

Materials Characterization Using Neutron Radiation Capabilities of the ICDD PDF-4 Databases

T. Blanton, J. Faber, J. Blanton, S. Kabekkodu, R. Papoular, T. Fawcett
International Centre for Diffraction Data, Newtown Square, PA 19073, USA

Worldwide neutron facilities offer sources and advanced optics and detector systems that can provide very high resolution. The growth of user facilities and mail-in programs has greatly expanded the general access to these facilities and the number of global users processing and analyzing neutron diffraction data. Structure elucidation, phase identification, and phase quantification are three key methods of materials analysis performed using neutron radiation diffraction techniques.

The International Centre for Diffraction Data, ICDD, has developed a series of tools for the analysis of neutron diffraction data, based on input from our users and ICDD members that work at neutron facilities around the world. All data entry references with atomic coordinates in the Powder Diffraction File PDF-4 annual releases can be converted to neutron diffraction patterns through the use of pattern simulations. Instrument functions for neutron experiments are incorporated in the software. In addition, ICDD sponsors the collection of new neutron radiation diffraction data for new reference patterns for inclusion in PDF-4 databases. User raw data patterns can be imported and analyzed for phase composition and phase quantity. In addition, over 270,000 PDF entries with atomic coordinates can be imported for use in Rietveld refinement analysis programs.

An overview of the PDF database, data entries, neutron pattern analysis, and case studies will be presented that demonstrate the application of the Powder Diffraction File for materials characterization, through the analysis of neutron radiation diffraction data.