

What's hot and what's not? The essential features of reflectometry analysis software.

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Motofit is a neutron/Xray reflectometry analysis package that has been developed to meet most needs of beginning and advanced reflectometry users. It was created out of a frustration that most programs often lack the remaining parts that make them indispensable. For example, you can have a graphical user interface, but you can't refine multiple datasets. Or, you like the analysis, but you don't know how the program does what it does because it's a black box.

Here I describe the essential features of Motofit, its strengths and weaknesses, as well as its possibilities for future extension. As an example I will present the Genetic Optimisation module, which is becoming widespread in reflectometry analysis, but is not as common in small-angle scattering software. This module allows the user to start with poor initial guesses for a model, yet still find the best fit available. Its ability to find a global minimum is essential for most scattering analysis, as some functions are topologically complex, made worse when fitting multiple contrast neutron and X-ray reflectometry data.

References

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3. R. Storn and K. Price, "Differential Evolution - a simple and efficient scheme for global optimization over continuous spaces." TR-95-012-ICSI, (1995)