, a limited-steps procedure that can quickly generate 2D/pseudo-3D maps of elements distribution on the material surface. The initial motivation behind RICOCHET's development was to serve the quick-and-dirty analysis of data sets obtained at ANKA synchrotron facility [1].

THE SYNCHROTRON FACILITY AT KIT (ANKA)

ANKA is a synchrotron facility located at Karlsruhe Institute of Technology (KIT) that offers a range of beam energies and avails a variety of analytical techniques based on X-ray microbeams. The ANKA SUL-X beamline (Fig. 1) focuses on environmental studies and combines diffraction, absorption and fluorescence measurements on environmental materials with microfocusing capabilities.

SUL-X data are provided to the user in ASCII format, where spectra and full details about the running experiment are stored. In the μ-XRF technique, the microbeam of X-rays (typically 20 μm x 20 μm beam size) irradiates the sample at specific coordinates of

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a predefined 2D grid. The intensity of the emitted characteristic X-rays is used to generate elemental maps from the few hundred spectra generated per run. This information needs to be processed during or immediately after the end of the run to provide quality assessment and guidance for follow-up spectroscopic techniques (such as μ-XANES, μ-EXAFS).

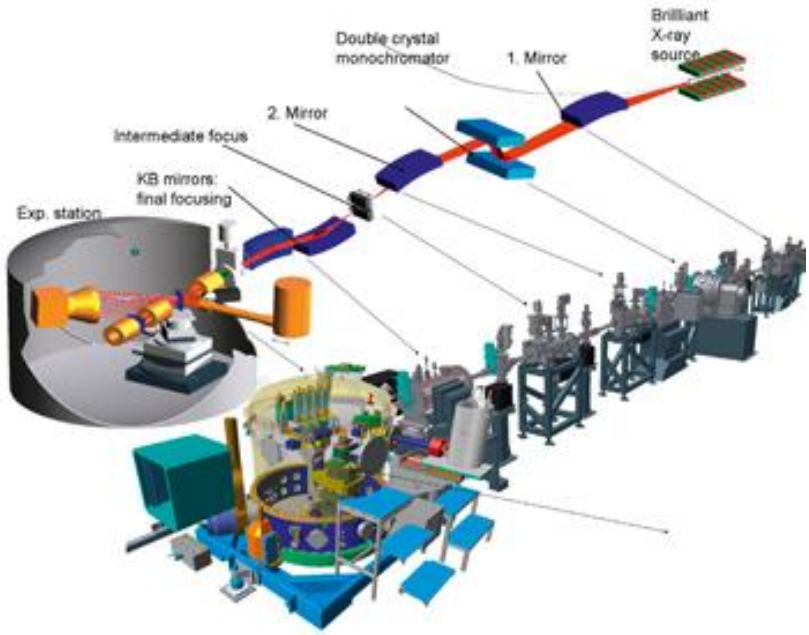

Figure 1 An outline of the SUL-X end station at ANKA Synchrotron

THE CODE RICOCHET

RICOCHET is a GUI-less tool that processes μ-XRF data in a fast and easy way during the experiment. It uses open-source scripting languages (*awk, sed, bash*) to process a large number of sequential spectra and extract all information needed to construct graphical 2D and pseudo-3D maps of elements found in the irradiated sample. Elemental hotspots, distributions and spatial correlations are studied in a concise way.

The user intervention is kept to a minimum level and simplicity in operation is the key advantage with respect to expensive proprietary software suites.

In brief, the main characteristics of RICOCHET are:

- It uses widely available, standard, open-source utilities that exist natively on Linux and Mac OSX platforms (e.g. *bash*, *sed*, *awk* and *gnuplot*)
- It operates fast on hundreds of data. Typical processing time for a 25x25 grid is in the order of minute on standard laptop computers. The processing includes ROI integration and plot generation
- It does not require experienced users
- It offers upscaling/expansion in an easy, straightforward way
- It offers high quality 2D/pseudo-3D plots, prepared at publication quality standards (PDF, EPS or scalable outputs)
- It can be adjusted to serve μ-PiXE analysis at a proton μ-beam facility.
- It is freely available and accompanied by a detailed tutorial

EXAMPLES OF APPLICATION

A few examples of application are demonstrated below in Fig. 2. The data are from earlier unpublished experimental studies at ANKA. Both 2D heatmaps (left column in Fig. 2) and pseudo-3D plots (right column in Fig. 2) have been generated. A grey-shades palette is available to be used in black and white printouts.

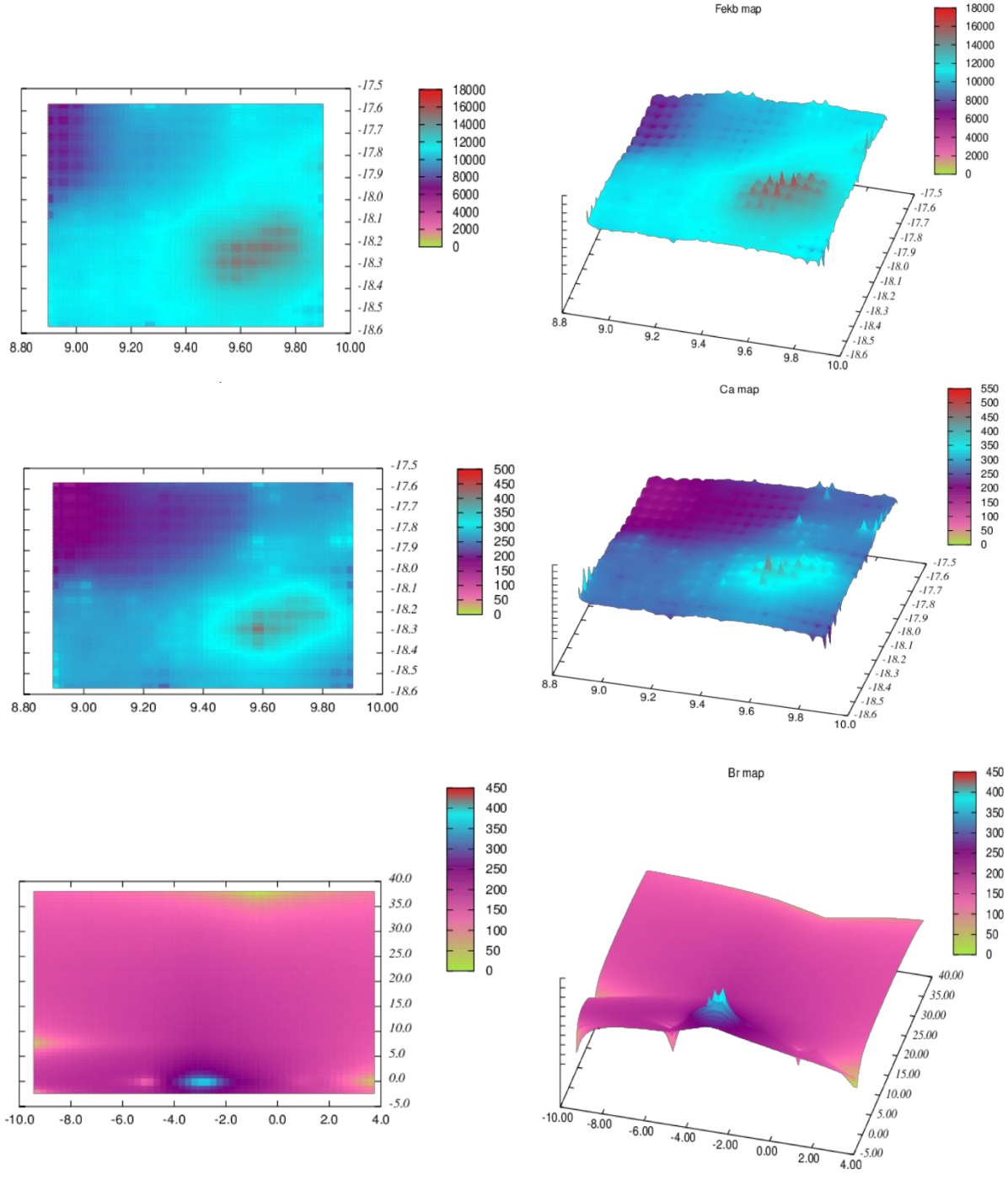

Figure 2 Examples of 2D (left) and pseudo-3D elemental maps (right). Spatial correlation is observed between Fe and Ca spots in the top and middle maps that come from the same experiment. Sharp peaks at the edges are algorithm artifacts.

CONCLUSIONS

A fast, efficient, user-friendly, open-source code (RICOCHET) has been developed for processing μ-XRF data from a synchrotron accelerator. The code has been tested successfully with real-data from recent experiments at ANKA. Future upgrades will focus on a Graphical User Interface (GUI).

Acknowledgements

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References

[1] ANKA SUL-X beamline, http://www.anka.kit.edu