Product Sheet XRD 53

DIFFRAC.XRR

- Software Feature Overview

The physical properties of surfaces, ultra-thin single or multilayer coatings on a wide variety of materials are of paramount importance for their use. X-ray reflectivity (XRR) is a unique analysis technique for the non-destructive and calibration free investigation of structural properties of thin films down to the sub-nanometer scale. These properties include layer thickness, roughness, mass density or chemical composition. Furthermore it is irrelevant whether the coating is amorphous or liquid, polycrystalline or epitaxial.

DIFFRAC.XRR is the powerful and easy-to-use software suite designed to analyze X-ray reflectometry measurements. It features two different analysis approaches to best fit the users requirements: Direct layer thickness estimation from the XRR curves with a single mouse-click and fitting of a sample model against the measured data.

The software also features automated analysis and display of series of XRR measurements as well as the evaluation of wafer mapping data including customizable contour plots and statistical analysis.

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 can be changed by selecting 2θ or q.
- The scaling of the y-axis can be set to linear, square root or logarithmic.
- Dedicated 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.

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 and crystalline materials, including mixed crystals up to quaternary compounds.
- Comprehensive definition of crystal structures via 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.

Estimation and model-based fitting

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

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.

Operating system and language support

- Windows 8, 8.1 and 10 (64-bit).
- English

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