## Integrated Thin Film Analysis Software GlobalFit (Reflectivity Analysis)

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#### 1. Overview

Recently, various thin film and multilayer materials are being developed and produced for use as functional devices. The characteristics of such a device are often influenced by layer parameters such as film thickness, film density and surface/interface roughness. X-ray reflectivity (XRR) is one of the techniques widely used to evaluate these parameters quantitatively.

XRR has various advantages over other characterization techniques: there is no need to treat the sample before measurement or measure reference samples, it is non-destructive, and it can be used with multi-layer systems and opaque materials.

XRR analysis is preceded by a pattern fitting process between the measured and the calculated XRR pattern. During pattern fitting, layer structure parameters are refined, commonly by using the least square method. However, it is very hard to find the best-fit model using only this method when the initial values of the structural parameter are quite different from the real ones. Therefore, practitioners of XRR analysis were often required to have a specialist's understanding of material science as well as enough experience to construct appropriate structure models.

GlobalFit (Reflectivity Analysis), the newly released XRR analysis software from Rigaku Corp., overcomes these difficulties with the use of two powerful tools for data analysis and automatic profile fitting.

#### 2. Features

### 2.1. Optimization method for structure parameters

The first tool is *Extended Fourier Analysis*. This tool analyzes the measured XRR profile, performs Fourier transformations, and then picks a reasonable structure model, all within an easy-to-use interface. Figure 1 shows an example of data analysis using Extended Fourier Analysis.

The second tool is a global optimization method named "GlobalFit". This method performs a global search for the solution and finds the neighborhood of the optimal solution. There are several approaches used for global optimization, including simulated annealing, parallel tempering, and genetic algorithms. GlobalFit software uses the parallel tempering method, which does not require complex settings for parameter fitting. Global optimization is efficient in cases where the initial values of the structure parameter are far from the actual values, or where Fourier analysis is inefficient.

Figure 2 shows the program window during the global optimization procedure. Measured and calculated patterns are displayed in the profile window. The R-value plot window (lower left) displays changes in the R-value, an indicator of agreement between the measured and calculated patterns, showing the discrepancy between them in real time while the global optimization is performed.

Optimization

Refinement



Layer Parameter List

Fig. 4. Analysis report.

procedure: load measured data, create layer structure (the extended Fourier transform and the global optimization are performed here), refine (the leastsquare method is applied here), save project, and create report. It is possible to save the analysis conditions and layer parameters, and then import them for use in another analysis. Using this feature, it is also possible for the user to set up automated analyses. The analysis report created shows the details of fitting results and generates a visual representation of the analysis results and layer structure model (Fig. 4).

If you are a user of GlobalFit (Extended Rocking Curve Analysis), you can switch between "Reflectivity Aanalysis" reported above and "Extended Rocking Curve Analysis" with the task list placed on the upperleft part of the main window.

If you have the former reflectivity analysis software GXRR, you can upgrade it to GlobalFit (Reflectivity Analysis).

#### The flow-bar is located on the left side of the main

Data input and output

2.2.

value: 0.0

Flow-Bar

Fig. 2. Globalfit processing window.

software and GlobalFit (Reflectivity Analysis). When

only using the least squares method, the operator has to

examine the initial parameters of the structure model

with regard to a personal knowledge of the material's

characteristics and their own experience with XRR

analysis. GlobalFit (Reflectivity Analysis) lets us search for a suitable initial layer model using either extended

Fourier transform or a global optimization process,

window. It guides the user through the proper operation

making the analysis procedure smooth and painless.

The schematic shown in Fig. 3 illustrates the difference between traditional commercially available

R-value Plot

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