X-RAY DIFFRACTION

DIFFRAC.LEPTOS X

Product Sheet 59

High-Resolution X-ray Diffraction (HRXRD) and X-ray Reflectivity (XRR) are non-destructive techniques that provide detailed insights into the physical properties of surfaces and ultra-thin single layer or multilayer coatings. These methods probe the sub-nanometer scale with high accuracy, evaluating layer thickness, solid solution concentrations, surface roughness, crystallographic lattice relaxation, lattice strain and stress, mass density, mosaicity, and other physical parameters.

These techniques are essential for the characterization of new materials in research and development, as well as for quality and process control in the mass production of electronic devices.

DIFFRAC.LEPTOS X, Bruker's next-generation thin film analysis software, sets a new standard by combining flexibility and accuracy with user-friendly, efficient workflows. Its intuitive design ensures a quick and smooth start for beginners, while offering the flexibility and high performance that experts demand. Providing the functionality for the analysis of measurements from thin film samples, DIFFRAC.LEPTOS X includes loading and pre-processing of 1D scans and reciprocal space maps (RSMs) as well as reduction of RSMs to 1D scans for further in depth analysis.

Material and sample databases are seamlessly integrated, providing full compatibility with the PLAN.MEASURE.ANALYZE workflow of DIFFRAC.SUITE.

Robust peak search and Fourier Transform based routines enable quick data analysis of the measurements, for example layer thickness estimation from XRR data. More advanced analysis is based on the simulation of XRR and HRXRD data. By combining high-accuracy simulations using dynamical scattering theory with robust optimization algorithms, these modules enable powerful data fitting, providing detailed and accurate analysis results.

DIFFRAC.LEPTOS X feature list

General layout

- Organization of data in folders
- Saving the entire evaluation in a single file
- Fully customizable user interface with project tree structure
- Undo/Redo capability

Supported data/scan types

- Import of 1D data brml, .xy or .xye format
- Import of single- and multi-range measurements
- Support of Reciprocal Space Maps and series of 1D measurements

1D Scan display

- The X-axis displayed as 2θ or q
- Y-axis can be set to linear, square root or logarithmic
- q^4 I(q) scaling to display XRR curves properly
- Display of counting statistics via error band
- Display in counts or cps
- Customization of graphics and text properties for creation of publication-ready figures
- Waterfall display for series of 1D measurements with variable x- and y-offsets

1D Data processing

- Scaling and shifting of the intensity
- Shift and scale of 2θ or the momentum transfer
- Peak search
- Addition and subtraction of scans
- Normalization and merging of scans
- Computation and display of statistical errors

Reciprocal Space Maps

- Display of Reciprocal Space Maps (RSM) in angular or q-space
- Intensities can be displayed on linear or logarithmic scale
- Merging or accumulating of multiple RSMs
- Cropping of RSM
- Automated and manual peak search
- Advanced peak search providing FWHM and angle of the peak ellipsoid
- Export of peak list in csv format
- Determination of general angles in RSMs
- Miscut determination tool
- Graphics export in bmp, png or jpg format
- Integration of RSM to extract 1D scans along predefined scan directions as well as arbitrary sections in reciprocal or angular space
- Various color legends with flexible customization and import/export of color schemes

Material database

- Support of amorphous and crystalline materials, including mixed crystals up to quaternary compounds
- Definition of crystal structures via all 230 space groups, lattice parameters and Wyckoff positions of individual atoms or ions
- Definition of mixed crystals up to quaternary compounds
- Transformation to higher or lower crystal symmetries
- Calculation of X-ray properties like penetration and information depth, dispersion and absorption
- Import and export of crystal structures in .cif and .str file format
- Structure factor calculation for any wavelength
- Operator Method for calculation of X-ray atomic scattering factors and Debye-Waller coefficients
- Various tables for the calculation of X-ray scattering factors, e.g. Henke, Brennan-Cowan, Sasaki, Cromer-Mann

Sample modelling and Sample Database

- Direct connection to the Material Database for creation of new samples
- Definition of layered samples including super-lattices
- Linking of sample parameters including free variables and formula editor
- Various models for description of interface roughness: error function, tanh, linear or sine transition function

Estimation and model-based fitting

- Fourier transform analysis and automated peak search for on-the-fly extraction of layer thicknesses

Reporting and data exchange

- Two-click or fully automated report generation
- Creation of customizable, high quality analysis reports in .pdf or .docx format – or direct printing
- Creation and storage of report templates
- Graphics exchange options to other Windows applications: copy and paste or export as .bmp, .jpg or .png file

Automation and Workflow support

- Creation of new workflows via direct recording
- Editor for changing and fine-tuning workflows
- Step-by-step execution with undo/redo capability
- On-demand user interaction to refine workflow parameters
- Capability to run workflows in batch mode
- External execution of workflows via command line/console for fully automated analysis
- Selection of workflows from database for fast and easy execution

Batch and Wafer Analysis

- Automated analysis of measurement batches
- Display of analysis results as function of batch parameters, e.g. temperature, humidity, stress
- Automated recognition of Wafer & Area Maps
- Fully customizable Wafer Plots for displaying the fitted parameters: color maps, contour lines
- Statistical evaluation of selected regions: Min, Max, Average, StdDev, 3σ, etc.
- Export of statistical results and plots in various formats
- Plot of sections through the wafer

XRR module (requires additional license)

- Atomic scattering factors calculated according to Cromer-Mann or by the operator method
- Dispersion and absorption corrections according to Henke, Sasaki, or Brennan-Cowan
- Simulation of XRR data using the extended Parratt formalism
- Eigenwave method for ultra-fast calculation of XRR measurements on samples with superlattices
- Accurate simulation by including effects of beam- and sample size as well as background and instrumental resolution
- Multiple optimization algorithms for fast, robust and effective fitting: Levenberg-Marquardt, Quasi-Newton method, Nelder-Mead and eXtended Genetic Algorithm
- Selection of multiple fit regions with different weightings
- Direct display of intermediate results and change of the cost function
- Display of standard deviations and correlation matrix of the fitted parameters
- Full integration of XRR data fitting into the workflow to enable automated analysis

HRXRD module (requires additional license)

- Module for the comprehensive and flexible description of epitaxial relations between crystalline layers, including non-polar and semi-polar layers
- Atomic scattering factors calculated according to Cromer-Mann or by the operator method
- Dispersion and absorption corrections according to Henke, Sasaki, or Brennan-Cowan
- Simulation of common HRXRD curves in angular or reciprocal space at symmetric and asymmetric reflections using 2x2 or 4x4 recursive matrix formalism
- Eigenwave method for the ultra fast simulation of measurements from superlattice structures
- Advanced convolution method to account for instrumental resolution. The divergence of the incident beam and the angular acceptance of the detector side can be chosen separately
- Use of multiple, individually weighted wavelengths selectable according to anode-specific lines or freely selectable in eV or nm
- Freely adjustable peak to account for additional diffuse scattering
- Multiple optimization algorithms for fast, robust and effective fitting: Levenberg-Marquardt, Quasi-Newton method, Nelder-Mead and eXtended Genetic Algorithm
- Selection of multiple fit regions with different weightings
- Direct display of intermediate results and change of the cost function
- Display of standard deviations and correlation matrix of the fitted parameters
- Full integration into the workflow for automated analysis of HRXRD data

Language support

- English

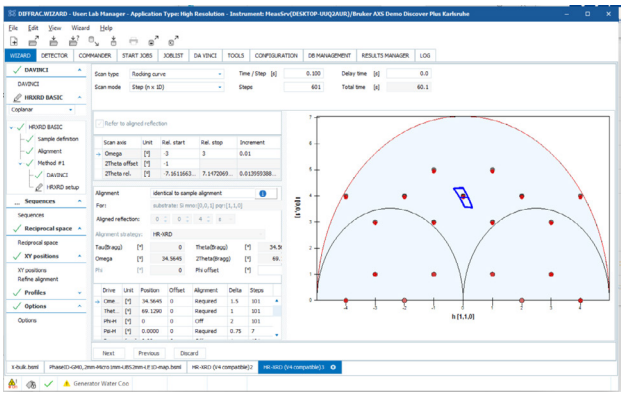
Hard- and Software requirements:

- Operating system: Windows 10 or 11 (64-bit)
- Minimum RAM size: 16 GB (recommended ≥32 GB)
- Minimum number of CPU threads/cores: 4
- Minimum screen resolution: 1024 x 600 pixels (recommended 1920 x 1080 pixels)

PLAN.MEASURE.ANALYZE
Workflows with Bruker's DIFFRAC.SUITE

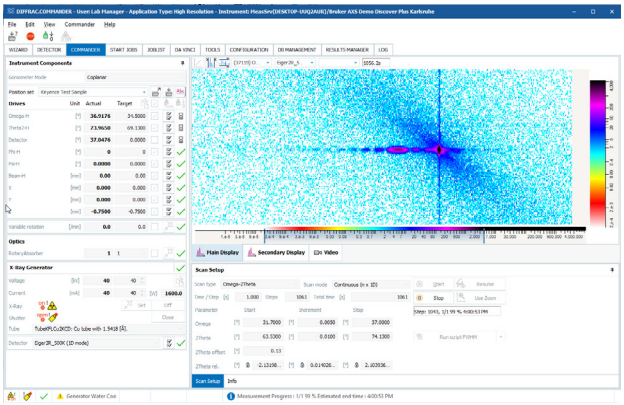
PLAN in DIFFRAC.WIZARD

- Create sample definition using customizable material database
- Graphical interface for instrument component settings including optics, slit sizes, and detector opening
- Setup 1D or 2D measurements at multiple sample points or under non-ambient conditions



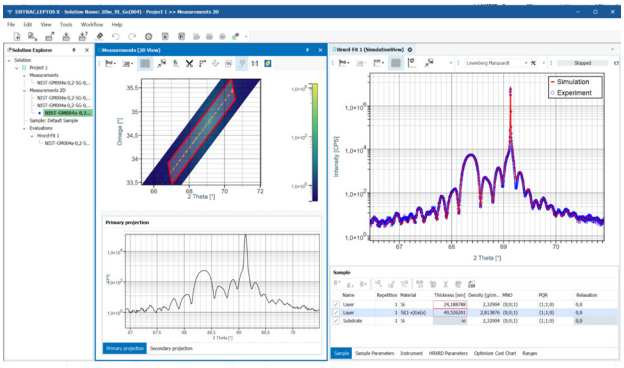
MEASURE in DIFFRAC.COMMANDER

- Direct measurement control or launch predefined experiment methods
- *rapidRSM™* technology for efficient and fast acquisition of 2D maps
- Automatic sample alignment for increased efficiency
- Real-time data monitoring
- Easy-to-use script designer to create and modify automated measurement scripts



ANALYZE in DIFFRAC.LEPTOS X

- Estimate layer thickness from XRR data using FFT
- Extract 1D data from measured 2D data for detailed analysis
- Set up complex sample models using a flexible sample editor, including material and sample database support
- Simulation of XRR and HRXRD data using dynamical scattering theories
- Multiple available fitting algorithms
- Clear, concise report generation



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