

Refinement of X-ray Diffraction/reflectivity Data Utilizing Genetic Algorithms and Direct Methods.

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One of the largest obstacles in determining the detailed structure of materials with diffraction techniques is the model building and subsequent fitting of the model to the data.

In this talk, I will present two modern tools that aid an efficient analysis of the measured data.

The first is the use of a genetic algorithm, as implemented in the computer program GenX [1], to fit a model to x-ray reflectivity and surface x-ray diffraction data. This method significantly reduces the manual refinement work thanks to its robustness. The second method is the use of a direct method, known as DCAF [2], to obtain a model-independent three-dimensional image of a surface unit cell from SXRD. It will also be shown that the obtained image can be used for subsequent model buildings and refinements.

[1] M. Björck and G. Andersson. *J. Appl. Cryst.*, 40, 1174 (2007).

[2] M. Björck, C.M. Schlepütz, S.A. Pauli, D. Martoccia, R. Herger and P.R. Willmott. *J. Phys.: Condens. Matter* 20, 445006 (2008).