The New PDF-4+ 2005: A Relational Database (RDB) with Atomic Structure Information and On-the-fly Total Pattern Analysis Capability

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The ICDD is continuing to develop new RDB database capability for the Powder Diffraction File™ (PDF®) [1,2]. The PDF-4+ 2005 will be released in August, 2005. This database will contain approximately 84,000 new entries with complete atomic coordinate information. Using the structure data, powder patterns will be calculated for electron, neutron and x-ray diffraction; these are calculated on-the-fly (as needed). Scattering contrast studies as a function of probe and wavelength can be used to aid experiment design. In addition to the standard peak intensity listing in the PDF, integrated intensity information will be available for all unique hkl's within each entry. Elemental composition data (available for all entries in the PDF) can be used as filter criteria for effective searches in the RDB. We will show how atomic evironment data can be used to help understand classes of materials properties. One of the aims of these initiatives is to enhance our ability to perform materials design studies. Fully digitized powder patterns are a first step in the realization of this process.

[1] Faber J., Fawcett T., *Acta Cryst.*, 2002, **B58**, 325-332. [2] Kabekkodu S. N., Faber J., Fawcett T., *Acta Cryst*.,2002, **B58**, 333-337.

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