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THE POWDER DIFFRACTION FILE (PDF): A RELATIONAL DATABASE FOR ELECTRON DIFFRACTION

John Faber*, Tim Fawcett* and Raymond Goehner**

* International Centre for Diffraction Data, Newtown Square, PA 19073
**Sandia National Laboratories, Albuquerque, NM 87185-0886

The PDF has been the primary reference for powder diffraction data for over 50 years. The primary information in the PDF is the collection of d-I data pairs, where the d-spacing (d) is determined from the angle of diffraction, and the peak intensity (I) is obtained experimentally under the best possible conditions for a phase-pure material [1]. These data provide a "fingerprint" of the compound because the d-spacings are fixed by the geometry of the crystal and the intensities are dependent on the contents of the unit cell. Hence, d-I data may be used for identification of unknown materials by locating matching d-I data in the PDF with the d-I pairs obtained from the unknown specimen. Identification is the most common use of the PDF, but the presence of considerable supporting information for each entry in the PDF allows further characterization of the specimen. Examination of the crystal data, Miller indices, intensity values, scale factors, physical property data and the comprehensive literature reference data provide extraordinarily useful information concerning the specimen under study [2].

The ICDD is in the midst of an exciting transition to relational database formats for the Powder Diffraction File (PDF). The PDF-4+ 2005 will be released in August, 2005. This database will contain approximately ~82,000 new entries with complete atomic coordinate information. Powder patterns will be calculated for x-ray, electron and neutron diffraction. In particular, electron diffraction patterns will be calculated for all entries that contain atomic coordinate information. Integrated intensity information will be available for all unique hkls within each entry; both the standard peak intensities and integrated intensities listings will be available for each entry. The aim of these initiatives is to enhance our capability to perform materials design. Fully digitized powder patterns are a first step in the realization of this process.

Search-indexing techniques that involve Hanawalt, Fink and Long8 searches are currently available in the SIeve+ plug-in to the PDF-4 database [3]. Chemical and compositional constraints to search indexing are available in the DDView+, a Boolean logic driven database base search and display program. In particular, the Long8 search does not consider the intensities of the low-angle hkl's. Taken together, all of these features provide an extraordinarily powerful set of analysis tools since chemical constraints and search-indexing methods are linked to experimental methods, for example SEM/EDS combined with EBSD.

References

[1] J. Faber and T. Fawcett, Acta Cryst. B58 (2002) 325-332.
[2] S. N. Kabekkodu, J. Faber and T. Fawcett, Acta Cryst. B58 (2002) 333-337.
[3]. J. Faber, C. A. Weth and R. Jenkins, Materials Science Forum, 378-381 (2001) 106-111.

2004 Release		**(PDF-4/Full File 2004)**	
Total No. of Datasets	163,835		
Classification		**Crystallographic Data**	
No. of unique empirical formula	95,775	No. with cell parameters	133,936
No. of alternates	9,825	No. with reduced cells	133,936
No. of deletes	16,217	No. with calculated Z	122,680
No. of elements	1,348	No. with calculated density	120,053
No. of binaries	24,570	**Bibliographic Data**	
No. of ternaries	53,804	No. of References	262,978
No. of quaternaries	46,837	No. of Journals	1,854
No. of quint	24,937	No. of Authors	66,617
No. > 5 elements	12,303	No. of Titles	64,942
No with Pearson symbol	122,283	**Physical Property Data**	
No with prototype assignment	16,820	No of entries w/Physical Properties	48,259
No. with Organic Functional Groups	41,552	No. of Melting Points	9,309
Diffraction Data		No with colors	31,418
No. of Indexed Patterns	134,083	No with optical properties	7,288
No with I/Ic	77,887	No. with Molecular weight	163,340
No. of Structure Factors	65,986	No. with measured density	29,951
2005 Release	~246,604	**(PDF-4+ 2005)**	
Data from MPDS (Linus Pauling File derived new entries)	78,769	Complete atomic coordinates, temperature factors, Wyckoff Sequences, 3D structures, elemental weight fractions for all compounds	Calculated electron diffraction patterns
Data from NIST	~4,000		

Table 1. Summary of selected properties of the ICDD PDF-4/Full File 2004 database and new entries for PDF-4+ 2005.

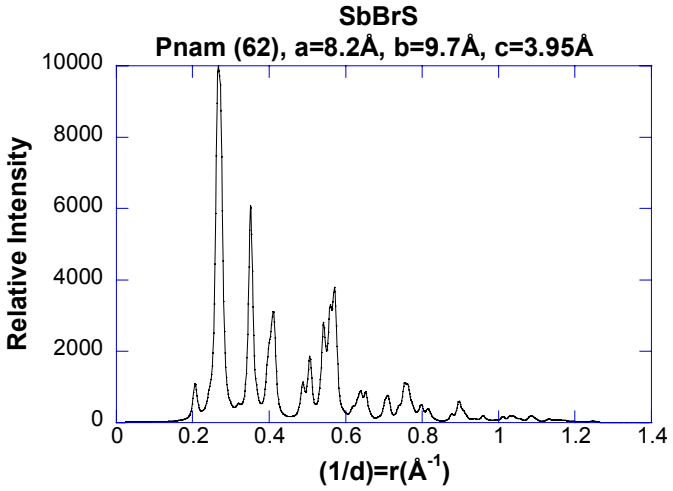

Figure 1. Calculated electron diffraction pattern for SbBrS, using $\lambda = 0.1$ Å

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