Materials Characterization Capabilities Using the Powder Diffraction File ™

How SMART is your database? Can your database visualize a modulated structure; identify unknowns in a neutron, X-ray or electron diffraction pattern; analyze a pharmaceutical tablet with a polymeric excipient, or an amorphous active ingredient; or study crystallite size and molecular orientation in a nanomaterial? You can do all of these analyses and more with the PDF-4+ database.

The International Centre for Diffraction Data (ICDD) is a global scientific non-profit organization whose mission and vision not only encompass the production and distribution of the Powder Diffraction File (PDF™) databases, but also promotes education and advancing methods of materials analysis. This results in a database that is designed specifically to analyze solid state materials, both crystalline and non-crystalline, powders and single crystals, with unique analytical capabilities. This workshop will describe both new data collections and methods of analysis embodied in PDF-4+ databases that result from ICDD's collaborations with global scientists.

X-ray Diffraction Analysis of Polymers – Expanding Materials Characterization Capabilities – T. N. Blanton, International Centre for Diffraction Data

Polymers often can pose a challenge for XRD investigations. Variations in macromolecule chain length, the occurrence of chain branching, and processing conditions often results in polymer materials that can be amorphous, semi crystalline, highly crystalline, randomly oriented, or preferentially oriented. In commercial applications, many composites are comprised of a polymer base with inorganic or organic additives present. Inclusion of raw data XRD patterns for polymers in the PDF database provides a more complete picture to help identify crystalline and amorphous components of a polymer XRD pattern. The original discussion of including full pattern polymer data in the PDF began with an ICDD member's task group and is now a reality with over 100 polymer raw data XRD patterns in the PDF, focusing on high volume commercial polymers.

Crystal Structures of Large Volume Commercial Pharmaceuticals – J. A. Kaduk, Illinois Institute of Technology, Chicago, Illinois

The crystal structures of a surprising number of the largest dollar volume commercial pharmaceuticals are unpublished, and the structures for many other pharmaceuticals have only been determined at low temperatures. To provide high-quality reference data for the Powder Diffraction File database and to determine the crystal structures, synchrotron powder diffraction patterns have been collected on many materials at ambient conditions. Density-functional geometry optimizations enable detailed analysis of the bonding in the solid state, particularly the hydrogen bonding. Powder diffraction patterns of these materials, as well as 9 compounds for which the crystals structures have been determined and 10 amorphous pharmaceuticals will be incorporated in the 2014 release of the Powder Diffraction File.

New Neutron Diffraction Data Analysis Capabilities in PDF-4+ - T. G. Fawcett, International Centre for Diffraction Data

Neutron powder diffraction is a useful tool because elemental scattering contrast is quite different when compared to X-rays. Elements in the periodic table often have quite different scattering amplitudes (the scattering cross sections are not strictly proportional to atomic number, Z). Unlike standard laboratory X-ray sources, neutrons are available both at nuclear reactors and pulsed sources. In this discussion, we treat the constant wavelength (CW) neutron case. The PDF-4+ Release 2014 will have ~230,000 entries with atomic coordinates used to calculate neutron powder diffraction reference patterns as well as new search and identifications features specifically developed for neutron diffraction analyses.

The Modulated Structure Subfile and Graphics - T. N. Blanton, International Centre for Diffraction Data

Modulated and composite crystals are fascinating and complex structures which violate the traditional idea that a perfect crystal structure must possess a 3-dimensional periodicity. Generally considered aperiodic, these structures actually do obey rules of periodicity but their description requires 4 or more dimensions for this periodicity to become obvious. These modulations are a result of fluctuations in the position or occupation of the atoms that compose the crystal. The ICDD has created the largest modulated structure database in the world with the addition of 178 new modulated entries to be released in 2014 for a total of 463 entries, all of which have been extensively edited through custom editorial programs developed from collaborative efforts. New for Release 2014 is a visualization graphics program specifically designed for modulated structures.

The Analysis of Nanomaterials by Powder Diffraction – P. Scardi and M. Leoni, U. of Trento, Trento, Italy

The International Centre for Diffraction Data (ICDD) has worked with its international membership of scientists to develop a series of software tools and simulations to be able to study and characterize nanomaterials. Simultaneously the ICDD has developed reference data and editorial procedures for experimental nanomaterials as well as amorphous materials. Methods have been developed that are generically grouped under the title of "Total Pattern Analyses" whereby the entire digital profile of a diffraction pattern is used to study degrees of order, domain sizes, and contributions from scatter and background in order to extract information about all the materials present in the solid state independent of their crystallinity.

Acknowledgements

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Nanomaterials

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