

notes and news

A Crystallographic Information File for specular reflectivity data

Since the early 1990s, X-ray and neutron specular reflectivity have been the scattering techniques of choice for materials scientists who want to study the vertical density profile of thin films, whether crystalline, amorphous or liquid. Important structural parameters, such as the electronic or nuclear density, the thickness, and the interfacial roughness of thin layers, can be deduced from specular reflectivity data using more or less straightforward modelling techniques (Lu *et al.*, 1996). Although initially developed by physicists, the technique is now used by chemists and biologists; however, each tend to speak their own reflectivity language.

This has led to a large variety of ways in which results from specular reflectivity experiments are presented, making reflectivity papers sometimes rather difficult to read, even for specialists in the field.

Some of us working in the field have thought it worthwhile to standardize the terminology by defining a Crystallographic Information File (CIF) dictionary for specular reflectivity data. The benefits provided by CIF for single-crystal diffractometry are well known (*International Tables for Crystallography*, 2005), and the CIF developed for powder diffraction (pdCIF; Toby &

Ashcroft 2005) has become more popular with the development of CIF-exporting modules in programs such as *GSAS* (Toby *et al.*, 2003). In view of these developments, it is expected that a CIF for specular reflectivity data (rfCIF) could make it easier to exchange specular reflectivity measurements between researchers working in different or multidisciplinary fields. It would also simplify archiving and interpreting this information.

An informal working group of specialists worldwide has recently been formed to produce a reflectivity CIF dictionary (rfCIF). A draft version of the dictionary is being prepared in collaboration with COMCIFS, the committee that oversees the CIF project for the International Union of Crystallography. A number of practitioners in the field have already commented on a first draft of the dictionary and any one else with an interest in this project is invited to contact one of the members of the working group listed below.

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