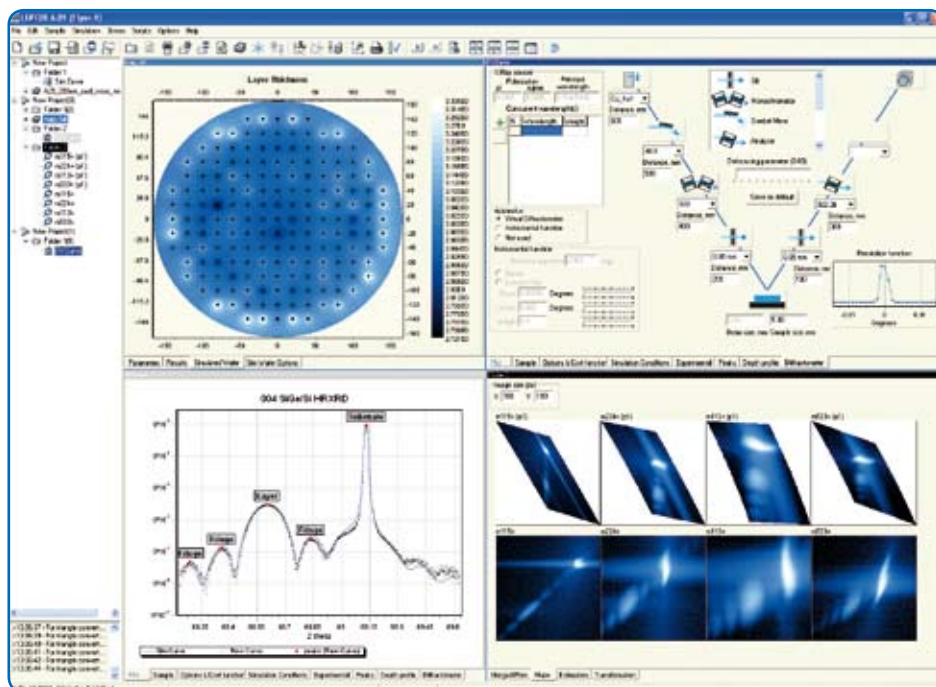


DIFFRAC^{plus} LEPTOS

The Comprehensive Nanometer X-ray Analysis Tool

DIFFRAC^{plus} LEPTOS V6 is the only commercially available software package that can combine data from all relevant X-ray investigation methods for thin-films to perform a synergistic analysis. This built-in flexibility includes the ability to process multi-dimensional data, whether it was obtained in real space or reciprocal space. In addition, the data can come from a 0-D, 1-D or a 2-D detector, to LEPTOS it does not matter.

The theory behind LEPTOS is based on well-established, fundamental descriptions of the interaction of X-rays with matter. It also incorporates scientifically found new approaches that are advantageous to the calculations. In particular, novel mathematical and physical models, as well as the wide selection of fitting routines enable accurate and reliable data analysis.



The LEPTOS user interface can be customized, ensuring that the user interface matches the various demands from specialists to automated assembly-line operations.

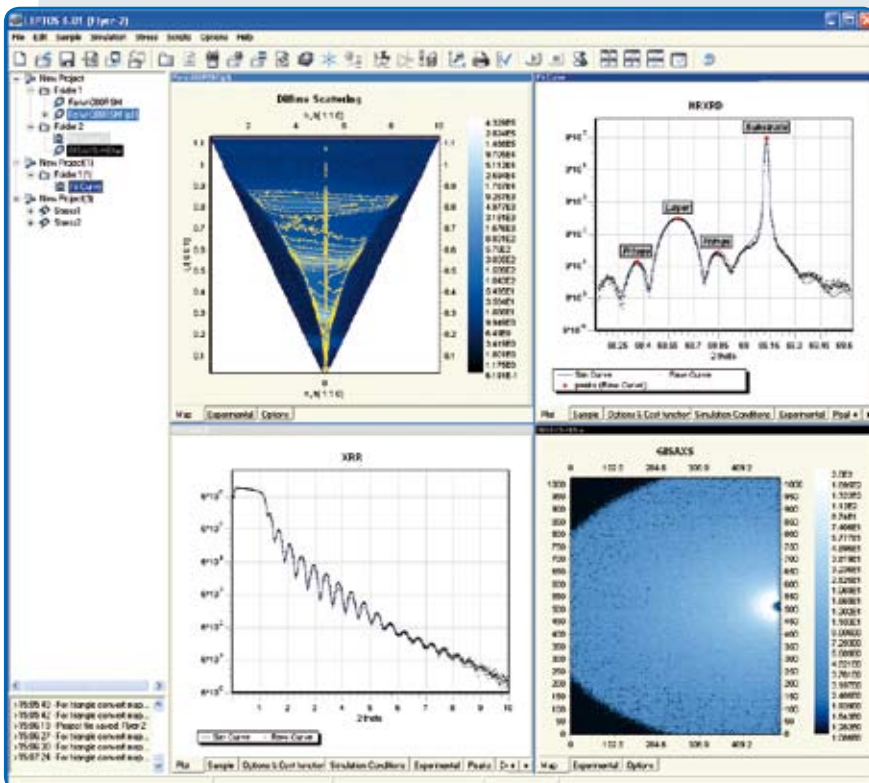
LEPTOS principle features

- Joint evaluation of multiple XRR, HRXRD, GISAXS, and Stress data
- Powerful patented physical and mathematical methods for data analysis
- Broad selection of fitting algorithms
- User Manager for customization of the GUI complexity levels
- Flexible automation capabilities including scripts and Area Mapping module
- Straightforward and fast evaluation via Estimate tool
- Precise and accurate evaluation via Fitting methods
- Comprehensive and extendable material database with all 230 space groups included
- Powerful customizable sample editor plus superlattice tools
- Graphical definition of instrumental set up via Virtual Diffractometer
- Evaluation of data measured with 0-D, 1-D and 2-D detectors

LEPTOS – One Software for Diverse Data and Methods

Thin film technology with its increasing importance in our daily lives has dealt with the nanometer scale for decades. Not astonishing though, X-ray radiation, with its perfectly-matched wavelength for the nm range, was and still is widely used for non-destructive testing of thin film and bulk samples. A variety of measurement methods can be used to determine a long list of physical and crystallographic parameters that characterize the thin film sample comprehensively. Accordingly, a variety of X-ray diffraction and scattering instrumentation based on the Bruker AXS D8 DIFFRACTION SOLUTIONS family was developed for meeting analytical requirements from quality control and process development to pure science for the field of thin films.

LEPTOS is the universal software suite for the interpretation of XRR, HRXRD, GISAXS, Residual Stress, and X-ray Diffuse Scattering data. X-ray reflectivity (XRR) delivers detailed information on the vertical sample density profile, layer thicknesses, and interface roughness. High-resolution X-ray diffraction (HRXRD) measures the crystallographic structure of the sample. X-ray Diffuse scattering characterizes lateral and vertical interface morphology. Grazing-incidence Small Angle Scattering (GISAXS) is used for evaluation of nanoparticles and porosity. Residual Stress analysis probes the strain status of the bulk samples and polycrystalline coatings. All kinds of data can be interpreted in LEPTOS separately or consistently in different combinations.



- Joint evaluation of multiple specular and diffuse XRR and HRXRD data for an integrated single solution
- Naturally integrated 2- and 3-dimensional data sets for quantitative data analysis from reciprocal space or real space maps
- Easy traceability and continuation of the evaluation due to keeping and storing all data and evaluations in a single project file
- Residual Stress analysis providing the advanced $\sin^2\psi$ method (for 1-D data) and XRD^2 method (for 2-D data) including stress gradients in coatings and multiple $\{hkl\}$ handling

LEPTOS' basic constituents are innovative physical theories^[1-13], patented mathematical approaches, and a comprehensive material database containing all space groups according to the International Tables for Crystallography. Internally, LEPTOS uses both the dynamic and the kinematic descriptions of the X-ray scattering process, therefore allowing accurate and fast determination of all sample parameters. The most important methods implemented into LEPTOS are:

- RMF: Recursive Matrix Formalism to overcome Takagi-Taupin limitations.
- MEW: Method of Eigenwaves for fast simulation of and diffraction from superlattices.
- XGA: eXtended Genetic Algorithm for robust and effective fitting.
- Operator Method: calculation of X-ray atomic scattering factors and Debye-Waller coefficients.
- Modified $\sin^2\psi$ and XRD² methods for residual stress analysis
- Cell Builder module to evaluate conventional and non-polar thin films
- DWBA approach for diffuse scattering and GISAXS simulations

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LEPTOS' extendable database features

- Classification of materials according to the International Tables for Crystallography on the basis of space group and Wyckoff positions for every atom in the unit cell. LEPTOS comes with a default database of the most widely used materials.
- Straightforward input of any amorphous or crystalline material including solid solutions with variable stoichiometry, implanted and doped materials, user-defined elastic properties, etc.
- Internal exact calculation of Debye-Waller factor for thermal vibration of crystallographic lattice and stiffness tensor for elastic properties.

Material Database (default. dbm)

Database: Open, Save, Save As..., Help, Check validity, OK, Cancel

Name: Al(x)Ga(1-x)N
 Space Group: [186] P 63 m c
 System: Hexagonal
 Phase: Graded Solution
 Debye-Waller factor: Current Definition: Isotropic approximation
 Temperature (K): 293.00

Atom	Index	Chem. Index	Coordinates (x,y,z)	Wyckoff	Occupation, %
Al	x	1	-- -- --	b	100
N		1	-- -- --	b	100
Ga	1-x	1	-- -- --	b	100

Unit Cell: a=0.315090, b=0.315090, c=0.508360, alpha=90.00, beta=90.00, gamma=120.00, Volume=0.0437 nm³, Density=4.6725 g/cm³

Atomic positions: Stiffness

Graded Solution: Crystal (AlN a1, GaN a2), Vegard checked, Dislikes unchecked, User defined unchecked

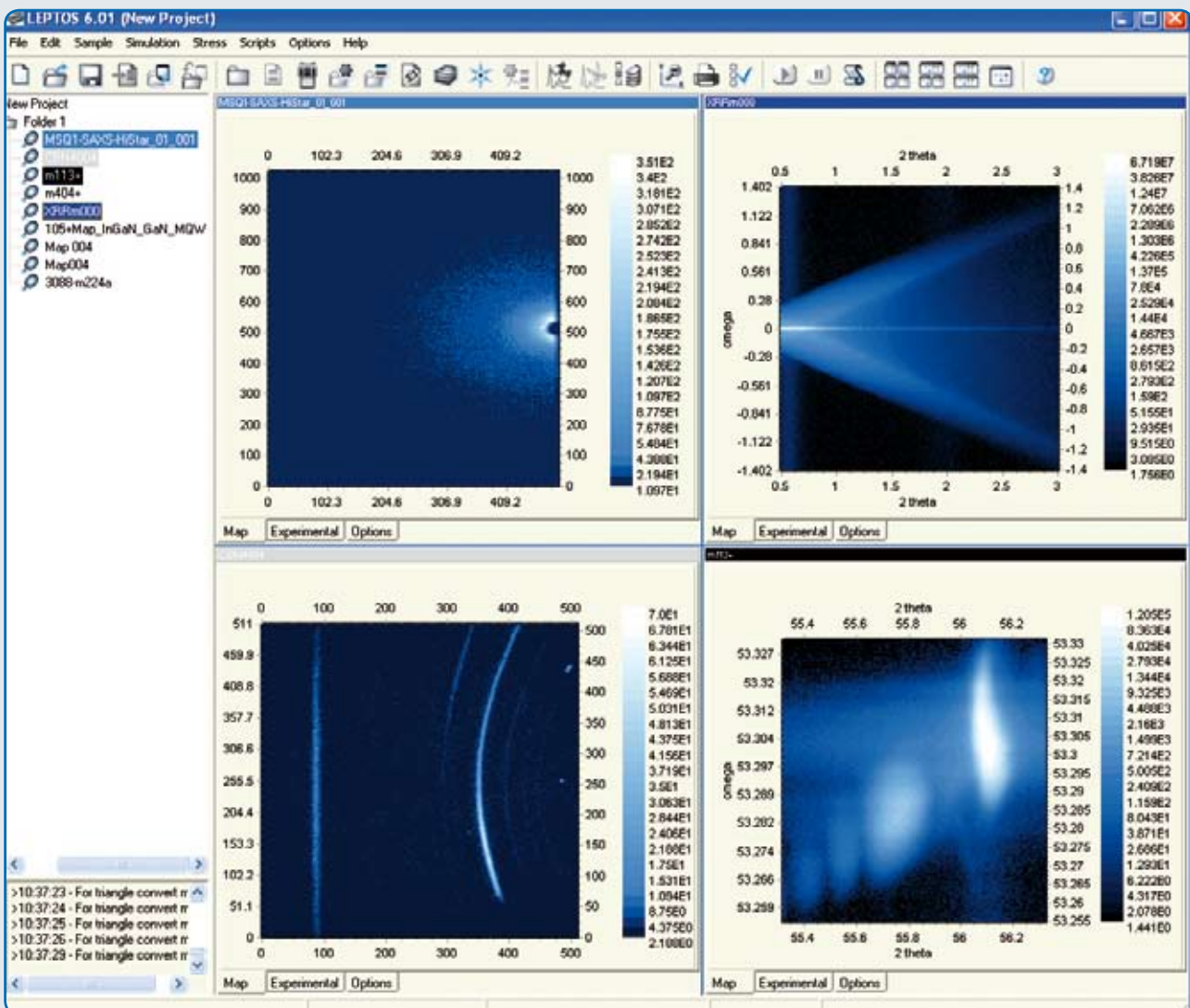
Concentrations: x=50, y=

Comprehensive Evaluation of Data Measured by 0-D, 1-D and 2-D Detectors

LEPTOS imports and evaluates the data from different detectors both in the Bruker data format and in external ASCII formats. The processing of the conventional one-dimensional scans are supplemented by equal handling of two-dimensional data (maps, frames), which provide more precise and accurate information on the sample physical parameters.

Along with the conventional single-curve scans, LEPTOS performs a treatment of high-resolution HRXRD and XRR reciprocal space maps, GISAXS and XRD² Stress frames, area mapping for HRXRD, XRR, and Residual Stress applications.

LEPTOS has numerous options for graphics customization, which include colors, fonts, line and point style, titles, legends, etc. These options allow a clear and informative data presentation. Transformation tools scale and shift data in several ways: manual drag-and-drop and transform, automated adjustment using user's criteria. The Peak Search engine delivers a tunable tool for peak recognition and search both on 1-D and 2-D data. The internal parameters of the engine help to customize the search procedure to any data type. The information on FWHM, peak location and peak quality is listed in the table. The Section tool makes an arbitrary cross-section and integration of 2-D data and extracts the curve into a separate object. Conversion between different units and scales is possible for both 1-D and 2-D data.

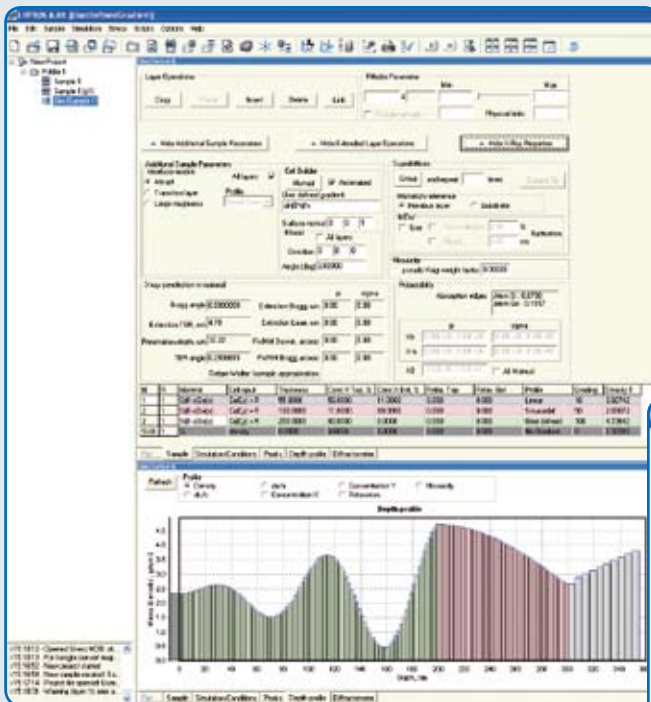


Customizable and Universal Sample Model Editor

- Comprehensive sample model for parametrizing any type of thin film and bulk samples
- Straightforward modeling of periodic or aperiodic superlattices for easy handling
- Powerfull layer-linking and gradient tools
- Diverse physical models for treating sample parameters
- Arbitrary orientations of the crystallographic lattice

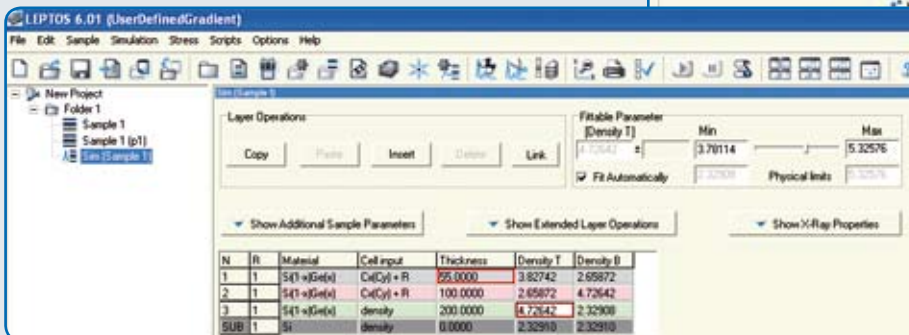
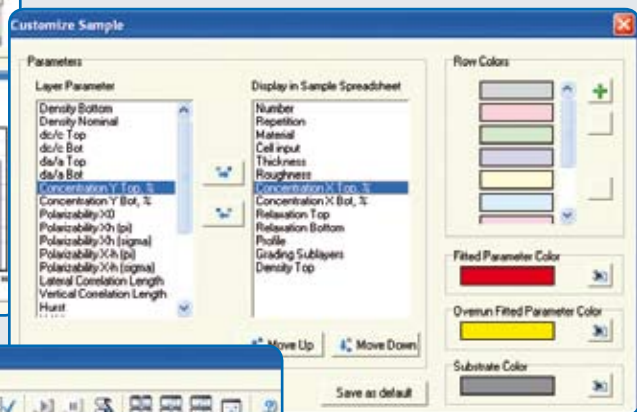
LEPTOS provides the possibility to set up a sample model using more than 40 physical parameters such as layer thickness, mass density, rms roughness, lattice mismatches, contaminations, etc,. For modeling sophisticated samples, depending upon the application. LEPTOS offers additional parameters, such as vertical and lateral correlation lengths, in-plane and out-of-plane

lattice mismatches, relaxation degree e.g.. Superlattices are easily constructed in the Sample Editor by a single mouse click. Any type of SL aperiodicity can be implemented in the sample model. The powerful and patented MEW method is used to accelerate the simulation of diffracted and reflected intensity from superlattices. The extended linking tool enables building functional dependences between different sample parameters. The gradient tool permits user-defined gradients of the fit parameter variation. The diverse crystallographic orientations can be selected to model nonpolar layer growth. The sample editor has a direct access to the stress and TFA databases for material selection. The Cell Builder module automatically adjusts the physically related parameters as lattice mismatches, concentrations, densities and relaxation degree. The sample spreadsheet is customizable to fit the needs of every particular application and user experience level.



Maximized view

Customization dialog



Minimized view

Estimation and Fit Approaches

LEPTOS provides a number of approaches for evaluating the measured data enabling a simple first guess of physical parameters or sophisticated modeling of the sample. In the Estimate mode, very fast evaluation of the sample parameters is performed on the basis of simple analytical formulas involving kinematical, semi-dynamical and dynamical theories, FFT method and elasticity relations. By using Estimate mode, the layer thicknesses, mismatches, concentration, and relaxation are evaluated straight from the data sets without fitting. Simple symmetrical scans, coupled asymmetrical scans, or reciprocal space maps can be used to determine the parameters.

In the Fit mode, the full dynamical theory or DWBA¹ is used to fit accurately experimental data by trial-and-error technique. The user-defined sample model is the starting point for the data analysis. The user simply clicks on the parameters to be fit. LEPTOS offers a unique combination of stochastic (eXtended Genetic Algorithm and Simulated Annealing) and gradient (Levenberg-Marquardt and Simplex) fitting algorithms. Whereas

the stochastic methods are indispensable for defined sample models, the gradient methods accelerate the fit process for models of high perfection. In order to tune the effectiveness of the fitting process, LEPTOS provides a selection of different cost functions. By choosing the appropriate function, specific data characteristics like covered dynamical range can be emphasized. All fitting methods supply evidence for the reliability of the results calculating the standard deviations, cross-correlations and goodness of fit.

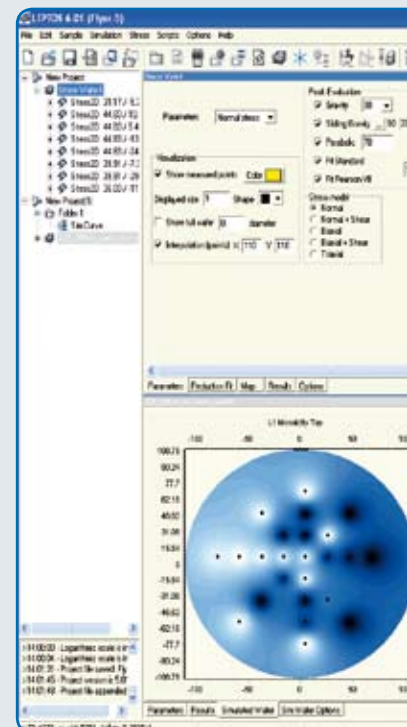
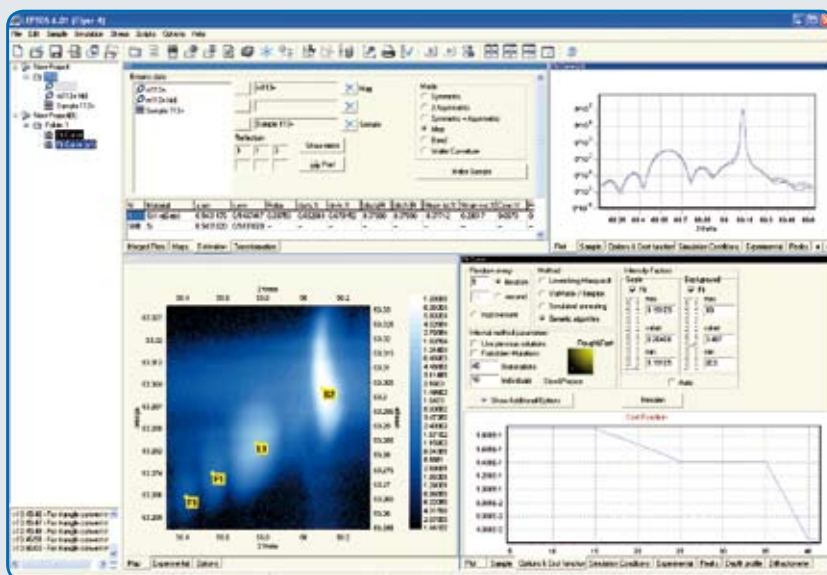
- Broad selection of fitting algorithms and cost functions for optimized data evaluation
- Quick thickness estimations by Fast Fourier Transformation
- Simple estimation of layer parameters from numerous data sets
- Accurate and robust fitting of different sample parameters
- Simultaneous and consistent fitting of multiple datasets

Multiple Data Processing, Script

- Area Mapping module for display and evaluation of HRXRD, XRR, and Residual Stress real space mapping measurements
- Simultaneous and consistent multiple datasets (e.g., HRXRD and XRR) processing on the basis of single sample model
- Script operation and batch mode for most of LEPTOS operations: Script Wizard and Macros Recorder tools

Any type of measurement batch across a sample area (mapping) can be processed by LEPTOS with minimal user intervention. The Area Mapping module determines the user-selected sample parameters fast and precise for all sampling locations, including layer thicknesses, lattice mismatches,

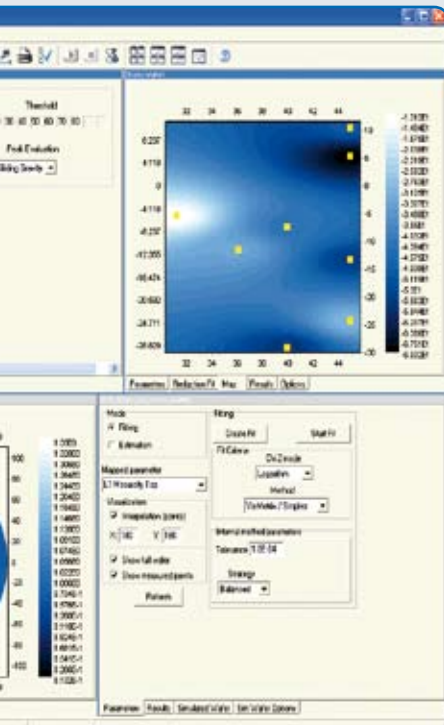
1 Distorted-Wave Born Approximation



Operation and Area Mapping

layer relaxation degree, residual stresses. The script option helps to completely automate the process of sample/wafer quality control in the industrial environment. The evaluated parameter distributions can be displayed, printed and saved in different file formats. The evaluation of the sample parameters can be conducted both by using Estimate and Fitting modes.

The script interface allows a construction of the fully automated and cycled evaluation procedure combined with the measurements automation. Script Wizard tool makes it easy to write a typical evaluation processes, whereas Macros Recorder stores in script file the operations made by user in LEPTOS GUI.



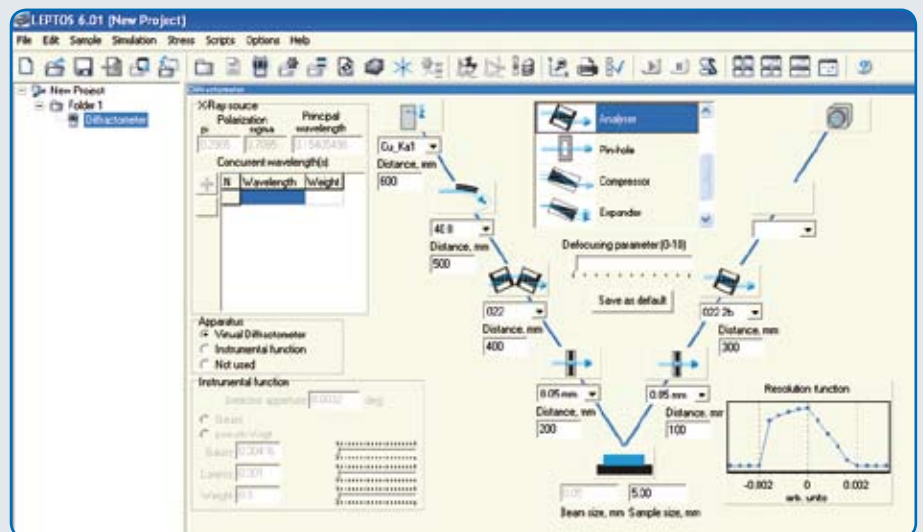
User Manager and Virtual Diffractometer

- Expert, Advanced and User levels to tune the software complexity and accessibility
- Graphical editor for a guided implementation of instrumental effects on the simulated data

LEPTOS provides three complexity and accessibility levels (Expert, Advanced, and User) in the GUI and physical kernel of the software. This allows the customization of the GUI from simple to extended one in view of the program and physics options available. The User level offers the simplified parameter access and most common physical models for data evaluation, whereas Expert level opens a wide access to the scientific modeling of the measured data.

The set up of the instrument defines the response and the resolution of the experiment. Therefore, it is essential to use the appropriate diffractometer components for the experiment and to use the fundamental knowledge about the components to simulate and to fit the parameters accordingly.

LEPTOS takes the instrumental effects into account for simulation and fitting of X-ray diffraction and reflection curves. To create the Virtual Diffractometer, LEPTOS offers an easy drag-and-drop construction using graphical X-ray optical elements, or alternatively statistical approximations. The Virtual Diffractometer permits to improve the fitting results essentially by taking into account all possible resolution effects and to achieve a perfect coincidence of the measured and simulated data.



LEPTOS Licenses and Applicability

The DIFFRAC^{plus} LEPTOS suite consists of the several modules protected by the licenses for different applications. Depending on the issued license set, the following modules are accessible:

- LEPTOS R: XRR module
- LEPTOS H: HRXRD module
- LEPTOS G: GISAXS and XRR modules
- LEPTOS S: Residual Stress module
- LEPTOS: all modules

Area Mapping module is accessible for all licenses. Operating within the single shell and providing an access to different modules by licenses, LEPTOS allows to work simultaneously and consistently with diverse applications. All the graphical functions are similar for each particular application.

Analytical Tasks	XRR	HRXRD	GIXRD ²	DS ³	GISAXS	STRESS
Layer thickness (amorphous)	✓					
Layer thickness (crystalline)	✓	✓	✓			
Layer mass density	✓	✓				
Chemical composition	✓	✓	✓			
Roughness	✓		✓	✓		
Vertical correlations				✓		
Lateral correlations				✓	✓	
Porosity, Nano-objects size and distribution	✓			✓	✓	
Lattice Parameters		✓	✓			
Strain, Relaxation, Mismatch		✓	✓			✓
Defects & Crystal Structure		✓	✓	✓		
Mosaicity		✓				
Residual stress (normal, shear, biaxial, triaxial)						✓

² Grazing-incidence X-ray diffraction

³ Diffuse Scattering

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