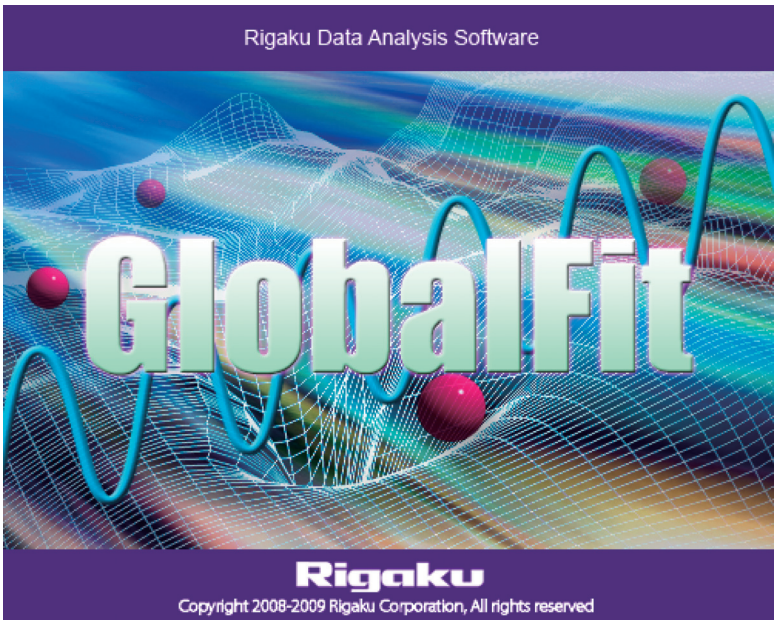
Integrated thin film analysis software

GlobalFit

(Extended Rocking Curve Analysis)



1. Overview

X-ray Rocking Curve (XRC) analysis is widely used with high resolution XRD systems for the evaluation of the layer thickness and periodicity of multilayer thin films, or for the composition of films in solid solution systems (also called mixed crystals). These parameters are crucial to the performance of electronic and opto-electronic device applications such as Si-Ge systems, GaAs-AlAs system, etc.

XRC analysis requires specialized software to compare the raw data with the calculated intensity profiles. It was not an easy task to find a best-fit model due to the wide variation of layer parameters, such as layer thicknesses, composition, strain, etc. — a simple least-square optimization procedure would have easily fallen into the traps of models with locally optimized states. In contrast, with the ever-increasing variation of functional thin film materials, an XRC analysis technique must be applicable to new material systems.

Here, Rigaku presents a sophisticated and powerful new XRC analysis program to respond to these requests. GlobalFit (Extended Rocking Curve Analysis) is equipped with a powerful fitting/optimizing algorithm and an expanded flexibility for applications in a wide range of material combinations. The main window is shown in Fig. 1.

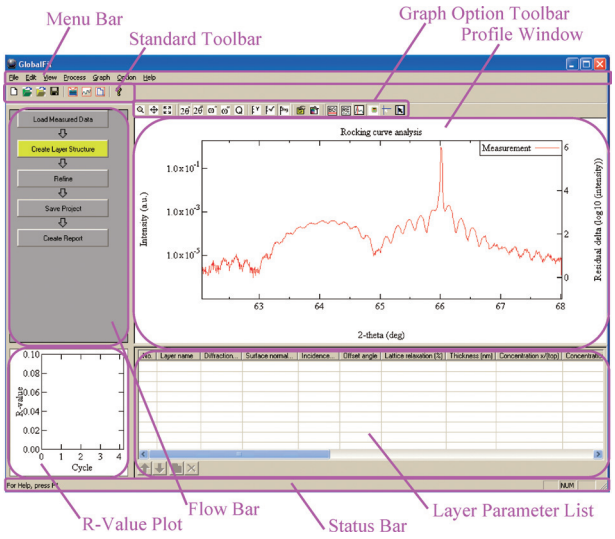


Fig. 1. Main window.

2. Features

2.1. Calculation engine

The diffracted intensity from samples of high crystallinity should be calculated by following the dynamical diffraction theory. Due to approximations in the calculation model, conventional XRC analysis

software could only be used to reproduce profiles in the vicinity of the Bragg diffraction peaks of a substrate.

Our GlobalFit (Extended Rocking Curve Analysis) software is equipped with a newly-developed calculation engine with which the diffracted intensity can be calculated from a layer just one atom thick, taking into account all contributions of reflected and transmitted waves from each atomic plane. Thus, this software can correctly calculate the diffracted intensity even in cases of extreme grazing-incidence geometry where specular reflections are non-negligible. This significant capability led us to name this software Extended Rocking Curve.

Additionally, there are no limitations on calculation with regards to crystal structures, crystallographic symmetry, Miller indices etc. This software enables you to add, edit and modify crystallographic information in the material database, even when working with hypothetical structural models.

2.2. Fitting/Optimizing functions

The best-fit model used to be determined through least-square optimization processes by varying the layer parameters. However, it was only successful in cases where the parameters of the initial model of layers were close to the ones for the reasonable model. Some optimizing tools to help users to find a reasonable model were proposed, including the Genetic Algorithm (GA) method and the Simulated Annealing (SA) method, but they were not easy to use, and the user needed to adjust the optimizing parameters for data analysis.

The optimizing tool proposed here is called the global fitting method. It is an advanced version of the Parallel Tempering (PT) method. Users are shown a globally-optimized model searched in a huge parametric space with varying numbers of layer parameters, and can smoothly move through the refinement process. This tool is customized for rocking curve data analysis, and there is no longer a need to set complex optimization parameters.

Figure 2 shows the window displayed in GlobalFit (Extended Rocking Curve Analysis) during the global optimization process. Deviation between the measured and calculated profiles is shown in the highlighted box on the bottom-left, allowing the user to track the progress of agreement between the profiles easily.

2.3. Other functions

In order to obtain a best-fit model, users simply step through the analysis procedure as shown in the main window (Fig. 1). The analyzing conditions can be saved as a "Project" file, and can be imported by other measurement data analysis processes.

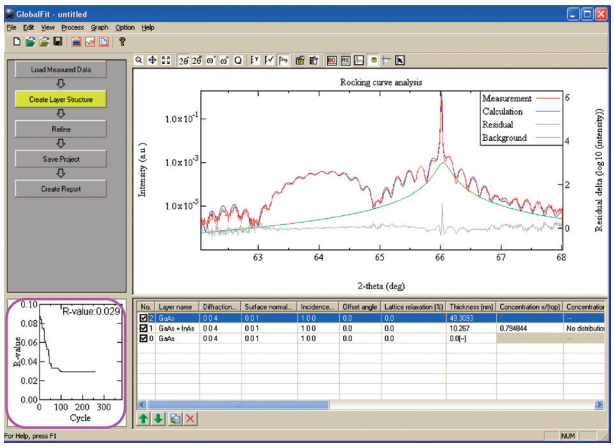


Fig. 2. Screen shot of the global optimization process.

Results are saved as analysis reports. Analysis reports present sample data along with a visual representation of the sample. You can add comments or memos to the report. Since the report is created in HTML, analysis results can be viewed on any computer with a web browser, making sharing analysis results exceedingly simple.

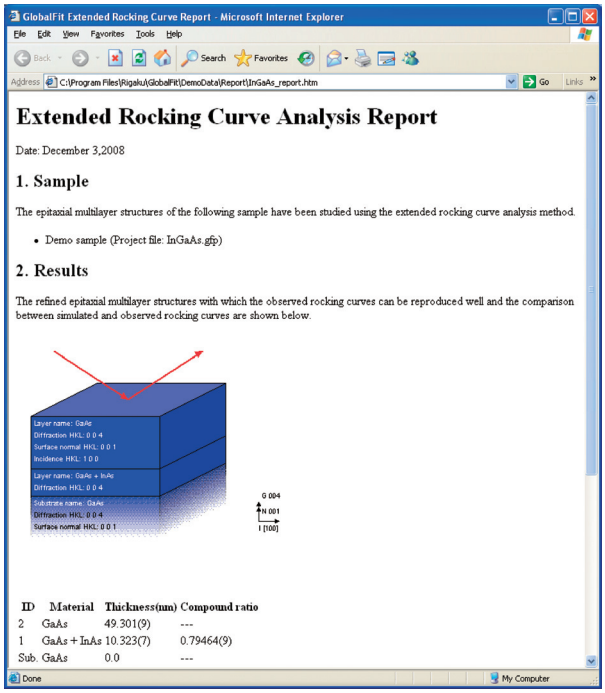


Fig. 3. Example analysis report.