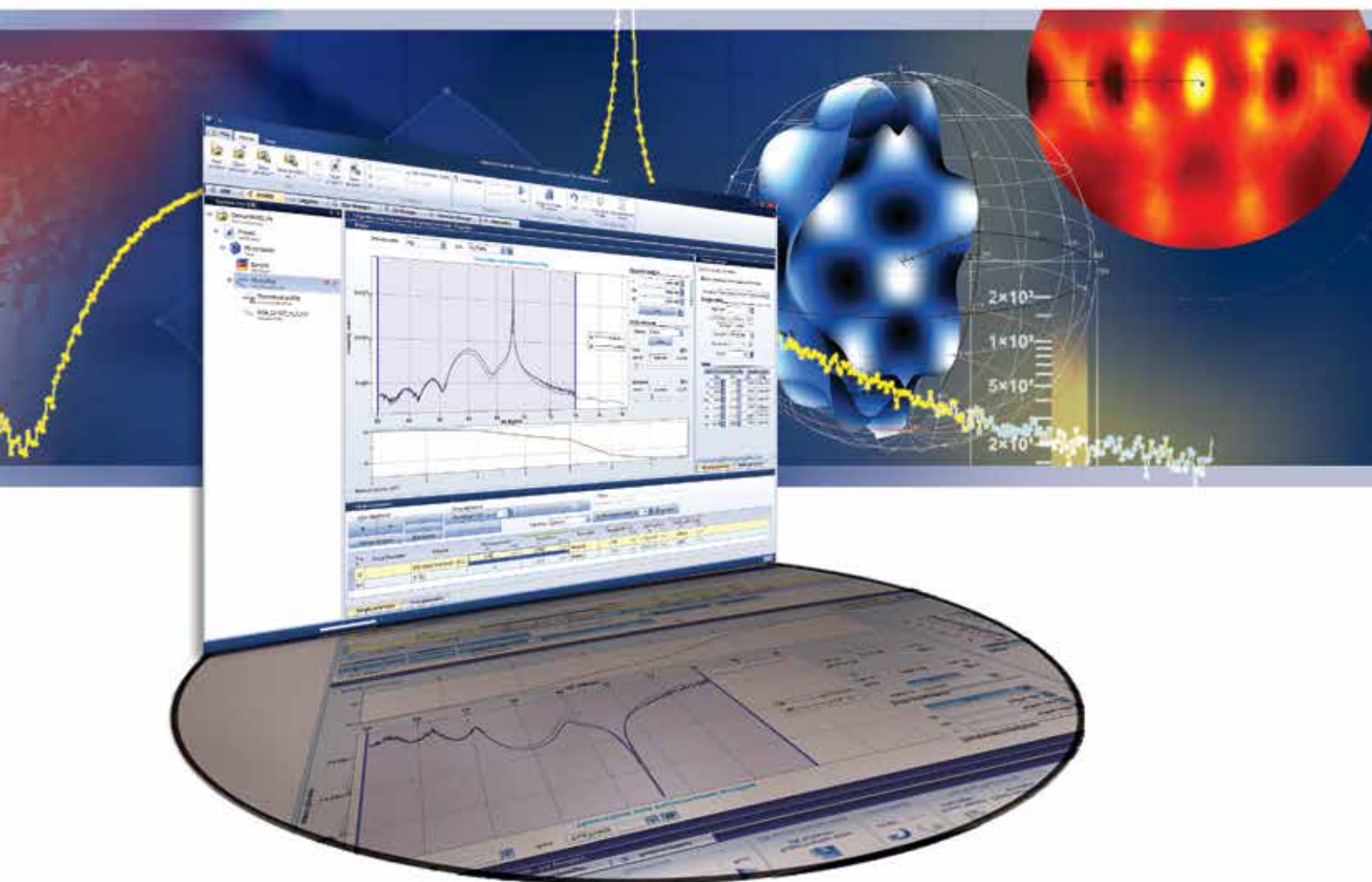


SmartLab Studio II

Measurement and analysis suite

Innovative modules for XRR and HRXRD



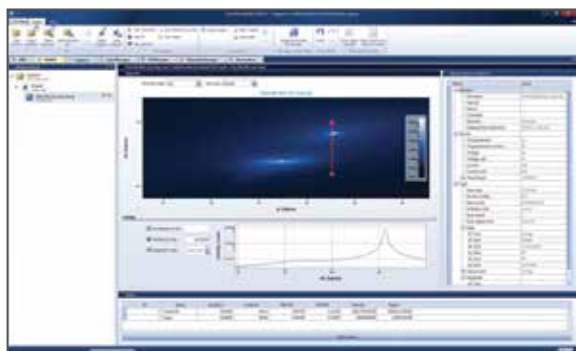
Rigaku

POWERING NEW PERSPECTIVES

Next generation software technology

Introduction

A variety of techniques are used to characterize thin solid films and bulk polycrystalline materials, but among them X-ray characterization techniques are favorable due to their non-destructive nature. High-resolution X-ray diffraction (HRXRD) and X-ray reflectivity (XRR) are the main methods to evaluate the layer thicknesses, concentrations of solid solutions, surface roughness, crystallographic lattice relaxation degree, lattice strain and stress, mass density, mosaicity and many other physical parameters. Reciprocal space mapping (RSM) is often used to investigate the structural properties of the epitaxial thin films (layer tilt, lattice relaxation, composition and quality of structures). The transition from a fully strained state to a relaxed state can be investigated with help of RSMs. The XRR technique provides information about thickness, density and surface roughness. Measurement of pole figures and evaluation of the orientation distribution function delivers the information of the preferred orientations of grains in polycrystalline materials. There are many various techniques to measure residual stress in both thin coatings and bulk polycrystalline samples. Rigaku diffractometers are designed to utilize all these and many other X-ray techniques and to meet Users' requirements in different ways: from pure science to quality control.



SmartLab Studio II software is designed to be easy to use by both experts and beginners, providing powerful tools for data interpretation. Based on the selected user level, the graphical user interface may change from a very simple one; with the minimal number of settings, up to a level that satisfies demanding professional researchers. Accurate analytical results are guaranteed due to many new and improved evaluation algorithms. The calculation and analysis of data in a module is based on complex mathematical calculations with the use of the latest developments in physics in the field of materials

analysis. The software works with 1D- and 2-D data allowing fast and convenient data evaluation and presentation.

Plugin-based software suite

SmartLab Studio II is a new software suite for measurement and analysis of data obtained from different X-ray diffraction techniques. The module (plugin) architecture of this application allows to choose and to load only necessary functional components. Customers can choose which plugins to buy and which plugins to load based on the purpose of their analysis. With a single shell application and different loaded plugins and services set, the user can have a lightweight app for specific needs, or a big app with rich functionality. SmartLab Studio II is a 64-bit application and offers all the benefits of Windows® 7.

The advantages of plugin technology:

- **Create set of plugins on demand**
- **Ability to deliver different packages with required functionality or plugins separately**
- **Direct and shell-managed communication between plugins**
- **Common look and feel, functionality and behavior of software**
- **Common user level management**
- **Single database for all applications; convenient access and backup**
- **Flexible common/unique settings for the main shell and plugins**
- **Ability to upgrade (update) plugins independently**

When running SmartLab Studio II, the software functionality is defined by the loaded plugins and services and can be different depending on the installed software or selected plugins. SmartLab Studio II provides the following general purpose plugins and services available for every license:

- **Logging plugin** displays messages addressed to the user with the information about the status of the application, plugins and services, about running and completed operations in the application.
- **User Manager plugin** is responsible for management of users and user groups.
- **Database Manager plugin** allows the manager to save and to reset the copies of database and displays the information about the status of the database tables.

Powerful XRR algorithms

- **Materials Manager plugin** serves for storage, creation and editing of the materials used for data analysis in analytical plugins (for example, X-ray reflectivity plugin or high-resolution X-ray diffraction plugin).
- **Automation plugin** is designed to create and to automatically perform the necessary sequence of actions on the application without user intervention, including measurement and data analysis.
- **Undo/Redo services** allows the user to restore the application status to one of the previously saved states.
- **Printing/Reporting service** automatically generates a report based on all application elements and displays them in the form of a report with the possibility of extensive reformatting.

Unique features:

- **Plugin architecture**
- **Flowbar**
- **Extended user management**
- **Centralized DB storage**
- **Extendable materials DB**
- **Individual user options and fully customizable UI layouts**
- **Automation with visual flow editor**
- **Rich Printing/Reporting with visual report layout editor and the ability to export to dozen of formats**
- **Localization**
- **Undo/redo**
- **Multiple packages in a single shell: XRR, HRXRD and others**
- **Extended sample model**
- **XRR: Oscillation analysis and fitting of XRR profiles**
- **HRXRD: Fast evaluation of sample parameters based on peak positions from an arbitrary set of RSMs and RCs and fitting of an arbitrary amount of profiles**

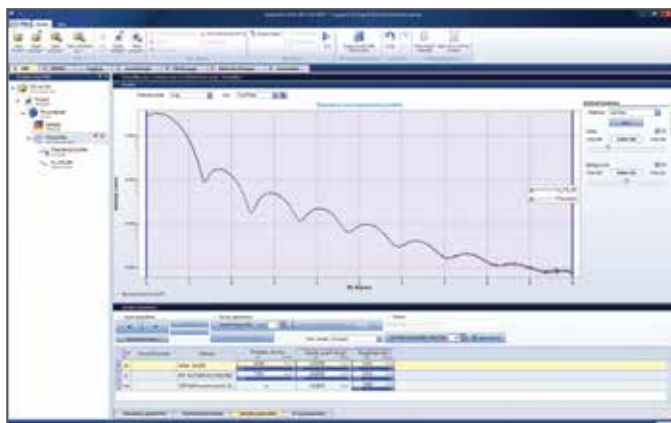
XRR plugin

XRR plugin is designed for the interpretation, display and analysis of data as well as for evaluation of the sample structural parameters based on the measured XRR data. Using this plugin, the layer thickness, density and surface roughness can be evaluated using a dynamical scattering approach. The plugin contains the XRR simulation engine, which is used for both simulations as well as fitting of experimental data to refine sample parameters.

The special tool, Oscillation analysis, is used for the fast evaluation of the parameters. Oscillation analysis is based on a search of intensity oscillations in the experimental curve due to the interference of X-rays reflected from different boundaries of layers. Then, the received list of oscillations is analyzed with the aim to build the structure of sample layers.

Main features of XRR plugin:

- **Fast evaluation of the sample data using Oscillation analysis**
- **Accurate data fitting using genetic and Nelder-Mead algorithms**
- **Advanced sample modeling including superlattices, density grading and parameter linkage**
- **Five interface roughness models**
- **Peak search tool**



HRXRD plugin

This plugin is designed to analyze high-resolution X-ray diffraction, measured with various geometries. The SmartLab Studio II software can operate with both 1D and 2D data and evaluate the sample parameters from single scans, simultaneously several scans, RSMs and combinations of all mentioned data. The layer thicknesses, concentration of the solid solutions, crystallographic lattice relaxation degree, lattice strain, mosaicity and many other physical parameters can be analyzed using this plugin. A Peak Search tool with customizable search parameters allows broad flexibility when working with the whole pattern. A Cutting tool makes an arbitrary cross-section and integration of 2D data and extracts the curve into a separate object. Using the Conversion tool,

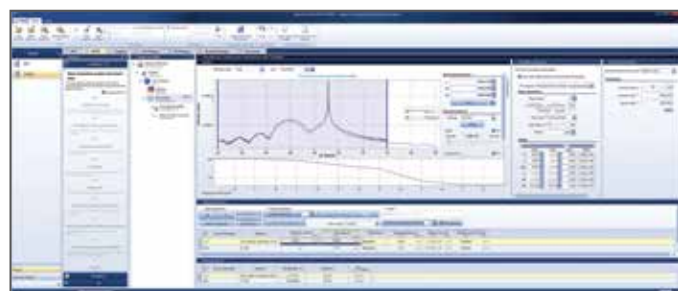
State of the art HRXRD analysis tools

the measured 1D and 2D data can be converted between different units. The HRXRD plugin works for pseudomorphic, partly relaxed and fully relaxed epitaxial layers by adjusting the dynamical diffraction theory for each state of the sample. A powerful simulation engine makes possible fast calculation of the various diffraction scans and robust data fitting to evaluate sample parameters.

The special tool *Evaluation* is used for the fast evaluation of the parameters. It is based on a search and association of various kinds of peaks present in rocking curves (RC) and RSMs. The peak positions are then used to find the physical parameters of the sample.

Key features of the HRXRD plugin:

- **Extended sample modeling by numerous physical parameters**
- **Advanced peak search procedure**
- **Fast evaluation of parameters based on peak positions in arbitrary set of RSMs and RCs**
- **Evaluation of pseudomorphic and partially relaxed layers**
- **Use of two- and four-waves approximations for dynamical diffraction theory**
- **Recursive Matrix Formalism for grazing incidence diffraction (GID)**
- **High-resolution RC simulation**
- **Rigorous high-resolution RC analysis by parameter fitting**
- **Fitting arbitrary number of profiles based on a common sample model**
- **Profile cutting option with ability to save as a data file**
- **Absolute and reciprocal coordinates systems for data processing**

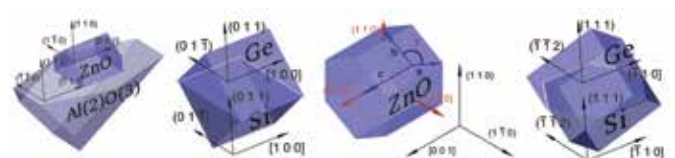


Advanced physics

The SmartLab Studio II kernel is based on modern published physical theories and approaches:

- **New approach with special parameters to characterize non-polar and semi-polar layers and anisotropic relaxation**
- **Recursive Matrix Formalism for dynamical diffraction theory and specular reflection**
- **Accurate treatment of grazing incidence geometries**
- **Two-wave and four-wave approximations for diffraction from pseudomorphic and partially relaxed layers**
- **Dual fit algorithms: genetic differential evolution and gradient Nelder-Mead**
- **Extended Fourier oscillation analysis**
- **Multiple models for interfacial roughness**
- **and many others**

Anchor method. Thin films and multilayered samples made of materials with non-cubic symmetry and/or nonstandard mutual orientation are being used in various technological processes for the production of blue lasers, LEDs, optical switches and many others electronic devices. The commonly used models for epitaxial relations are based on the assumption of cubic symmetry with the only characterization parameter, such as relaxation degree. These models are not applicable for X-ray diffraction analysis of samples characterized by non-cubic symmetry and/or nonstandard material orientation. A new approach has been developed and implemented in SmartLab Studio II for solution of these problems by utilizing special parameters (*Anchors*).



Advanced physics algorithms

A generalized covariant approach for strain analysis of multilayered epitaxial structures with an arbitrary mutual orientation, taking into account the anisotropy of the layers interaction, has been included in the new SmartLab Studio II software. The mutual orientation is determined by the epitaxial relations between two adjacent layers using the pair of coordinates of coincident lattice points of the upper and lower layers in the interaction plane. These coordinate pairs are called Anchors. Two relaxation parameters are introduced into the analysis; these are set in the strain tensor axes within the sample plane. These parameters describe the upper layer anisotropic strain. Such an approach allows one to analyze structures with cubic symmetry and simple orientation, for example, $\text{Si}_{1-x}\text{Ge}_x$ (0 0 1) on Si (0 0 1) substrate, the structures with arbitrary orientations such as $\text{Si}_{1-x}\text{Ge}_x$ (0 1 1) on Si (0 1 1) substrate, $\text{Si}_{1-x}\text{Ge}_x$ (1 1 1) on Si (1 1 1) substrate, and crystalline systems like ZnO (1 1 0) on Al_2O_3 (1 -1 2) substrate.

- [1] S. A. Stepanov, E. A. Kondrashkina, and R. Köhler, *Phys. Rev. B*, **V. 57**, 1998, 4829-4841.
- [2] T. A. Alexeeva, A. I. Benediktovich, I. D. Feranchuk, T. Baumbach, and A. Ulyanenko, *Phys. Rev. B*, **V. 77**, 174114-1-13 (2008).
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- [4] A. Benediktovich and I. Feranchuk, *Phys. Status Solidi A*, 1-4 (2009)
- [5] A. Zhylik, A. Benediktovich, I. Feranchuk, K. Inaba, A. Mikhalychev and A. Ulyanenko, *J. Appl. Cryst.* (2013). **46**, pp.7.
- [6] A. Benediktovich, I. Feranchuk, A. Ulyanenko, *Theoretical Concepts of X-Ray Nanoscale Analysis*, 2013, 318 p. (Springer, Heidelberg).

Common features and modules

Extended and centralized materials DB

To describe the sample SmartLab Studio II offers a variety of physical parameters: relaxation degree, lattice mismatches, layer thickness, concentrations, mass density, mosaicity, etc. The inter-dependence of layer parameters can be implemented using a linkage tool. For the modeling of complex or repeating structures, there is an opportunity to form the layer groups. The visualization of the sample model is customizable in forms of the displayed parameters set and order, table cell colors and presentation. The Anchors tool makes it possible to construct the arbitrary orientations of the crystallographic lattices.

Main features of the Sample tool:

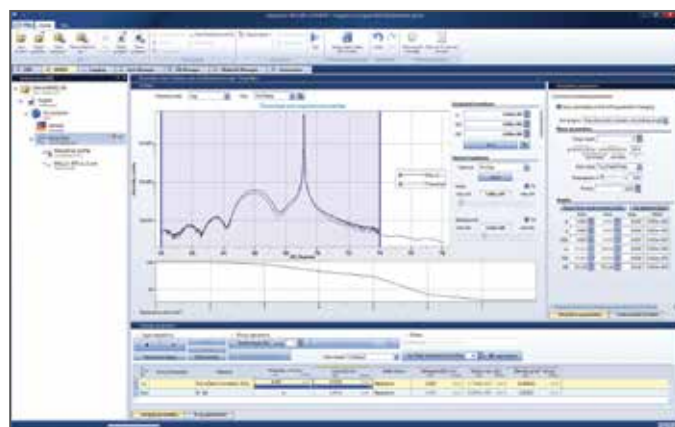
- **Isotropic and anisotropic samples**
- **Arbitrary cell orientation in the crystallographic layers**
- **Defining the relation between epitaxial layers**

- **Solid solutions up to four components**
- **Advanced mosaicity evaluation**
- **Accounting of the crystallographic layer misorientation**
- **User defined parameter linkage**
- **Advanced multilayer samples: extended graded layers and advanced superlattice models**



Dual fit algorithms

SmartLab Studio II offers several possibilities to perform precise fitting to measured data. Two optimization algorithms are available: Nelder-Mead simplex method and an advanced genetic algorithm. The internal parameters of both algorithms are chosen during the fit depending on the performance of optimization.



Nelder-Mead algorithm. The implemented high-speed algorithm is a modification of a classical Nelder-Mead optimization method with improved accuracy and stability of the algorithm.

Rigaku's signature flowbar

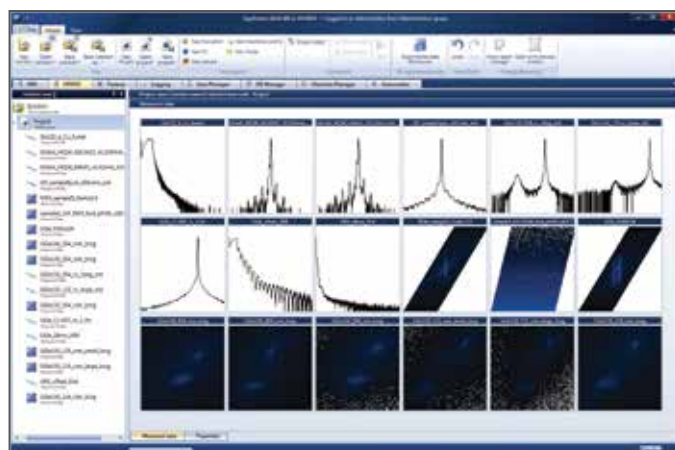
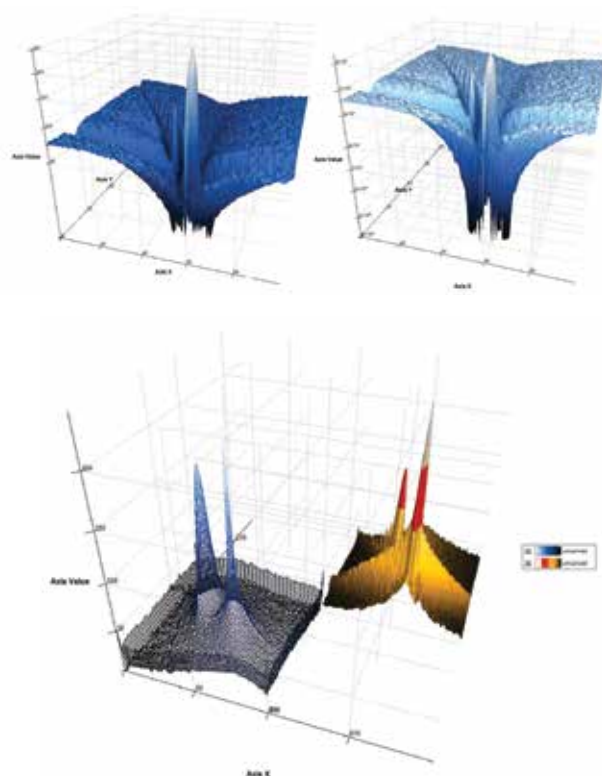
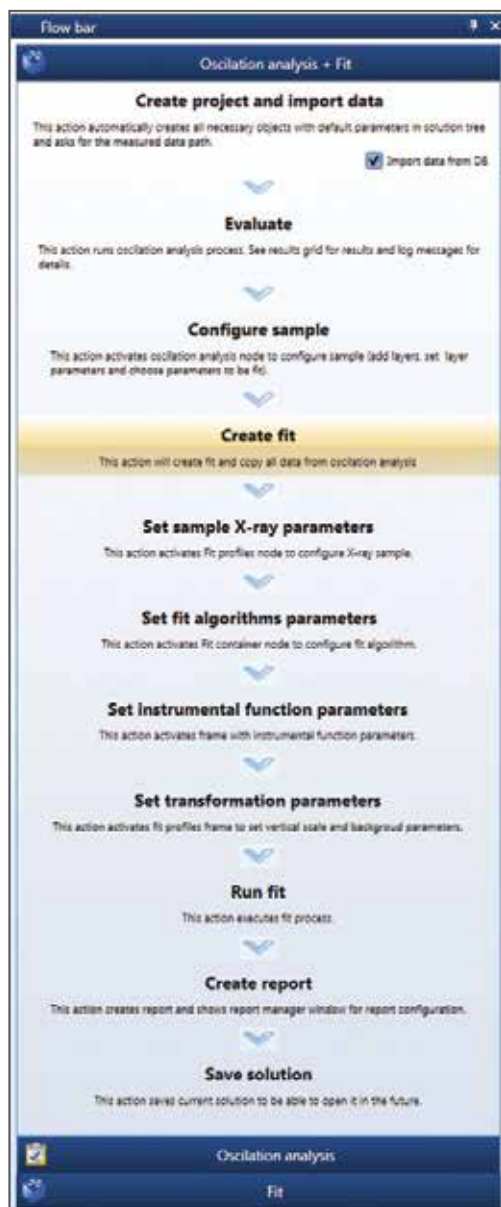
Genetic algorithm. The differential evolution algorithm has been improved and delivers highly stable performance as well as exceptional accuracy in the case of the presence of multiple minima of optimized hypersurface.

User flowbar

The flowbar simplifies standard evaluation procedures and may be used as step by step roadmap for unexperienced users. For different plugins there are several predefined flowbars, for example, Oscillation analysis and Fit for XRR, Evaluation and Fit for HRXRD. Each flowbar step contains a detailed description of the step and provides hints for the user.

Full-featured and fast data visualization

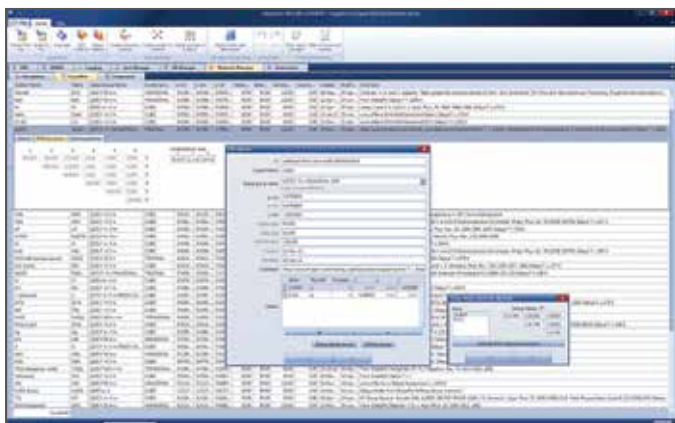
SmartLab Studio II works with the *.ras data format and has full-featured visualization tools. The graphical module represents the data as 1D (curves), 2D (maps) and 3D (surfaces) graphs in Cartesian, polar, and spherical coordinate systems. SmartLab Studio II offers a flexible customization of plot legends, colors, fonts, titles and other graphical attributes. The software supports different fill modes for surfaces like Solid,



Extensive Materials Manager

Wireframe and Waterfall and has advanced color legend control which enables in runtime to change map filling from gradient to stair-step style with highlighting of a specified region. SmartLab Studio II's graphical system can display data containing 1 to 64 million points without simplification and changing a point's structure. The graphical control uses the graphical processing unit and video memory for data rendering that results in high performance, high responsiveness and real-time modifications like data-scaling, projections, coloring, filling and etc.

Materials Manager and Extendable Material Database

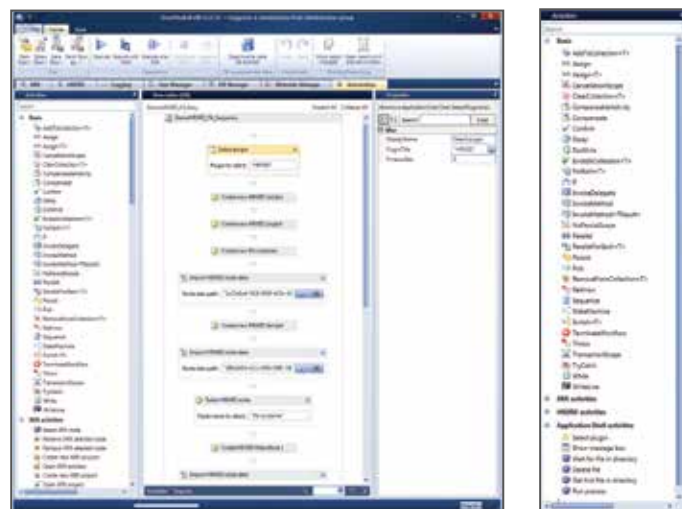


To perform the analysis of the measured data, the software uses the modeling of the investigated sample, part of which is a physical description of the crystalline, polycrystalline or amorphous material. Materials are described by crystallographic space groups, the linear dimensions of an elementary cell a , b , c ; angles of the elementary cell α , β , γ , the chemical structure of cell; Wyckoff position for the given type of atoms; the probability parameter that the specified position is occupied by the atom of certain type, Debye-Waller and stiffness tensors. The Materials Manager includes all necessary operations like create, edit, export, import, copy, print, etc.

Automation plugin

This plugin allows the user to create the sequence of actions (measurements and data evaluation) and to run them afterwards. Using the list of actions (Activity), a visual flow editor and the properties of the selected action one may easily create a necessary sequence. The set of actions that are available for inclusion in the sequence stream depends on the set of loaded plugins in the application as well as on the level of the user access. Each created flow can be saved for further use in the file system as a file or in a database.

The flow sequence can be run as *Easy start* (without the possibility of a pause), *Start with a mark of executable action* (highlighting of the current action and with the possibility to pause) and *Stepping* (execute flow actions step-by-step).



Printing/Reporting service

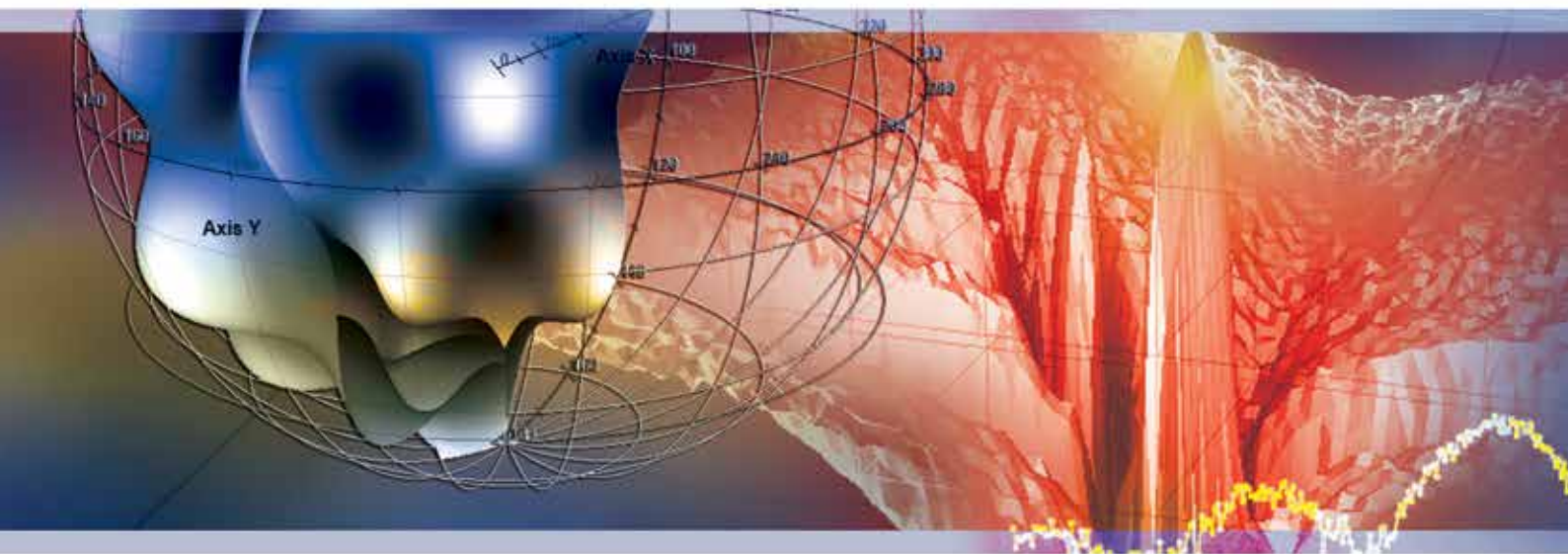
This service is designed to automatically generate reports based on all application elements as well as print separated GUI application components like charts and tables. All reports support layout customization (visibility, relative position, elements size) and customizable printing and exporting to dozens of accessible formats such as PDF, Microsoft Word®, Microsoft Excel®, etc.

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