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Fundamentals of Powder Diffraction and Structural Characterization of Materials

Second Edition

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Cover illustration, created by Peter Zavalij, follows the book content. It is inspired by Salvador Dali's painting "The Metamorphosis of Narcissus" where Narcissus (polycrystalline (Au,Ni)Sn4, courtesy Lubov Zavalij) falls in love with his own reflection (diffraction pattern), transforms into an egg (reciprocal lattice), and then into a flower (crystal structure in a physical space), which bears his name.

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this database. Nonetheless, the PDF is not a complete database, which is nearly impossible to achieve anyway. The information included in the PDF is mostly collected from published powder data and from records produced upon ICDD request.[31] At the time of writing this book, the ICDD database exists in two formats: PDF-2 preserves a classic text-based format that allows one to search-match using positions and intensities of several strong Bragg peaks in addition to searching a limited number of other fields; PDF-4 is build on relational database technology that is distributed in several subsets (see Table 13.3) and provides searchable access to all data fields.

In addition to a vast number of included entries and a comprehensive quality control, the usefulness of the Powder Diffraction File is established by the ability to perform searches based strictly on the digitized patterns, that is, without prior knowledge of the unit cell dimensions and/or other crystallographic and chemical information. Similar searches may also be carried out using several different existing databases: for example, Pauling File and Mineralogy Database and, perhaps, a few others (see Table 13.3), which are, however, not as comprehensive as the PDF. For example, the Pauling File is underdeveloped with respect to multinary compounds, while the Mineralogy Database is dedicated to naturally occurring and synthetic minerals. More detailed and recent (as of 2002) information about a variety of crystallographic databases can be found in a special joint issue of Acta Crystallographica, Sections B and D (also see references 6–13 in Sect. 13.4).[32]

When experimental data remain unidentified using a digitized pattern-based search-match, different databases should be checked before drawing a conclusion that a material is new. Continuing searches, however, usually require unit cell dimensions and therefore, a powder pattern should be indexed prior to the search. There are a variety of databases dedicated to different classes of compounds and containing different information, as shown in Table 13.3.[33]

For example, two comprehensive databases, ICSD and CSD, contain crystallographic data and structural information about inorganic, and organic and metal–organic compounds, respectively, while NIST database encompasses all types of compounds, but provides only crystal data with references. Other databases are dedicated to specific classes of materials, such as metals and alloys, proteins and macromolecules, minerals or zeolites. Search-match utilities are usually provided with databases, or they may be obtained separately.

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[31] ICDD makes limited funds available to researchers interested in processing and submitting new experimental patterns for incorporation into the Powder Diffraction File. More information about the ICCD's Grant-in-Aid program can be found at http://www.icdd.com.

[32] Acta Crystallographica is an international journal published by the International Union of Crystallography in five sections: Section A (Foundations of Crystallography); Section B (Structural Science); Section C (Crystal Structure Communications); Section D (Biological Crystallography), and Section E (Structure Reports Online). Special joint issue: Acta Cryst. **B58**, 317–422 (2002) and Acta Cryst. **D58**, 879-920 (2002). Table of contents is available at http://journals.iucr.org/index.html.

[33] Full list of databases related to crystallography can be found at http://www.iucr.org/resources/data.

Table 13.3 Selected computer searchable crystallographic databases.

Database	Content/Compounds	No. of entries
ICDD[a] – Powder diffraction file	PDF-2, original text based. Both experimental and calculated patterns.	199,574 total 172,360 inorganic 30,728 organic
	PDF-4+ (Full)	272,232 total 100,511 experimental 107,507 with atomic coordinates
	PDF-4/Minerals	25,861 4,316 with atomic coordinates
	PDF-4/Organics. Both experimental and calculated patterns.	312,355 28,677 (Experimental) 283,678 (Computed)
LPF – Pauling file[b]	Inorganic ordered solids. Contains structural, diffraction, constitutional (phase diagrams), and physical property data.	80,000 structure entries 34,000 patterns 52,000 property data 6,000 diagrams
ICSD[c] – Inorganic crystal structure data	Inorganic crystal structures, with atomic coordinates, 1913 to date.	100,000+
CSD[d] – Cambridge structural database	Crystal structures of organic and metal organic compounds (carbon containing molecules with up to 1,000 atoms)	436,436
CRYSMET[e] – Metals and alloys database	Critically evaluated crystallographic data for inorganic and intermetallic materials.	119,600
PDB – Protein data bank;[f] Nucleic acids database[g]	Structures of proteins. Structures of oligonucleotides and nucleic acids.	49,620 3,768
IZA[h] – Zeolite database	All zeolite structure types: crystallographic data, drawings, framework, and simulated patterns	179 types
Mineralogy database[i]	Mineral species descriptions with links to structure and properties. X-ray diffraction list (three strongest peaks).	4,442
NIST[j] – Crystal data	Unit cell, symmetry and references	237,671

[a] Release 2007. The International Centre for Diffraction Data (http://www.icdd.com).
[b] The multinary edition of database developed in cooperation between JST (Japan Science and Technology Corporation, Tokyo, Japan) and MPDS (Material Phases Data System, Vitznau, Switzerland); http://crystdb.nims.go.jp/.
[c] Release 2007-2. The ICSD is produced by FIZ (Fachsinformationzentrum) Karlsruhe, Germany (http://www.fiz-karlsruhe.de/icsd.html).
[d] As of January 1, 2008. Produced by Cambridge Crystallographic Data Centre (CCDC) (http://www.ccdc.cam.ac.uk/prods/csd/csd.html).
[e] Release November 2007. CRYSTMET® is maintained by Toth Information Systems, 2045 Quincy Avenue, Gloucester, Ontario K1J 6B2, Canada (http://tothcanada.com/databases.htm).
[f] Release March 2008. PDB is maintained by the Research Collaboratory for Structural Bioinformatics (http://www.rcsb.org/pdb/home/home.do).
[g] Release March 2008. Rutgers University, NJ, USA (http://ndb-mirror-2.rutgers.edu/).
[h] IZA (International Zeolite Association) zeolite database is maintained by IZA structure commission. Available on-line at http://www.iza-structure.org/databases/.
[i] Update January, 2008. Mineralogy Database is available on-line at http://webmineral.com/.
[j] Release January, 2008. National Institute of Standards and Technology (http://www.nist.gov/srd/nist3.htm). Distributed by ICDD.

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