SimulReflec

A NEW TOOL FOR THE SIMULATION OF REFLECTIVITY MEASUREMENTS

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In order to provide to the users a frienly interface for modelling polarised neutron reflectivity data we have developed this new fitting program.
This program allows to simulate reflectivity curves and to fit experimental x-rays and neutron data. The incident waves can be either neutrons or p-polarised x-rays. The multi-layer system has to be described by a series of discrete layers which model as accurately as possible the physical system. The layers in this model can be characterised by their thickness, their density, their scattering diffusion length, their magnetisation, the direction of their magnetisation, their RMS roughness, the in-plane correlation length and a critical exponent describing the fractal dimension of the roughness…
The program has advanced convolution possibilities and if necessary can use any arbitrary angular and wave-length distributions. The possibility of fitting Time Of Flight data is also offered.
The calculation is performed using an exact recursive matrix calculation. In the case of polarised neutrons, the program can handle any magnetisation configuration (in or out of plane) and any applied magnetic field (in direction or magnitude). The Zeeman energy splitting effects are taken into account in the calculation. They can lead to large effects in the case of the spin-flip signals.

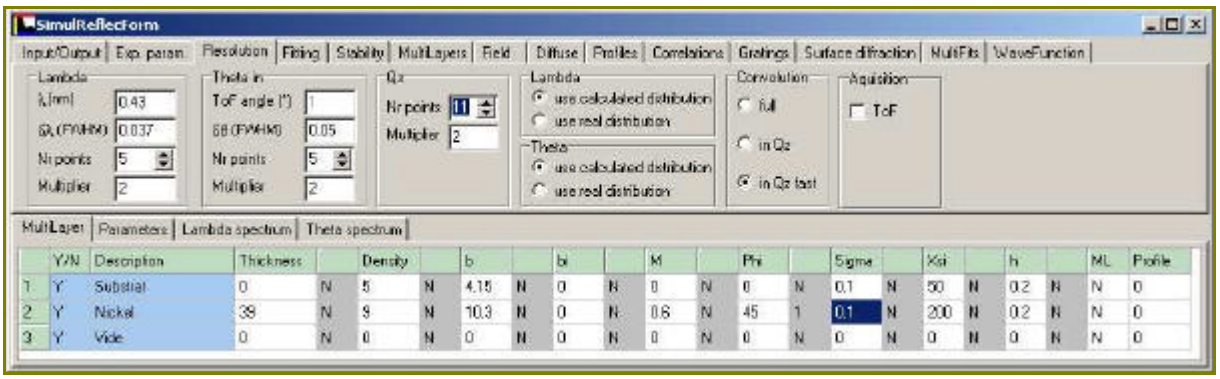

Figure 1. Main interface window for the modelling and simulation of reflectivity data

The figure 1 illustrates the main graphical window used to describe the system being studied. The system is described as a series of discrete layers. In the case of soft matter systems, it is possible to generate smooth profiles. The modelling user interface is coupled with a user friendly plotter (see figure 2).
Beyond simple specular reflectivity data fitting, the program offers some more advanced modules for experienced users. It is for example possible to plot the wave-function amplitudes and phase inside a multi-layer system as well as the reflection and transmission coefficients at each interface. The program also offers some possibilities in the field of off-specular reflectivity and surface diffraction simulations. A "grating" module is under development.

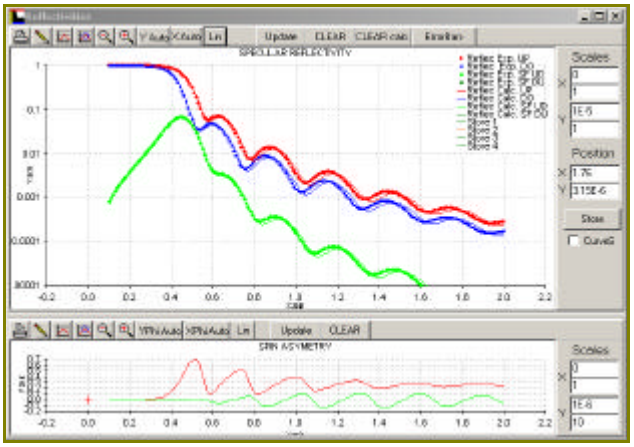

Figure 2. 1D graph window for displaying the experimental data and fits.

It is possible to simulate complex systems such as multi-layers and to include thickness and roughness fluctuations. The possibilty of fitting a two phases system is also available (which may mostly be encountered in the case of magnetic domains for example).

Additionnal modules include :

- An advanced 1D plotter for printing high quality graphics
- An analytical fitting modules (also usable for 2D fits)
- A parser allowing batch processing of data and arithmetic operations on spectra.
- Some utilities such as SLD conversion tools and interface to a SLD database.

The program is developed under the GPL license and can be downloaded at the following address : www-llb.cea.fr/prism/programs/programs.html
The most recent sources are also provided on the Web. The development is made under Delphi ™.
This program can be coupled with its twin brothers :

- SpectraProcessor (for data reduction)
- SpectroDriver (for data acquisition)

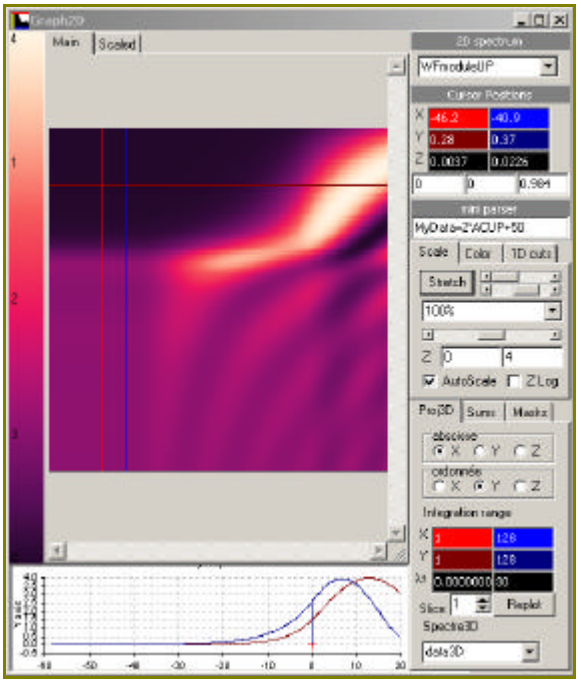

Figure 3. 2D graph window for displaying fits stabilities or wavefunctions amplitudes