PDF-4+, the material identification database

T. G. Fawcett[1], J. Faber[1], S. Kabbekodu[1] , F. McClune[1], D. Rafaja[2]

[1]International Centre for Diffraction Data, Newtown Square, PA, USA
[2]Institute of Physical Metallurgy, University of Freiburg, Germany

Keywords: Powder Diffraction File, PDF, Diffraction Data

Abstract. Release 2005 of the Powder Diffraction File (PDF) represents the next generation in the 64 years of continuous development of the PDF . The database has transitioned to a relational database format, been given a new housing with all new 32-bit display and viewing software. The latest product, PDF-4+ contains many new features from a collaboration with MPDS, codevelopers with Japan Science and Technology of the Linus Pauling File. The PDF-4+ database is tailored for identification and quantitation of solid unknowns by x-ray diffraction but can also be used for unknown identification by elemental analysis, electron and neutron diffraction and combinations thereof.

Introduction

Release 2005 of the Powder Diffraction File (PDF) represents the next generation in the 64 years of continuous development of the PDF. In the last decade the PDF has undergone explosive growth due to a series of collaborations between the International Centre for Diffraction Data (ICDD) and global crystallographic database organizations. These collaborating organizations include the Cambridge Crystallographic Data Centre (CCDC, United Kingdom), Fachinformationszentrum (FIZ, Germany), Material Phases Data System (MPDS, Switzerland), and the National Institute of Science and Technology (NIST, USA). The cumulative effect of these collaborations has resulted in the detailed characterization of approximately 475,000 materials by x-ray analysis with tens of thousands of new materials being added annually.

Data translation, standardization, editing, merging, and publication of multiple databases has had many effects in database development, some foreseen and others not. To handle large amounts of data the database has transitioned to a relational database format, been given a new housing with all new 32-bit display and viewing software. The latest product, PDF-4+ contains many new features from the collaboration with MPDS, codevelopers with Japan Science and Technology of the Linus Pauling File (LPF), and includes structural data and atomic parameters from the LPF in the PDF database.

Results and Discussion

The Powder Diffraction File (PDF) is a comprehensive compilation of materials identified by either powder diffraction or single crystal analyses. A comprehensive compilation was obtained through a series of strategic collaborations with international database organizations when added to the ICDD traditional sources of extracted bibliographic data, data from generous contributions, and data obtained through grants. This latter source enables the ICDD to keep current with major new material developments in superconductors, nanomaterials, electronic materials, drugs, pesticides and pharmaceuticals from research centers around the globe. In total the combined data in the PDF represents the published works of hundred of thousands of authors recorded from thousands of journals. In order to process large amounts of data both the ICDD and the database had to develop and evolve. The organization continuously strives to automate data review, standardization and analysis procedures with the end result that nearly all the entries have been improved through standardization, calculation of new properties, and removal of errors.

Release 2005 PDF database is available in three primary products PDF-2, PDF-4+, and PDF-4/Organics the first two are primarily metals and inorganic databases while the latter is primarily an organics and organometallics database. The word primarily is used because common materials are added to both databases to enhance identification efficiency. For example this would include common polymers, celluloses, and drugs in the former databases and inorganic excipients and common salts in the latter database..

In PDF-4+ Release 2005, new data has been added from a strategic collaboration with MPDS, that includes atomic coordinates, thermal parameters and a new structural prototyping system. These data, combined with developments in digitial pattern calculations, enables both identification and quantitation by techniques such as the Reference Intensity Ratio method (1), Rietveld Analysis (2) and total pattern analyses methods. The editors of the Linus Pauling File (3) have applied a new structural prototyping system to all inorganic materials facilitating unknown identification by isostructural and isotypical material analysis. As shown below, inclusion of atomic coordinates and thermal paramenters has resulted in a capability to simultaneously compare and utilize x-ray, electron and neutron diffraction patterns on a single material using user-defined instrumental functions typical of these methods.

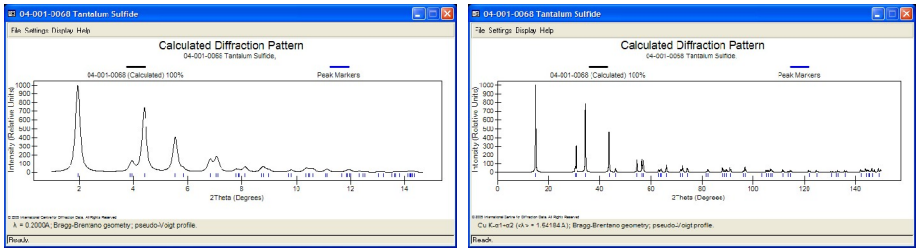

Figure 1. Electron and X-ray diffraction digital patterns for TaS_2

The inclusion of data from multiple sources has also led to the development of new methods to analyze entries and determine the degree of overlap and duplication between laboratories analyzing similar materials. The editorial review resulted in two new capabilities in the viewing programs, DDView and DDView+, for PDF Release 2005. Empirical formula and nomenclature searches have been supplemented with a composition search that can search by atomic or weight percent with a search window defined by either a range or an estimated standard deviation in the elemental analysis.

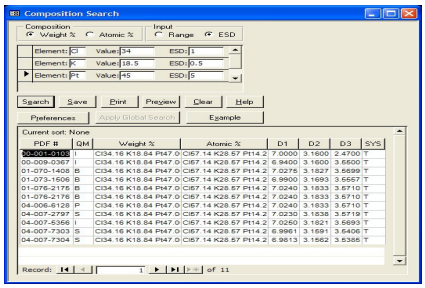

Figure 2. Composition Search in DDView and DDView+

Another feature is a quality mark developed for single crystal analysis. Several quality indicators have been used (4) to let the user know the performance of the data relative to a series of statistical analyses. Hundreds of thousand of editorial comments were added to the databases to let the user know the basis of the analyses so that they can judge whether the specific comment pertains to their particular material of study.

Finally, critically large numbers have been added to many searches, increasing their efficiency. This includes title searches, Pearson symbols, RIR values, unit cell parameters, and prototype assignments.

References

1. C.R. Hubbard, E.H. Evans, and D.K. Smith, "The Reference Intensity Ratio, I/I_c, for Computer Simulated Powder Patterns," *J. Appl. Crystallog.*, *9* 169 (1976).
2. H. M. Rietveld, "The Rietveld Method", *Energy Research Foundation,* ECN-RX-90-035April, (1990).
3. P. Villars, "New Structural Prototyping System" presented at the plenary session of the annual meeting of the International Centre for Diffraction Data (2004). Abstract available at www.icdd.com
4. S. N. Kabekkodu, D. Sagnella and V.Bosnic. "Quality Mark Distribution in Calculated Patterns", annual meeting of the International Centre for Diffraction Data (2004). Abstract available at www.icdd.com

Acknowledgements. The authors represent talented teams of editors and scientists at the ICDD including the publication, editorial, and science staffs who make the PDF possible. We would also like to acknowledge the continuous generosity of our volunteer members who ideas and knowledge continuously fuel new database concepts and developments.