

A REFERENCE DIFFRACTION DATABASE FOR NON-CRYSTALLINE, PARTIALLY CRYSTALLINE AND AMORPHOUS MATERIALS

Timothy G. Fawcett, John Faber, Suri Kabekkodu, Justin Blanton
International Centre for Diffraction Data, Newtown Square, PA 19073

The concept of having a diffraction database for non-crystalline materials has been discussed for nearly 40 years. Several specialty products, containing hundreds of diffraction patterns, have been produced, particularly in the material fields of polymers and clay minerals. In recent years, we find many natural products, nano-materials, thin films, modulated structures and glass ceramics that are not adequately explained by crystalline representations. The ICDD has been involved in two efforts, the sale and distribution of the Dow Polymer Pattern Collection [1] and the generation and production of a mineral pattern collection. The mineral patterns were displayed on PDF index cards and books for nearly a decade but they did not transfer to electronic formats (tape, CD, DVD).

Non-crystalline/amorphous databases are distinctly different from the standard representations made in the Powder Diffraction File (PDF) because data on crystalline materials can be easily reduced and represented by a d,I listing of position and intensity data pairs. This data reduction greatly facilitates data storage and the searching of thousands to hundreds of thousands of material data sets in an unknown analysis. The description and representation of non-crystalline, partially crystalline and amorphous materials in a reference database is made infinitely more difficult by the need to use the entire diffraction pattern complimented by extensive details on specimen preparation and data collection. This has historically limited most collections of non-crystalline materials to paper products.

The explosive growth in data storage capacity and processing capabilities in personal PC's is enabling the ability to rapidly search large data sets. Automated total pattern analysis capabilities, through full pattern analysis and Rietveld analysis techniques, are providing new capabilities of exploring large ranges in crystallinity and size domains. These developments, in turn, push the evolution of the PDF. The ICDD has collected tens of thousands of full experimental diffraction patterns which include subgroup collections of polymers and minerals. These are being processed into standardized formats for display and eventual inclusion in the PDF. This presentation will discuss the editorial efforts being made to generate the database and the necessarily developments required to make the database useful to the scientific community. Polymer examples will be used to demonstrate recent progress and the ICDD is soliciting dialog and feedback in developing new capabilities for the polymer community.

[1] "X-ray Diffraction Patterns of Polymers", J. W. Turley, The Dow Chemical Company (1965), published by the International Centre for Diffraction Data.

