

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

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Worldwide synchrotron facilities offer high brilliance sources and advanced optics and detector systems that 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 synchrotron diffraction data. Structure elucidation, phase identification, and phase quantification are three key methods of materials analysis performed using synchrotron radiation diffraction techniques.

The International Centre for Diffraction Data, ICDD, has developed a series of tools for the analysis of synchrotron diffraction data, based on input from our users and ICDD members that work at synchrotron facilities around the world. All data entry references in the Powder Diffraction File PDF-4 annual releases can be converted to synchrotron diffraction patterns through the use of pattern simulations. Instrument functions for synchrotron experiments are incorporated in the software. In addition, ICDD sponsors the collection of new synchrotron radiation diffraction data for structure elucidation of pharmaceuticals and 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, synchrotron pattern analysis, and case studies will be presented that demonstrate the application of the Powder Diffraction File for materials characterization, through the analysis of synchrotron radiation diffraction data.