

NEW DEVELOPMENTS AND CAPABILITIES IN PDF-4+: A RELATIONAL DATABASE WITH ATOMIC STRUCTURE INFORMATION AND ON-THE-FLY TOTAL PATTERN ANALYSIS CAPABILITY

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The ICDD is in the midst of an exciting transition to relational database formats for the Powder Diffraction File (PDF) [1,2]. The PDF-4+ 2006 will be released in August 2006. In addition to the steady annual increase in experimental data in the file, the entry population has risen by leaps and bounds since 1997. These dramatic increases are the result of institutional collaborations with FIZ (ICSD), NIST and most recently, the LPF (Linus Pauling File). The PDF-4+ 2006 database will contain ~98,000 entries with complete atomic coordinate information. Using the coordinate and structure data, powder patterns can be calculated for electron, neutron and x-ray diffraction; these are calculated on-the-fly (as needed). 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. 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, i.e., comparison with experimental data.

There are two central aspects to our new developmental work: utilization of an appropriate database housing to support powder diffraction and development of software tools that allow the user to better understand the content of the PDF. Better understanding of this content empowers the user to exploit and data mine the PDF. This year, DDView+ (our front-end program), is developed in Java (the size of the database and complexity of information queries require this) so that we can provide speedy response to our query structures.

In this paper, the front-end DDView+ will be used to illustrate problem solving and data mining using this new Java front-end. Over 50 broad classes of search conditions are available (many sub-classes are also available). Search-indexing techniques that involve Hanawalt, Fink and Long8 searches are currently available in the SIEVE+ plug-in to the PDF-4 database [3]. Coupling these search functions with chemical constraints provide an extraordinarily powerful set of analysis tools as applied for example, to SEM/EDS combined with high-resolution Electron Back-Scattering Diffraction (EBSD). This allows for the quantitative input of results from other analytical methods into our search and discovery functions.

References

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- [3]. J. Faber, C. A. Weth and R. Jenkins, *Materials Science Forum*, 378-381 (2001) 106-111.