DPDAK: Directly Programmable Data Analysis Kit for Online Analysis of 2D Scattering Data

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With modern area detectors (e.g. Pixel or CCD) on third generation SR-sources, frame-rates in the sub-second regime are not uncommon. Interactive experiment control by the user is frequently restricted to visual observation of the 2D patterns and - at best - tracking intensities in a pre-defined region of interest on the detector. Subtle changes of structural parameters of interest are, however, mostly not accessible this way, and the success (or failure) of an experiment is often discovered (months) later after detailed analysis of the data. It is therefore highly desirable that some simple but fast online analysis tools are available, allowing to classify the data e.g. for quality control and follow a number of parameters of interest predefined by the user as a function of the scanning parameters. The procedures imply typically some basic corrections (e.g. monitor correction of the intensity, background subtraction, etc.) and the extraction of scalar parameters from 2D patterns. These parameters should then be visualised in an efficient way (typically as an image or a profile in dependence on the scanning parameters) allowing an interactive experiment control by changing/adjusting the experimental protocol accordingly.

The goal of the project is to develop a general purpose software platform for preliminary online analysis of large data sets resulting from high throughput scattering experiments using large area detectors at synchrotron radiation sources, starting from the beamlines Bw4/HASYLAB, mµSpot/Bessy and MiNaXS/Petra III.

An important aim is that the platform should be independent of the beamline and/or experiment control software in order to be exchanged between different centres. Users should be able to use the software at their institutes. Therefore, the software package is developed as an open source project in Python and avoids commercial and license-based programs.

The software is designed as a framework with an easy plugin interface. Plugins allow to extend the software with new procedures for collecting, processing and visualise data. Plugins are Python files loaded at runtime. They have to be integrated in the software. A simplified layout of a plugin is shown in Figure 1. The analysis depends on the selected plugins and their configuration. Each analysis can be saved and redone afterwards. Figure 2 shows a complete screenshot of a GISAXS analysis.

DPDAK is currently under development. Most framework functionality is implemented and beta versions are tested. Plugins for rapid display of 2D scattering data, line, radial and azimuthal integration and plotting of parameters are included. Current aims in development are support for multicore CPUs and a more complex plugin configuration. Further analyses functions [1,2] will be included as new plugins.

MyPlugin

- Input & Output Definition
- Parameter Definition

Interface Functions
- allows DPDAK to access the plugin
- necessary to implement

Self Defined Functions
- the actual functionality of the plugin

Figure 1: Valid DPDAK plugins have to fulfil a specification.
Figure 2: A GISAXS analysis of in-situ sputter deposition.

References