

THE BRIDGE

MATERIALS ANALYSIS eNEWSLETTER AUGUST 2013, ISSUE 2

SmartStudio: The software command center for the SmartLab

A central software platform that simplifies X-ray analysis

SmartStudio is a platform that seamlessly integrates the software modules that operate and analyze data generated by the SmartLab diffractometer. It enhances the communication between the application software modules and increases ease of use. For example, data generated from one application module can be sent to another with a single mouse click using the Launcher, an interface that serves as the starting point for application software modules. When you select a data file, it will show you what applications can be launched. Various processes from measurement to analysis are automatically executed by using a recipe function. Using SmartStudio as the central point of all data measurement and analysis allows for a more efficient workflow and fewer possibilities for errors.



Files can be displayed in a thumbnail style that allows easy identification of the file contents

SmartLab Guidance

The Guidance package, based on built-in expertise, suggests the optimal hardware configuration and settings for specific application measurements. The program will determine which optics are most appropriate for a given application, determine the instrument settings and execute the measurement, offering a completely automated measurement sequence. Since the SmartLab has built-in component recognition, Guidance will not only tell you how you should configure the SmartLab for a given measurement, it will also warn you if you have not configured it properly. Expert advice coupled with hardware that will confirm the correct configuration is the foundation of the SmartLab system.



Guidance interface showing hardware configuration

<u>PDXL</u>: Integrated powder X-ray analysis software

Rigaku's PDXL is a modular full-functioned powder X-ray analysis software package developed to combine extreme ease of use with powerful state of the art analysis methods. The unique flow-bar makes PDXL the easiest to use in the industry.



In PDXL, multiple data files can be analyzed automatically under the same conditions. Comparing various analysis results, such as samples synthesized under different conditions and data obtained by a change in the measurement temperature, can be done easily. In addition, report generation can be done automatically for all analysis results.



List of detailed PDXL processing results obtained by profile fitting is shown

<u>2DP</u>: A tool to convert and view 2D data in various forms

2DP is a program for processing two-dimensional (2D) data. Functions include conversion to 1D data, background subtraction and merging while maintaining data in a 2D format, and the creation of actual movies depicting the changes in scattering data resulting from dynamical processes. Videos can be saved in AVI or WMV formats. There are various formats for displaying pole figures, residual stress and reciprocal space maps.

<u>3D Explore</u>: Analysis of crystal orientation and polycrystalline texture

3D Explore is used to display reciprocal space maps (for crystalline evaluation of single crystal thin films or structure evaluation of epitaxial films), as well as pole figures (for surface orientation evaluation of single crystal thin films or preferred orientation evaluation of multi-crystal thin films). Along with topography display and control of color mapping, equivalent-intensity surfaces and contours displays are supported. The measured data

can be overlapped with simulation data exported from the DSS module (Diffraction Space Simulation, i.e. reciprocal space map simulation) of SmartLab Guidance. In addition, smoothing, background subtraction, peak search and other data processing functions are also available.



3D Pole Figure

Data Mapper: Mapping display software

Data Mapper is a powerful tool to display the results of an XY mapping measurement performed using the SmartLab. Virtually any material property measured as a function of position on a sample can be mapped and displayed for simple visualization of anisotropic properties. For example, Data Mapper can map the results of phase identification obtained from PDXL or film thicknesses refined by GlobalFit.

GlobalFit: Thin Film Analysis Software

GlobalFit provides superior fitting methods for the most accurate results in thin film analysis. The GlobalFit algorithm (patent pending), available only from Rigaku, offers advanced parallel tempering base fitting methods that have been customized for analytical X-ray applications. Years of practical experience in the development of experimental methods for the X-ray analysis of thin films have been incorporated into the GlobalFit programs to complement and enhance the performance of traditional parallel tempering algorithms. As with all Rigaku software products, GlobalFit programs



offer an intuitive, user-friendly interface. Automatic reporting, macro driven operation, and Rigaku's trademark flowbar interface combine to offer users exceptional ease of use and productivity.



Periodic analysis of a super lattice using satellite peaks

<u>Nano-Solver:</u> Particle and pore size distribution analysis

Based on small angle scattering data, size distribution of particles and pores existing in media such as powders, bulk material, thin films, and liquids can be analyzed. Generally, a size of about 1 - 100 nm can be analyzed with data collected using standard SAXS, but NANO-Solver can also process length scales up to 1000 nm using USAXS data. Particles and pores of various shapes—such as spheres, core shells, cylinders, and spheroids—can be routinely analyzed. Additionally, a Debye model for analyzing indefinite shapes is also included.

PDF Analysis

Intensity corrections (e.g. subtracting Compton scattering intensity) of the X-ray scattering pattern allows for determination of the RDF (Radial Distribution Functions) and PDF (Pair Distribution Functions) by the Fourier transform method. Rigaku's PDF analysis software module can also refine RDFs and PDFs using the MEM (Maximum Entropy Method). This feature allows patterns with small ghost peaks to be obtained even from data with low spatial resolution, which often occurs when scattering is measured using Cu or Mo X-ray sources. Click here for more information on SmartStudio