X-RAY DIFFRACTION

DIFFRAC.XRR V2

Comprehensive Analysis of X-Ray Reflectometry Data

The physical properties of surfaces or thin-film coatings generated from a wide variety of materials using different processes are decisive for their use. X-Ray Reflectivity (XRR) is a unique analysis technique for the non-destructive and calibration free investigation of structural parameters of thin films which determines the physical and chemical performance. These parameters include layer thickness, roughness, mass density, or chemical composition. It does not matter whether the coating is amorphous or liquid, poly-crystalline or epitaxial.

The analysis of XRR data requires a comprehensive and sophisticated software. DIFFRAC.XRR is the powerful and user-friendly software suite based on the latest algorithms and software engines which takes all aspects of the analysis into account.

DIFFRAC.XRR adds the complete automation of XRR analysis to Bruker's powerful software solution DIFFRAC.SUITE including sample alignment and result reporting.

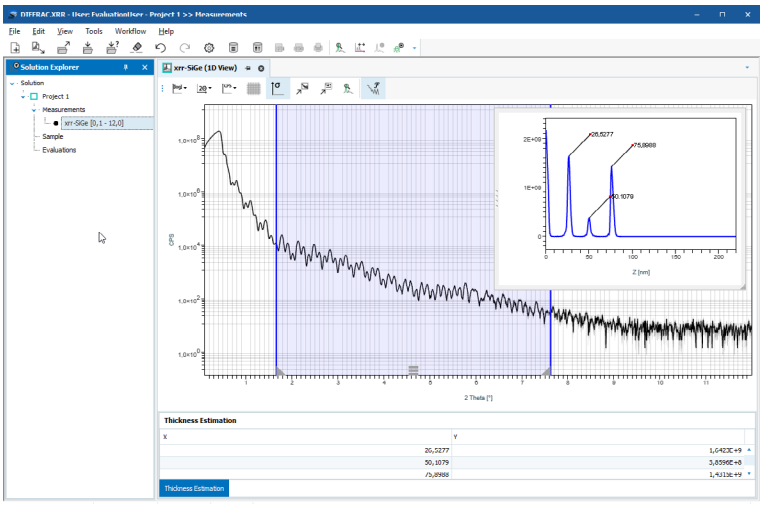
Main features

- Thickness estimation via Fast Fourier Transform.
- Model based fitting using dynamical scattering theory.
- Flexible formula-based parameter and free fitting variable modeling.
- Comprehensive and extendable material and sample databases.
- Advanced automation and workflow capabilities including macro-recording and the *WorkflowDesigner* with drag'n drop capability.
- Step-by-step execution or command line launching of workflows.
- Automated analysis and display of reflectivity measurement series.
- Customizable contour plots and statistical analysis of wafer mapping data.
- Powerful and extensive report generator featuring template capability.

DIFFRAC.XRR offers two approaches for evaluation of the measured data: instant thickness estimate and precise fitting.

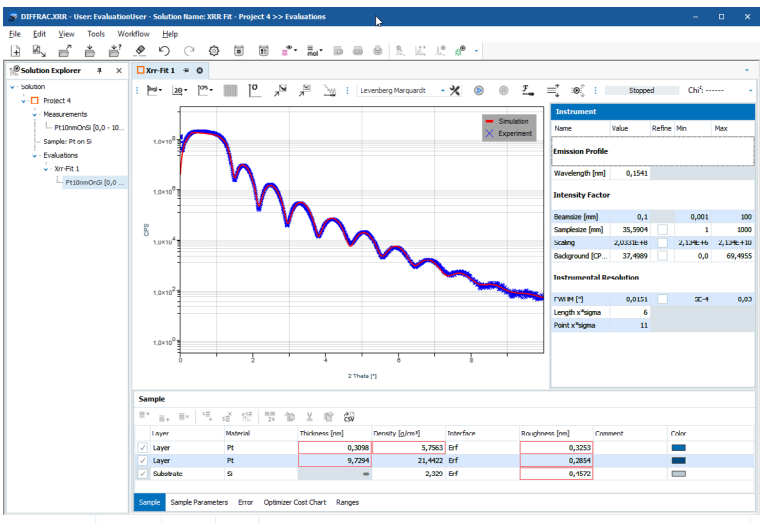
Instant XRR analysis using FFT analysis

When the analysis task consists in extracting a layer thickness, DIFFRAC.XRR sets the benchmark: With a single mouse-click, the Estimate tool evaluates the layer thicknesses via a Fast Fourier Transform and directly displays the result in the corresponding graph of the XRR measurement.



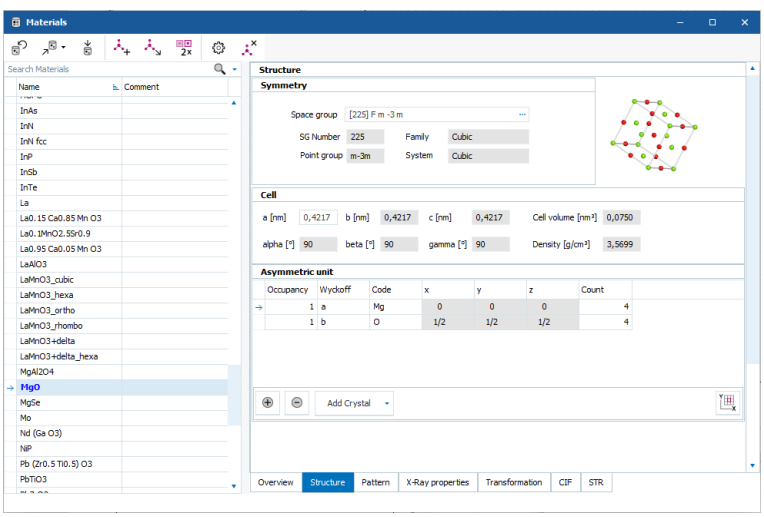
Detailed XRR analysis via full fitting

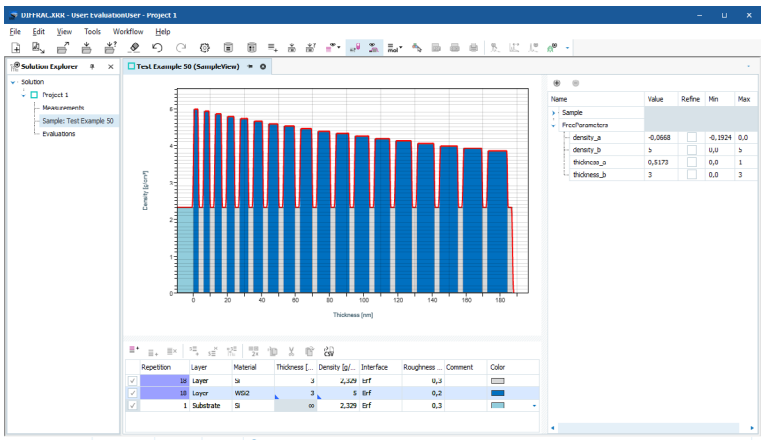
DIFFRAC.XRR applies the dynamical scattering theory to perform accurate simulations. The parameters of the sample model (e.g. thickness, roughness, mass density) are optimized by least-squares method to fit the XRR curve to the measured data. Experimental contributions like instrumental resolution, background, and the sample size are integrated to accurately describe the measurements. Different fast and stable fitting algorithms ensure best convergence and provide reliable results.



Comprehensive material database

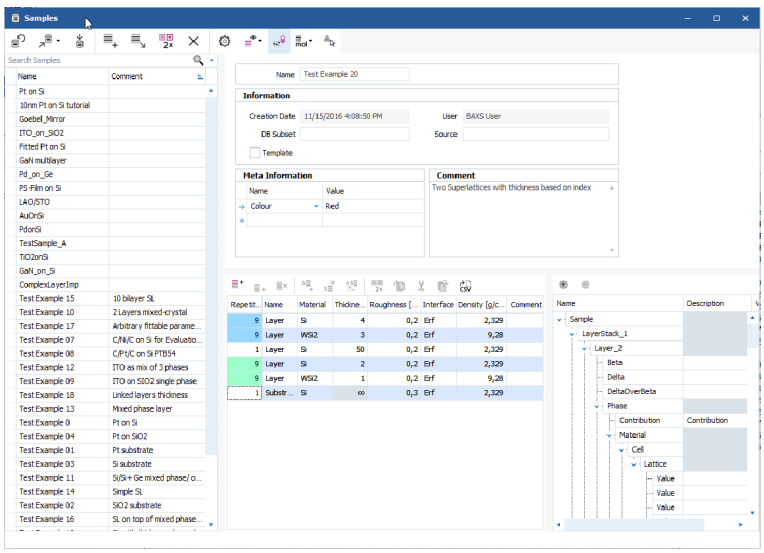
DIFFRAC.XRR features a comprehensive and extendable material database. It includes amorphous and crystalline materials as well as mixed crystals up to quaternary compounds. The database offers calculation of structure factors or hkl patterns as well as X-ray properties like absorption, penetration depth, index of refraction, and polarizability. To facilitate the creation of new database entries, .cif files, and .str files can be directly imported.





Sample-model definition with unparalleled flexibility

From simple single layer to highly complex samples containing superlattices and gradients - DIFFRAC.XRR masters them all. Various interfacial roughness models allow a precise description of the different growth morphologies. Layer parameters can be linked to impose constraints. And the availability of additionally user defined free variables sets new standards in the flexibility of sample modeling.

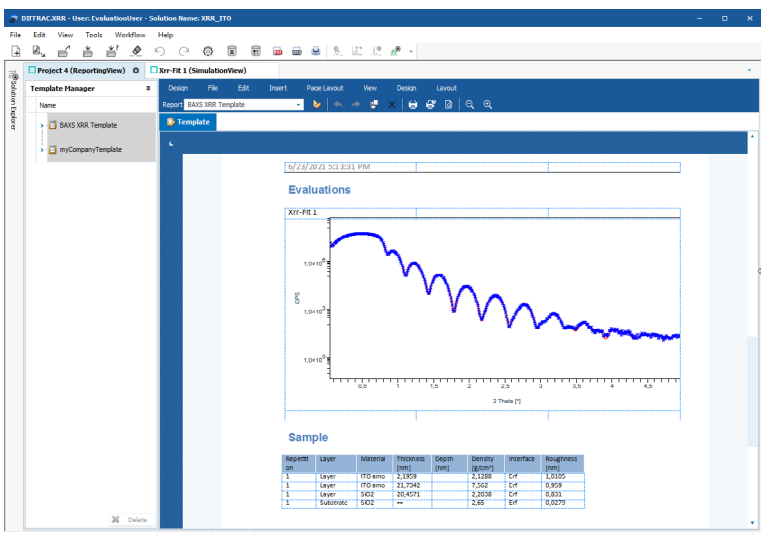


Sample database for faster and more efficient work

DIFFRAC.XRR comes with a powerful sample database.

Complex samples structures can be created, stored, and then directly loaded into the current analysis project. This significantly increases the efficiency in routine work.

Sharing the sample database with the measurement software DIFFRAC.SUITE also allows for a more efficient planning of the experiments and thereby greatly supports the PLAN.MEASURE.ANALYZE philosophy of the DIFFRAC.SUITE software platform.



Unrivalled reporting capabilities

DIFFRAC.XRR includes a professional printing and reporting system for the creation of reporting or publication-ready graphics and full analysis reports.

User-defined and fully customizable report templates can be generated. Reports can be printed directly, shared as .pdf files, or further edited as .docx files.

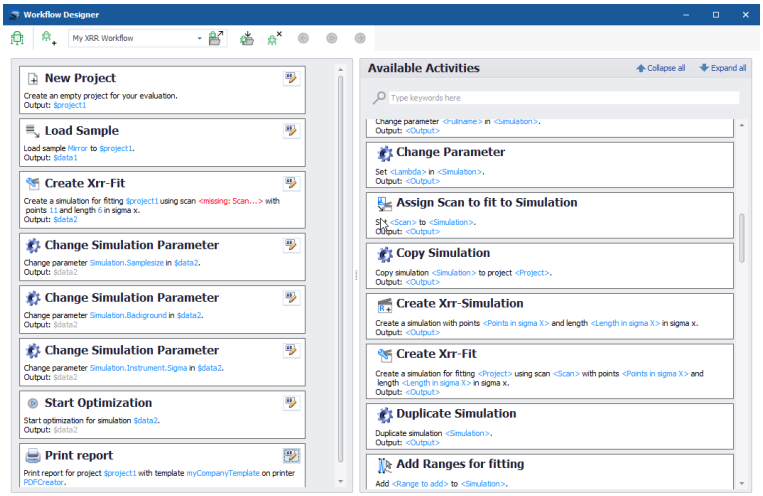
DIFFRAC.XRR: Fully automated XRR analysis

Automation

With DIFFRAC.XRR, X-ray reflectivity analysis has become easier than ever before:

- Capture a workflow as you create it and reuse it anytime.
- Use the intuitive *Workflow Designer* to create customized workflows.

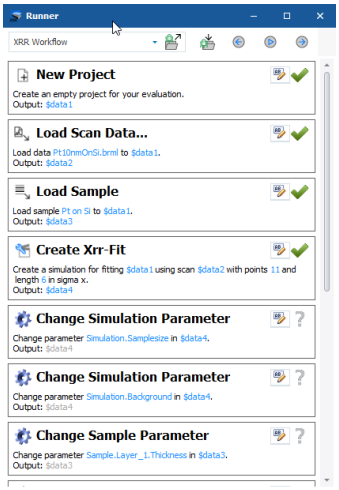
From importing of the measurement data to the reporting of the results, DIFFRAC.XRR offers intuitive user guidance and automation.

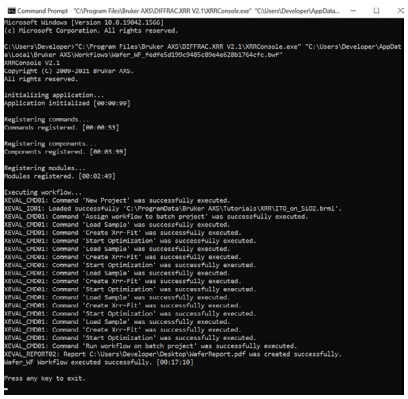


Executing workflows

DIFFRAX.XRR offers two different implementations to execute workflows:

- Workflows can be launched by an external program, called console mode. This is enabling an integration into fully automated thin-film analysis solutions.
- The Runner allows step-by-step and step-back excecution of workflows for maximum control and user interaction.





Exporting results

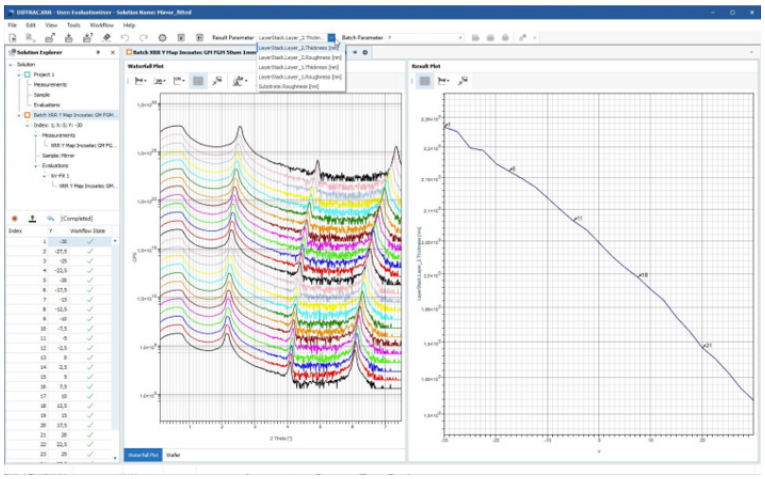
The results of an XRR analysis often need to be exported for reporting or further processing. DIFFRAC.XRR allows exporting of the following parameters into csv format:

- Refined sample models.
- List of free sample parameters.
- Peaklists from PeakSearch and FFT analysis.

	B	C	D	E	F	G
1	Name	Material	Thickness [nm]	Density [g/cm³]	Interface	Roughness [nm]
2	Top C Layer	C amorphous	1,6983	1,9778	Tangential	1,2718
3	Ni Layer	Ni amorph	55,078	8,7507		
4	First C Layer	C amorphous	2,8878	1,7441		
5	Substrate	Si	0	2,329		

	A	B	C	D
1	Name	2 Theta [Â°]	Q [1/nm]	Counts
2	Super lattice #1	0,9301	0,6621	7,52E+05
3	Super lattice #2	3,3545	2,3875	1,12E+07
4	Super lattice #3	6,6252	4,7133	9,21E+04
5	Super lattice #4	9,9263	7,0569	7618,937

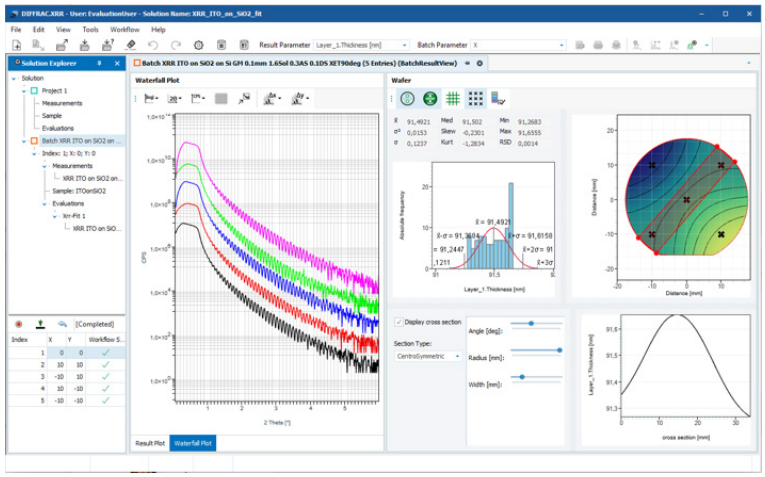
	A	B
1	d [nm]	P [a.u.]
2	11,4864	4,26E+15
3	22,0892	3,86E+15
4	33,5756	3,19E+15
5	44,1785	2,52E+15
6	55,6649	2,04E+15
7	67,1513	1,47E+15
8	77,7541	1,12E+15
9	89,2405	7,88E+14
10	99,8433	5,17E+14



Analysis of a measurement series

Frequently, XRR investigations are performed with the sample under changing conditions like temperature or stress, for example.

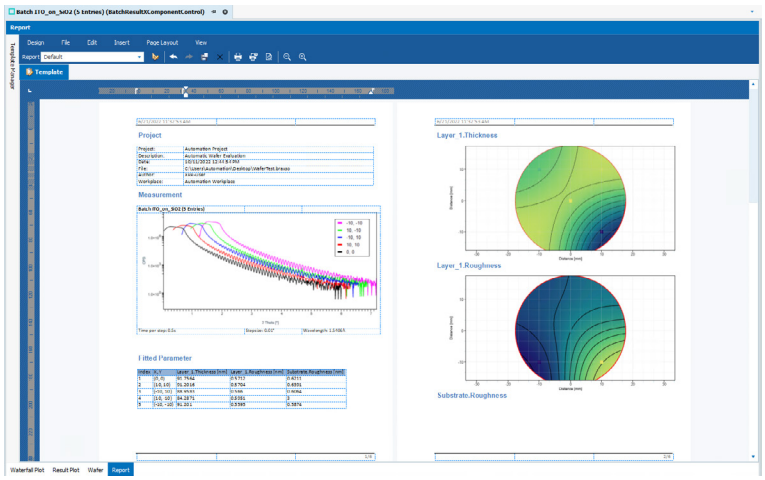
DIFFRAC.XRR enables the easy and fast analysis of such data series: each refined parameter of the sample model can be evaluated individually as a function of the condition. Additionally, the statistical analysis can provide maximum insight into the sample's properties and behavior.



Detailed Wafer analysis

Wafer or area mapping allows for the determination of lateral homogeneities of the sample.

DIFFRAC.XRR features full wafer analysis: each refined sample parameter can be displayed as a contour plot, detailed statistics on the parameters can be displayed, and sections along the surface allow for an in-depth look at the local sample properties.



Flexible reporting of measument series

DIFFRAC.XRR supports the reporting of results from wafer mappings and other XRR measurement series: customized templates can be created including waterfall plots, contour plots for the different sample parameters, or tables to present the results in a more compact way; reports can be saved in .pdf format.

DIFFRAC.XRR feature list

Supported data/scan types

- Import of 1D data in .raw, .brml, .xy or .xye format
- Single- and multi-range measurements

1D Scan display

- The x-axis: 2θ or q
- The y-axis: linear, square root, or logarithmic
- Dedicated q4 I(q) scaling to display XRR curves for optimum data weighting
- Display of counting statistics via error band
- Display in counts or cps
- Customization of graphics and text properties for creation ofpublication-ready figures.

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 of statistical errors

Material database

- Support of amorphous, poly-crystalline, and crystalline materials, including mixed crystals up to quaternary compounds
- Comprehensive definition of crystal structures considering all 230 space groups, lattice parameters and Wyckoff positions of individual atoms or ions
- 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: 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 Materials Database for easiest creation of new samples
- Definition of layered samples including superlattices
- Multiple phases per layer with different ratios: molar, volume and weight
- Easy and flexible 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

Operating system

- Windows 10 (32-bit or 64-bit)

Language support

- English

Estimation and model-based fitting

- Fourier transform analysis and automated peak search for on-the-fly extraction of layer thicknesses
- Recursive Matrix Formalism for accurate XRR simulation
- Effective Density Model (EDM) for calculation of XRR from thin layers with large roughness
- Fastest XRR simulation for superlattices via patented Method of Eigenwaves (MEW)
- Multiple optimization algorithms for fast, robust and effective fitting: Levenberg-Marquardt, Quasi- Newton method, Nelder-Mead, and eXtended Genetic Algorithm

Data exchange and reporting options

- 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

Workflow Designer

- Fast and easy creation of new workflows via direct recording
- Step-by-step execution with undo/redo capability
- Capability to run workflows in batch mode
- On-demand user interaction to refine workflow parameters
- Commandline launch mode for a complete integration into automated XRR solution

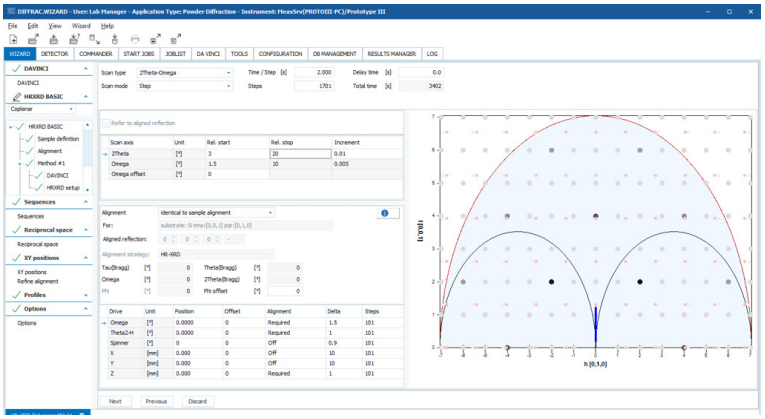
Batch and Wafer analysis

- Automated analysis of batches of measurements
- Display of analysis results as function of batch parameters, e.g. temperature, humidity, stress
- Automated recognition of wafer & area mappings. 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
- Extended reporting capabilities for Wafer mapping and series of measurements

DIFFRAC.SUITE
Workflow for X-Ray Reflectometry

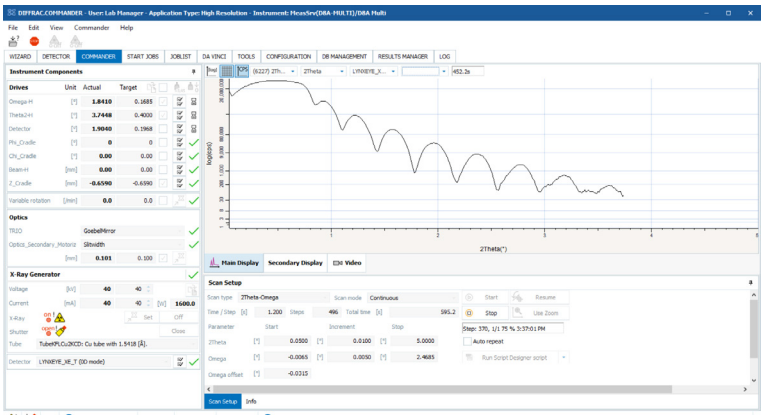
PLAN in DIFFRAC.WIZARD

- Create sample definition using customizable material database
- Graphical interface for instrument component settings including optics, slit sizes and detector opening
- Measure at multiple points with mapping



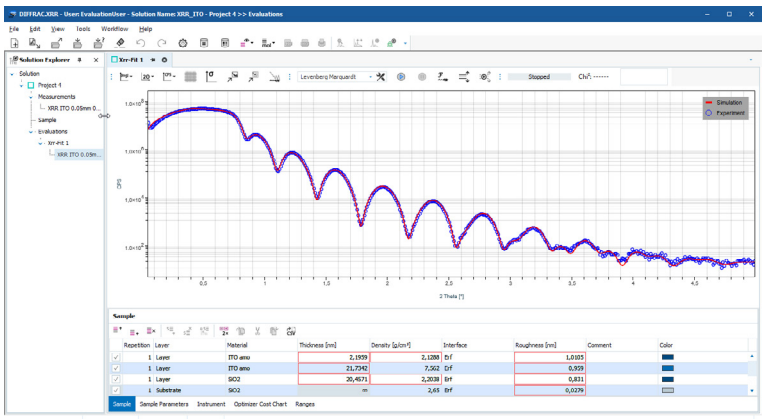
MEASURE in DIFFRAC.COMMANDER

- Direct measurement control or launch predefined experiment methods
- 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.XRR

- Estimate layer thickness using FFT
- Model complex data using a flexible sample editor including material and sample database support
- Multiple available fitting algorithms
- Clear, concise report generation



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