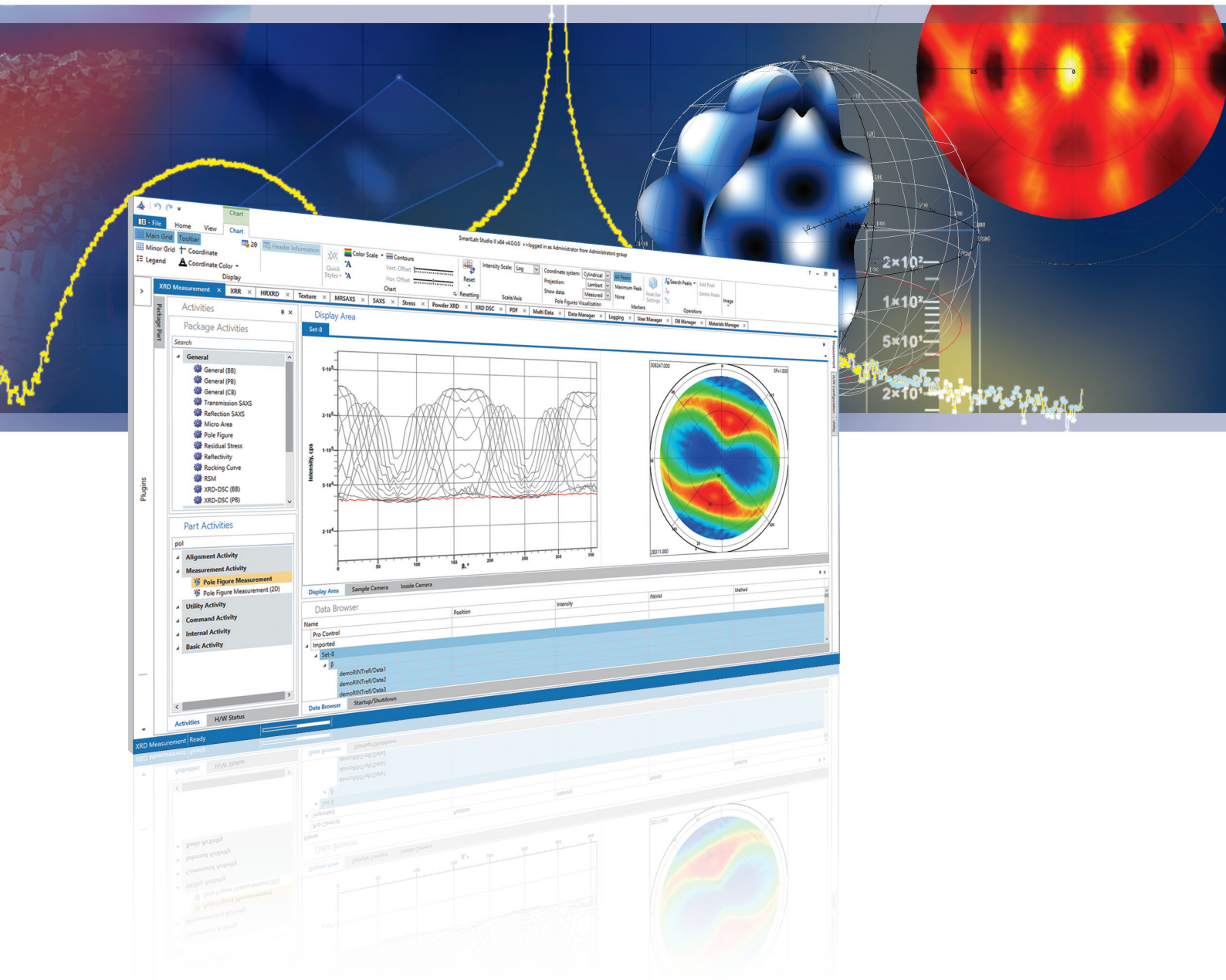
SmartLab Studio II

Integrated X-ray analysis software

All-in-One Integrated Software Platform for XRD Analysis



Rigaku

Leading With Innovation

SmartLab Studio II

All-in-One Integrated Software Platform

SmartLab Studio II is an integrated software platform for the SmartLab SE fully automated multipurpose diffractometer, covering the full spectrum of operations such as alignment, measurement, analysis, and report creation. This software employs plugin technology, which divides the necessary functions into several modules. The XRD Measurement plugin of SmartLab Studio II contains "Part Activities"*1, which incorporates the experience and know-how of Rigaku's expert scientists, allowing even novice users to obtain the best results. Analysis plugins contain an innovative flow bar to guide users through complete analyses with ease, as well as a solution tree intended for more advanced analyses.

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Centralized information management with an original Rigaku database

SmartLab Studio II stores not only the information on materials and users, but also other details such as measurement data, analysis results, and analysis conditions in its own databases to facilitate information management*2. This makes data backup and restoration easy and reduces the administrator's work.

User privilege management

In SmartLab Studio II, user privileges can be set in detail for each user group. As this software has extensive functions, administrators might not want certain users to access certain functions. In such cases, they can specify user levels, thereby "hiding" unwanted or unneeded functions, to customize the software for improving operability.

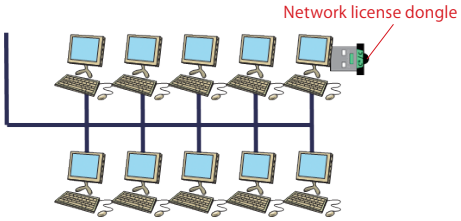
ER/ES mode and Audit trail

SmartLab Studio II offers an ER/ES mode and audit trail function (optional) to comply with electronic records/electronic signature of regulatory standards such as FDA 21 CRF Part 11. When users are logged in using ER/ES mode, all data are managed in the database, and all activities are traced by an audit trail. This function is recommended for situations that require traceability or integrity, as well as in the pharmaceutical industry.

Note: The ER/ES mode is available for the following plugins: XRD Measurement, Data Manager, and Powder XRD (as of April 2017), and will also be available for XRD-DSC Analysis plugin in October 2017.

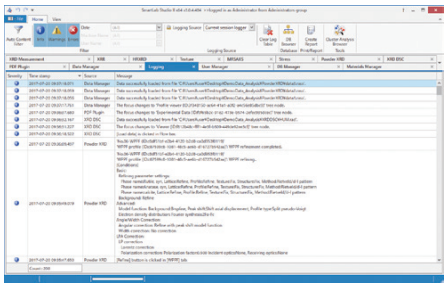
A single network license for sharing SmartLab Studio II

A single network USB dongle allows users to share SmartLab Studio II on up to 10 PCs on the same network, which eliminates the need for inserting a USB dongle into each computer. In addition, measured data and analysis results obtained from different PCs, as well as the information on users and materials, can be managed on a network database.



Quick log viewing

The Logging plugin stores all log messages generated in all plugins, and displays them in a single list. This allows users to immediately recognize any problems by viewing this log list if an error occurs.



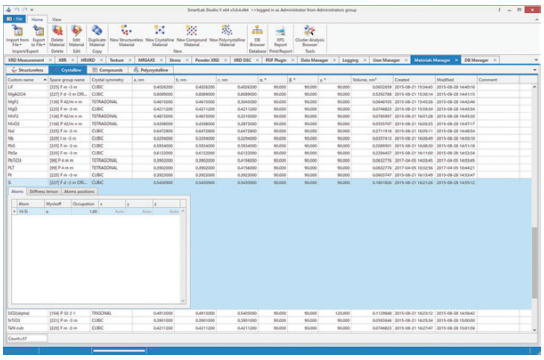
*1 A sequence of measurement activities including scans and axial movement is called "Part Activities" (*e.g.* Optics Alignment Part, Sample Alignment Part, Reflectivity Measurement Part, etc.)

*2 Data can be saved in the Windows® file system as well.

for XRD Analysis

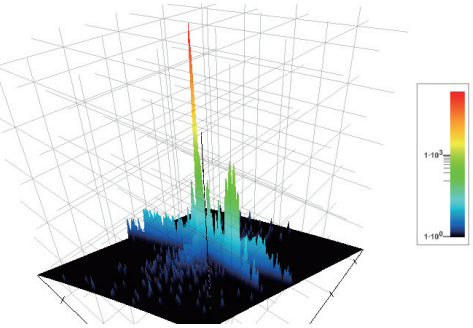
Common material database

Previously, each software application had to have an individual material database. SmartLab Studio II has consolidated those databases into a single database as a plugin module. This material database is classified into four material categories. Once a database is created on a server PC, multiple users can share it simultaneously via a network license.



Common chart control

The chart control is used to display data, graphs, 3D maps, etc. SmartLab Studio II uses common chart controls in all plugins, making mouse operations easier for enlarging or reducing any graphs or maps.
Color, line thickness, label font can also be changed freely in Chart options. This chart control has been developed using Microsoft® DirectX®, which supports high-performance applications, and can reduce the stress in operating graphics.

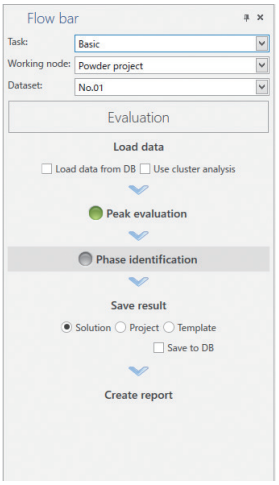


Report creation tool

The report creation tool is available on the flow bar or the ribbon tab. Users can choose their desired information from contents already provided by the tool, or use preset report formats.

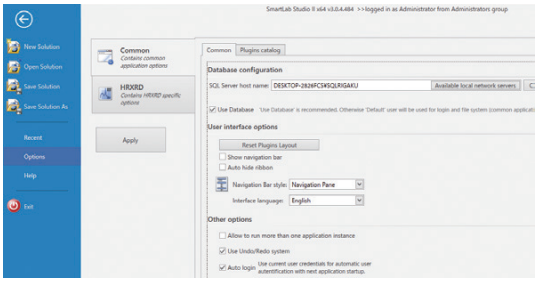
User-friendly flow bar navigation

SmartLab Studio II contains one or several flow bars in its analysis plugins to guide users through the necessary steps from loading measurement data to saving measurement data and creating reports. Even novice users are able to perform analyses with a good understanding of each step.



Other remarkable features

- Flexible GUI layout change
- Undo/Redo function
- Auto log-in
- Multiple applications launching
- Easy switching of languages (Japanese/English)
- New data format (RASX) for XML format

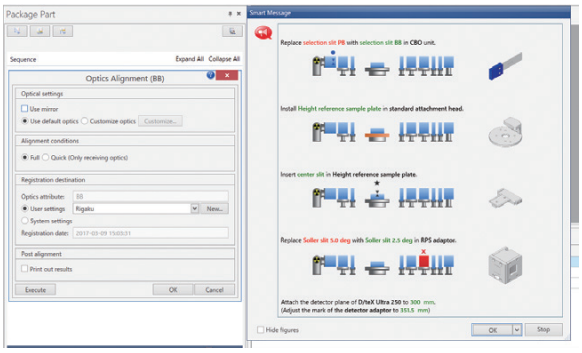


XRD Measurement

A measurement package built by experts in XRD

Leading-edge user guidance

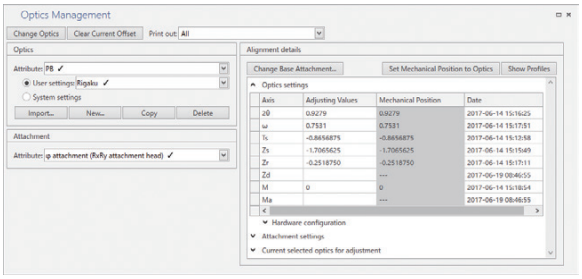
SmartLab Studio II incorporates the guidance function highly-admired in the SmartLab series. This function suggests the optimal hardware configuration and settings for specific application measurements, a task that normally requires expert advice. The software will determine which optics is the most appropriate for a given application, configure the required instrument settings and execute the measurement. It allows inexperienced users to master advanced measurements, which are usually only performed by experienced users*3.



Optical devices are changed following the instruction guidance (Smart Message) that appears during a measurement process.

Auto sample and optics alignment

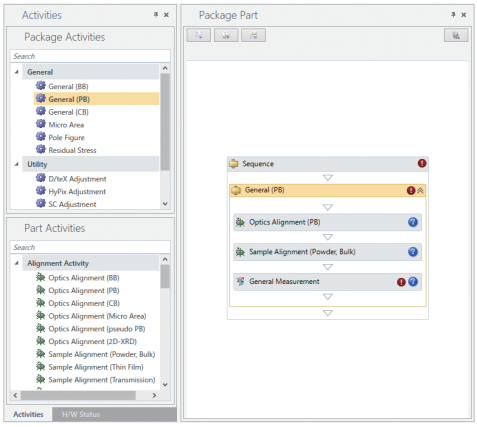
Sample and optics alignments are very important and require expert experience. The XRD Measurement plugin automates complicated alignment functions to allow users to conduct high-precision measurements every time. Since alignment results are saved with each optics and attachment, the aligned positions can be restored readily even when optics are changed.



Alignment results are saved with each optical device and attachment, making the change of optical and attachment settings easy.

Creating measurement flow and automating measurement

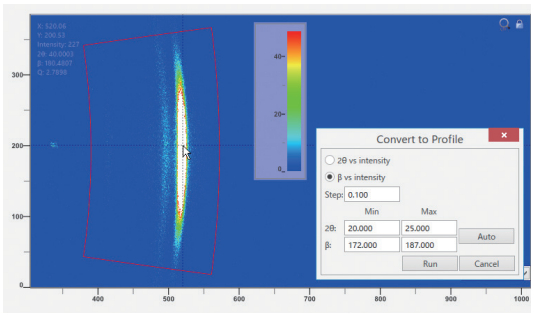
The XRD Measurement plugin offers "Package activity," which is grouped by measurement technique and contains optical alignment, sample alignment, and data measurement. It enables all users to execute alignment and measurement without expert knowledge.
In addition, users are able to create measurement flows according to their own needs. Basic functions can be combined to create users' own recipes for measurement or automatic maintenance.



A flow of alignment through measurement appears when opening a "Package Activity".

HyPix-400 next generation 2D detector

The HyPix-400 2D hybrid pixel array detector is capable of obtaining 2D diffraction data. In addition, it can also be used as a 1D or 0D detector without changing the actual detector itself, simply by switching 1D/0D mode in SmartLab Studio II. In the XRD Measurement plugin, the measured 2D diffraction data can be zoomed in/out or converted into a 1D profile.



XRD Measurement plugin is capable of showing 2D images (zoomed in/out) and converting 2D images to 1D profiles.

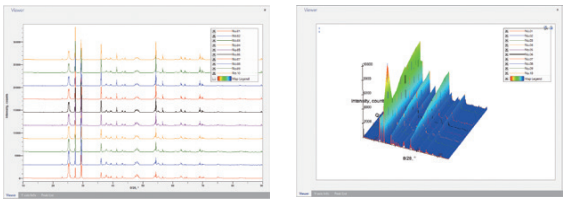
*3 SmartLab Studio II offers experienced users a function for freely customizing optics, which was not available in SmartLab Guidance.

Data Manager

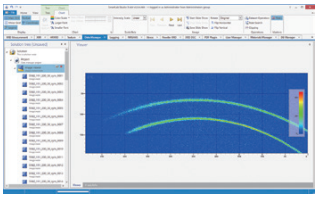
Simple mouse operation for data display, processing, and calculation

1D/2D data display

The Data Manager plugin is designed to compare several sets of measured data, using an offset graph, a map of 1D profiles or playback of 2D data slides in order to observe any changes in 1D or 2D data.



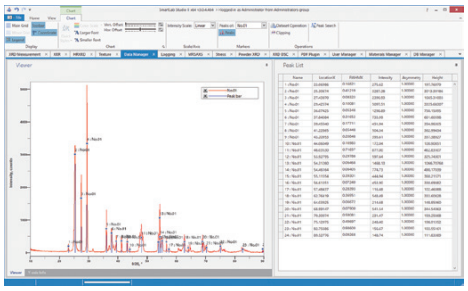
Offset graph and mapping of 1D profile data



2D image data

Quick data processing

Data Manager plugin contains several data processing tools, such as smoothing, background subtraction, and peak search, which are applicable to both 1D and 2D data.



Peak Search

Data calculation

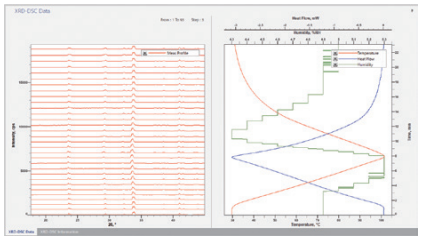
This plugin is designed to conduct simple calculations, *e.g.* addition, subtraction and scalar multiplication, as well as data normalization based on intensity (of a specific peak or at a specified position), and data clipping.

XRD-DSC Analysis

User-friendly tool for simultaneous XRD-DSC measurement

XRD-DSC data display

The XRD Measurement plugin is capable of displaying XRD-DSC data, but the XRD-DSC Analysis plugin features more advanced functions, such as changing the temperature range or thinning data to display graphs.

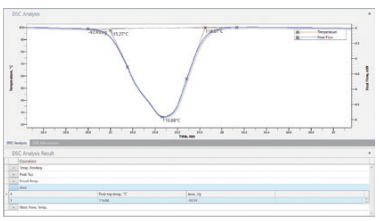


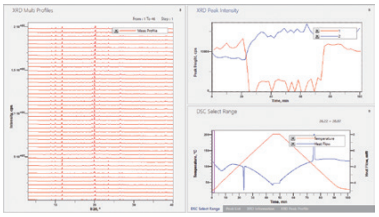
Linking XRD data and DSC chart

Measured XRD-DSC data demonstrate how changes in a diffraction pattern relate to thermal changes in a DSC measurement. This plugin is designed to present a graph of diffraction pattern or X-ray intensity and the DSC chart at the same time, allowing users to determine the changes in the crystal structure of the material.

DSC analysis

The XRD-DSC Analysis plugin incorporates an automatic DSC chart analyzing feature, which was not supported in earlier versions of Rigaku's software. This feature facilitates the estimation of melting point and phase transition point, as well as endothermic/exothermic calorimetry of dissolution, solidification, etc.





Powder XRD

The state-of-the-art consolidated powder X-ray analysis package

Hybrid Search/Match enhancing qualification analysis

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Hybrid Search/Match is crystalline phase identification based on two types of measured data: peak position and profile shape. Using this method, the accuracy of phase identification has drastically improved. It can also be used to identify crystal phases with preferred-orientation or heavily distorted lattices.

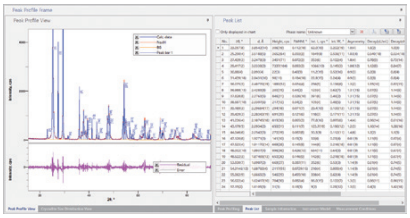
User-friendly operations for Rietveld analysis

SmartLab Studio II provides a user-friendly interface for Rietveld analysis, which enables users of any experience level to load crystal structure parameters from a database, set analysis conditions, display graphical images of crystal structures and quantify results without difficulty.

Basic package

▶ High-speed search with fully automated profile fitting

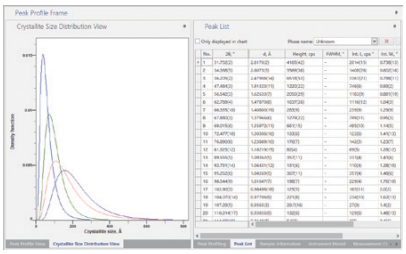
Simply by loading measurement data, SmartLab Studio II executes fully automated profile fitting to calculate peak position, FWHM, integrated intensity, and crystallite size (using the Scherrer method).



Peak list This list shows detailed processing results obtained from Profile Fitting.

▶ Crystallite size distribution analysis

Using the fundamental parameter method (FP method), theoretical peak shapes are calculated based on optical information to obtain more detailed analysis results, such as crystallite size distribution.



Crystallite size distribution Based on diffraction peak shape, crystallite size and size distribution are analyzed.

Quantification package (optional)

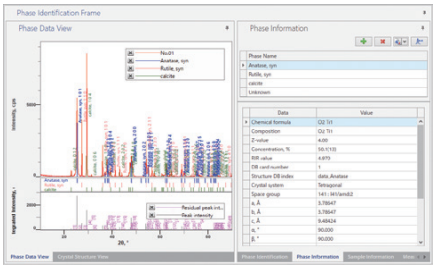
▶ Simplified procedure for creating calibration curves

This optional quantification package supports various calibration methods: Internal standard method, External standard method, Standard addition method. Peak intensity can be extracted and plotted with the software to create and use calibration curves. Quantification using the calibration method is suitable for quantification and management of specific crystal phases.

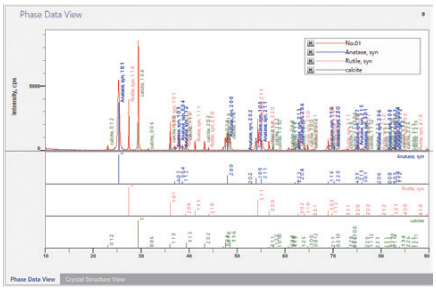
Qualitative analysis package (optional)

▶ Flexible search using Hybrid Search/Match

Rigaku's unique "Hybrid Search/Match" uses peak-base qualification, which detects heavily distorted lattices, to identify solid solution phases that are generally difficult to be identified. In addition, it determines whether preferred orientation exists based on separated peak intensities, which cannot be determined by the profile-base qualification.



Samples with preferred orientation or of solid solution Preferred orientation or heavily distorted lattices can be determined automatically, using the intensities of separated peaks.



Stacked display This facilitates comparison of identified phases.

Comprehensive analysis package (optional)

▶ A variety of analyses

This package is capable of providing analysis results such as crystalline size, lattice strain, lattice parameters refinement, %crystallinity based on fully automated profile fitting executed when loading measured data. The obtained information helps understand the relationship between structure and physical properties, and allows users to compare the results of different samples.

Rietveld analysis package (optional)

▶ Using the results of phase identification analysis

When a phase included in a sample is unknown, this package performs phase identification and then Rietveld analysis. Initial parameters required for Rietveld analysis are automatically estimated based on the measurement data right after phase identification. This makes Rietveld analysis easy even for inexperienced users.

▶ Using Rietveld method for quantitative analysis

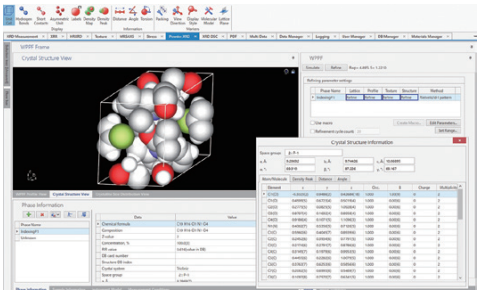
Rietveld method obtains quantitative results directly from the measurement results of the sample in question, unlike the calibration curve method, which requires adding a standard reference substance to the sample and creating a calibration curve.

▶ Using WPPF method for lattice parameter refinement

Lattice parameter refinement performed by Rietveld method or whole powder pattern decomposition method (Pawley method) is based not only on the measured peak positions, but also on the peak shapes (WPPF method). More accurate values are obtained with the angle correction, performed using an internal standard phase or external standard sample.

▶ Using FP method for theoretical peak profile calculation

The fundamental parameter method (FP method), which is used to calculate theoretical peak profiles taking into account the used optics and crystallite size distribution, shows great results for analysis of samples including several crystal phases, such as cement samples.

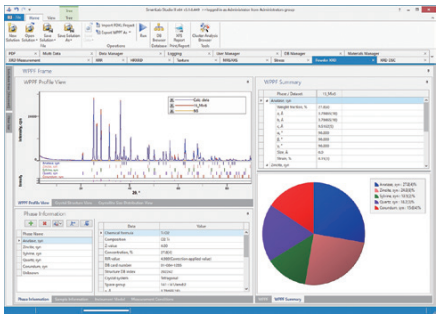


Crystal structure refinement of an organic compound

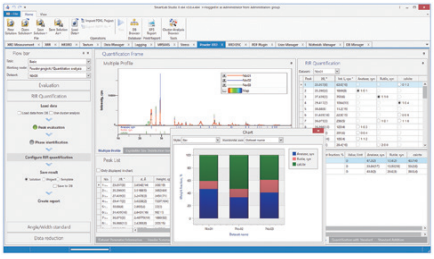
Flow bar

▶ Enhanced flow bars guide users through the analysis procedure

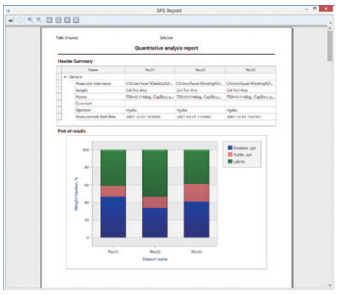
No need to worry about getting lost in operations anymore – there are 12 flow bars for various analysis purposes supporting all steps from loading data to creating reports. The flow bar allows effortless creation of the calibration curve, angle standard and width standard curve.



Analysis profile and quantification result



RIR quantification analysis with flow bar



Analysis result report

Available databases*4 in Powder XRD plugin (as of 2017.07.01)

Database name	Contents	Number of entries	Structure parameters*5	License term*6
ICDD PDF-2	Mainly inorganic compounds	291,119	None	Five years
ICDD PDF-4+	Mainly inorganic compounds	384,613	70%	One year
ICDD PDF-4/Minerals	Mainly inorganic compounds (minerals)	44,341	75%	One year
ICDD PDF-4/Organics	Mainly organic compounds	516,054	20%	One year
NIST-ICSD (for Powder plugin)	Inorganic compounds	170,000	100%	Unlimited (Conditions apply)
COD	Inorganic 25%, organic 75%	308,000	100%	Unlimited (Free of charge)
Rigaku cement DB	Cement based compounds	220	100%	Unlimited (for purchase)

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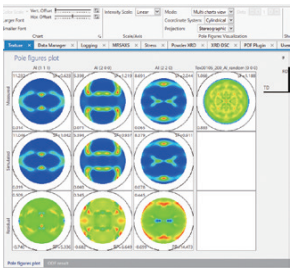
*4 These databases do not support network licenses, and must be purchased for every PC in use.
*5 The rate of structure parameters stored in each database.
*6 Each database may be renewed.

Texture

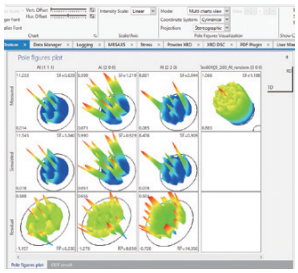
Step-by-step instructions on the flow bar allow smooth calculation of the crystal orientation distribution map

Creating and displaying pole figures

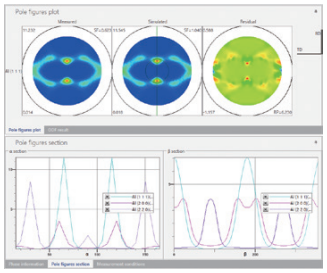
Texture plugin is designed to analyze the ODF (Orientation Distribution Function) from pole figure data measured with 0D or 2D detectors. The plugin supports defocusing correction and absorption correction of pole figures. In addition, the plugin includes functions such as smoothing, rotation and regrid of the pole figures. Measured 2D data, 2D images polarization correction and absorption correction are also available. Pole figures can be displayed in different formats.



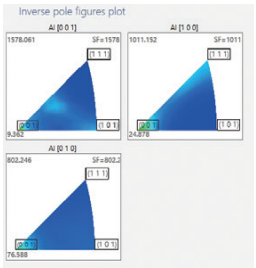
Stereo projection



3D view of pole figure



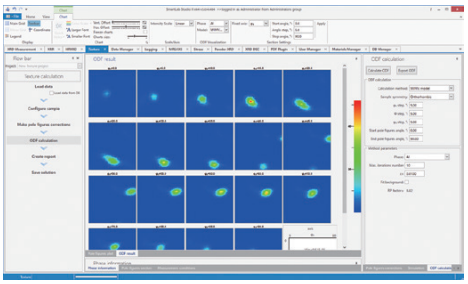
Pole figure cutline



Inverse pole figure

ODF calculation

Two methods of ODF calculation are available: WIMV *7 and component approximation analysis method. Both methods are suitable for the calculation of a crystal orientation distribution map and recalculation of whole pole figure corresponding to an arbitrary index. One of the optimization algorithms for component approximation is the genetic algorithm. When using this algorithm, there is no need to match parameters with a measured pole figure beforehand.
Also, the inverse pole figure can be created using the obtained crystal orientation distribution map.



Crystal orientation distribution map

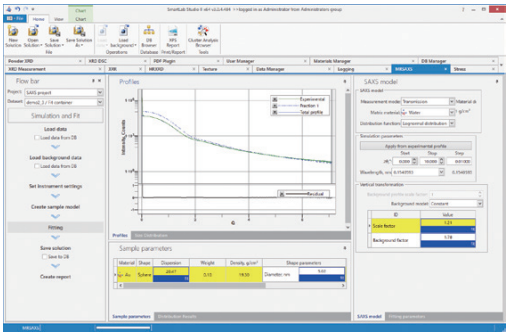
*7 Williams-Imhof-Matthies-Vinel (WIMV) method [Williams 1968, Imhof 1982, Matthies et Vinel 1982]

SAXS

Determination of particle/pore size distribution ranging from nano- to submicron order

Particle/pore size analysis

Particle/pore size analysis determines the size distribution of particles/pores in powder, bulk, film samples and liquid. Generally, particles/pores on the order of 1 to 100 nm are available for analysis. Using ultra-small angle X-ray scattering (U-SAXS) optics, users can analyze particles/pores 1000 nm in size. Particle/pore shapes such as sphere, core-shell, cylinder and spheroid can be analyzed. The plugin also features the Debye model, which performs analysis without the shape being specified. In the case of high density particles, the structure factor is taken into account for a more accurate size distribution calculation.



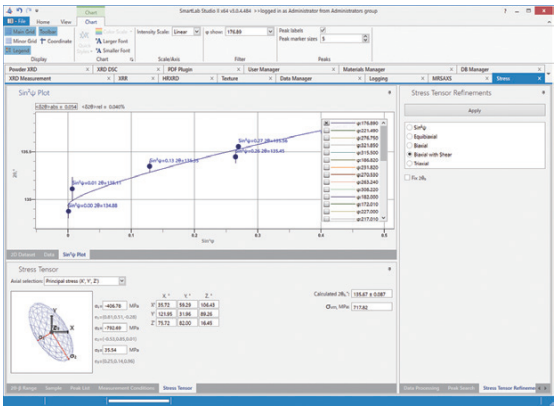
SAXS pattern fitting

Stress

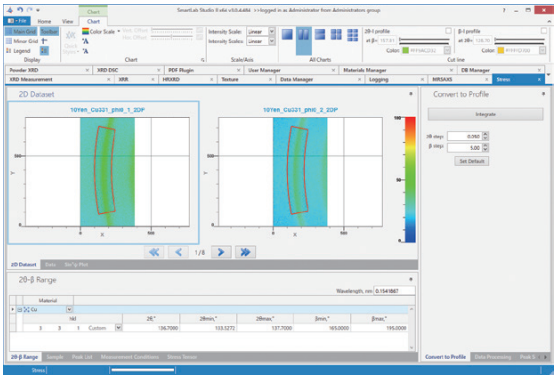
Stress analysis plugin suitable for activities from quality control to R&D

Residual stress analysis

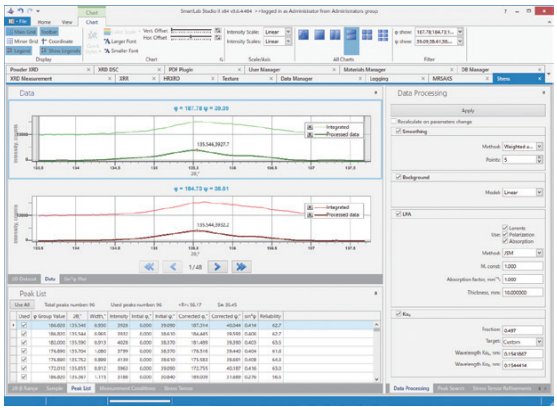
Stress analysis plugin is designed not only for stress analysis with the conventional $\sin^2\psi$ method but also for stress tensor or principal stress analysis under the assumption of biaxial and triaxial stress state.
Multiple-HKL method is also available, which uses diffraction peaks with different indices, and is effective for film material stress analysis. This plugin contains the following data processing functions: loading data measured with 0D, 1D, or 2D detector; cutting out 2D image data; processing 1D profile data peaks (smoothing, background subtraction, LPA correction, $K\alpha 2$ removal, peak search). In addition, extensive material database and X-ray elastic constant calculations are also available. The following grain interaction models can be selected: Reuss, Voigt, Kröner, Neerfeld-Hill. High usability and enhanced functionality assist convenient stress analysis in the areas from quality control to R&D.



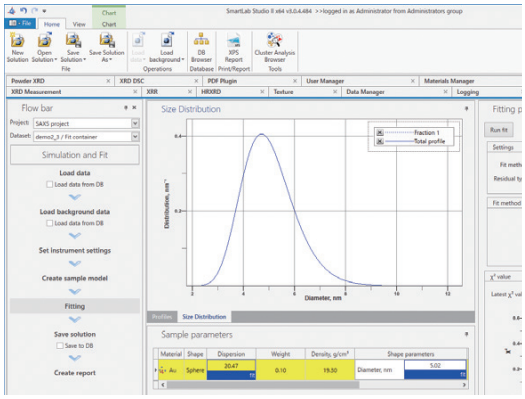
$\sin^2\psi$ plot



2D image data processing



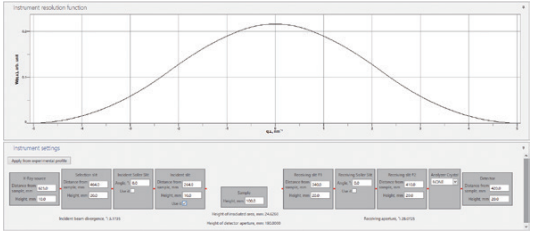
1D profile data processing



Size distribution graph

Slit correction

Due to the Rigaku original correction method, the theoretical profile is accurately repeated and more precise size distribution analysis is performed.



Slit function

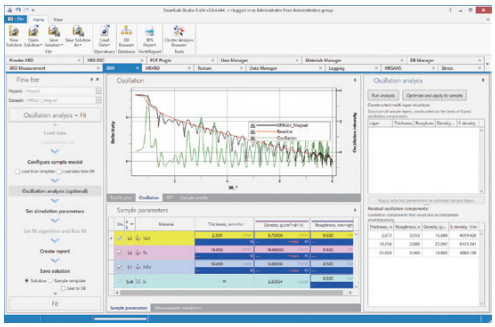
XRR / HR-XRD

An X-ray reflectivity analysis plugin for a wide range of applications from film thickness to multilayer structure analysis

The XRR plugin is designed to analyze thickness, density and surface/interface roughness of multilayer thin films, using the X-ray reflectivity method. The conventional non-linear least-squares method for reflectivity analysis, which provides a local minimum as a solution, had a problem that the final solution varied depending on the initial analysis model and the operator's skill. Our plugin uses the innovative fitting algorithm (genetic algorithm), which automatically searches multiple solutions to provide analysis results with no dependence on the initial model or the operator's skills.

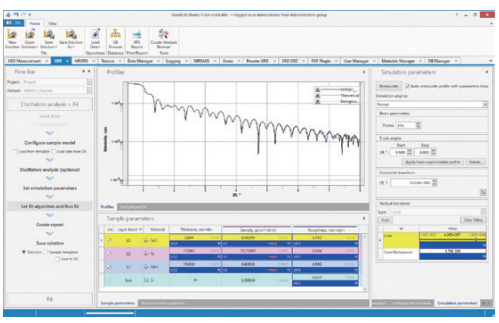
Extended Fourier analysis of film thickness

With extended Fourier analysis, the information on film thickness can be approximated in just one click. The approximated film thickness value can also be applied to fitting the initial model, which shortens the analysis time.



Diverse modeling functions

Modeling of the density gradient in a film provides an analysis that regards such complicated phenomena as interface diffusion. By setting the density and film thickness gradient for superlattice structures, the plugin can be applied to unequal multilayer structures. Five models for interface roughness provide detailed analysis of the interface state and precise consideration of the diffuse reflections caused by roughness.

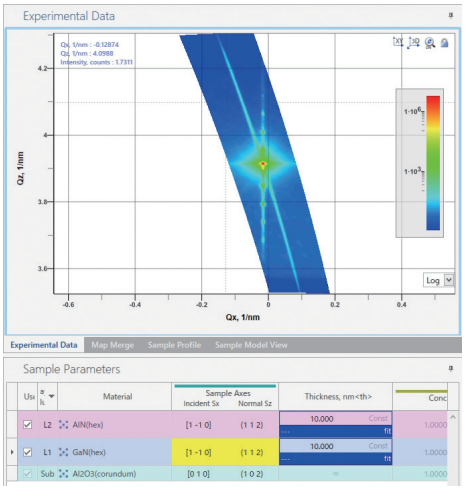


An integrated reciprocal lattice map and high-resolution rocking curve plugin for epitaxial films analysis

This plugin enables both reciprocal lattice map and high-resolution rocking curve analysis to be executed in a single plugin module. It performs seamless analysis of epitaxial films such as compound semiconductors. The plugin enables reciprocal lattice map analysis, which estimates crystal orientation and strain state, as well as high-resolution rocking curve analysis, which estimates film thickness and composition ratios.

Designed for advanced materials

This plugin supports analysis of epitaxial growth with anisotropy within the surface plane of the substrate. Employing "anchor parameters," which specify orientation in two directions of the sample surface plane, allows users to analyze anisotropic elastic deformation of epitaxial films in in-plane anisotropic tensions. The method can be applied to cutting-edge materials such as epitaxial films deposited on silicon (110) substrate or a-plane and m-plane sapphire substrate.



Diverse thin film structure models

Smooth structure modeling of samples with complicated multilayer structure is now possible, using parameter functions such as interlayer link and superlattice modeling. Relaxation in-plane strain and lattice mismatch in two directions of the sample surface plane can be selected as parameters for strain state description. Orientation deviation (inclination, twist) settings and mosaicity evaluation function have been added.
The upper and lower limits for each parameter can be set, which enables analysis considering film deposition conditions. The color coding for each crystal phase of the sample structure makes even complicated sample structures easy to distinguish visually.

Cluster Analysis

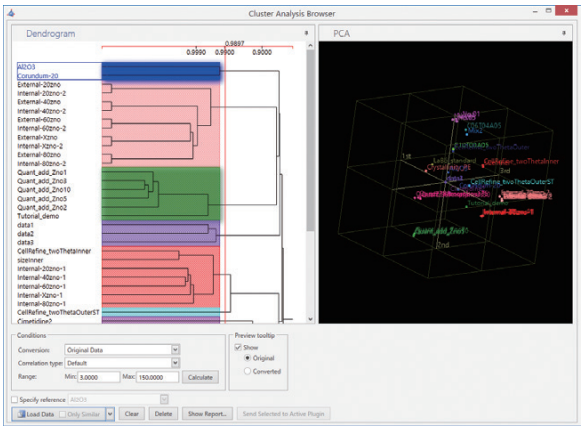
Categorization and extraction of large amounts of data

Dendrogram and principal component analysis

The cluster analysis module of SmartLab Studio II is designed to perform clustering regardless of data type and dimension (categorizing data based on the degree of similarity). Clustered data are displayed as a dendrogram. The number of clusters is freely varied by simply changing the threshold of the similarity degree. The correlations between similar data are clearly displayed in the PCA view.

Extracting data similar to reference data

SmartLab Studio II has a data extracting function. By setting reference data beforehand, data similar to the reference data will be extracted from a specified folder. This function is useful for searching previously collected data.



System requirements

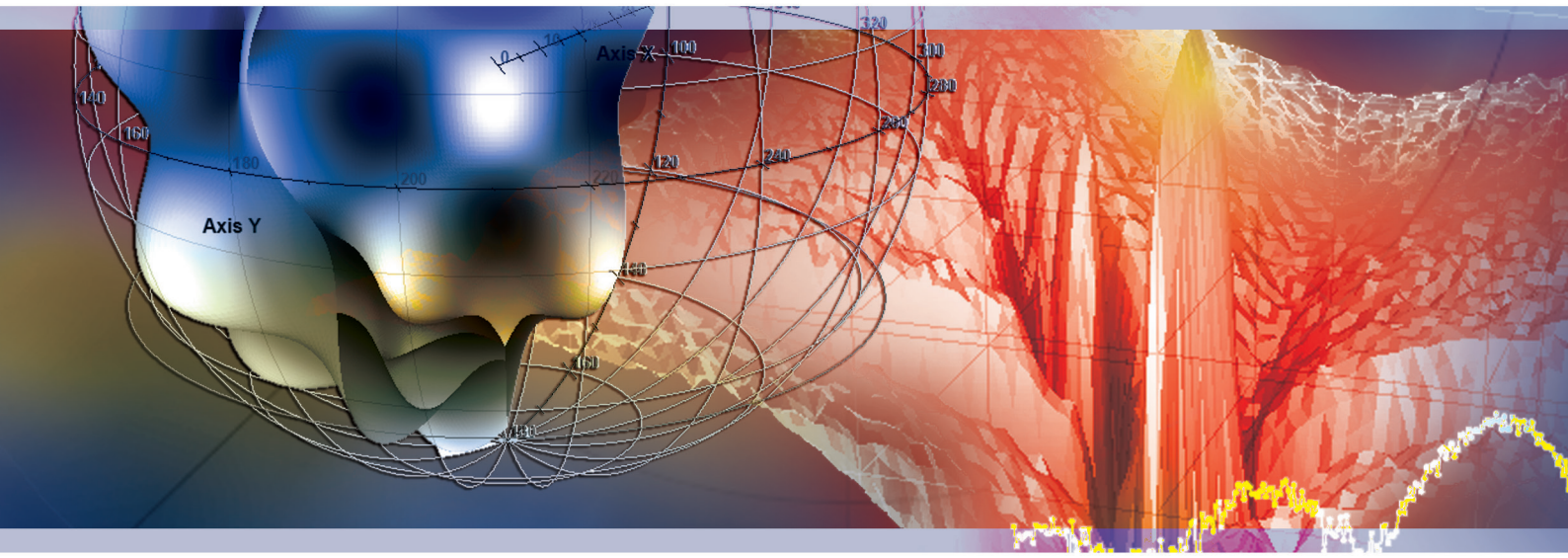
OS	Windows® 10 Pro (64-bit)*8 (Japanese or English (United States))
CPU	Intel® Core™ i5-2500 equivalent or greater (Core™ i7-3770 or greater recommended)
Video adapter	Microsoft® DirectX® 10.1 and Shader model 4.0 supported Video memory 512 MB (1 GB or higher recommended)
Network	Ethernet adapter Connection speed 100 Mbps (1 Gbps or greater recommended)
Monitor	Resolution 1920×1080 or higher (1920×1200 or higher recommended)
Memory	8 GB or higher (16 GB or higher recommended)
HDD free space	3 GB or more*9
USB port	1 USB port is required for using USB dongle (USB1.1 or USB2.0)
Other	DVD drive, Adobe® Reader (for displaying user manuals)

*8 Windows® 7 Professional SP1 (64-bit) and Windows® 8.1 Pro (64-bit) are also supported on all plugins except the XRD Measurement plugin.
*9 For installation of ICDD database additional 2.3 GB of free space is required.

SmartLab Studio II

Integrated X-ray analysis software

www.Rigaku.com



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