WORKSHOPS

WS-01 Workshop on Protein Data Bank

WS-02 Workshop on Crystallographic Databases for Chemical and Material Analysis

WS-02.01 OVERVIEW OF THE WORKSHOP ON CRYSTALLOGRAPHIC DATABASES. By Winnie Wong-Ng* and Alan Mighell, Materials Science and Engineering Laboratory, National Institute of Standards ad Technology, Gaithersburg, MD 20899, U.S.A.

Characterization and identification of materials have become increasingly important in the areas of materials design and preparation. A vast source of reference data and a logical strategy of using them are needed for selecting candidate materials for desired chemical, physical and structural properties. Two x-ray diffraction databases: ICDD/Powder Diffraction File and NIST Crystal Data serve these purposes extensively. As the material sciences are rapidly moving toward the identification and design of substances at the atomic level, the newly developed NIST/Sandia/ICDD Electron Diffraction Database will also play a vital role in material science. The need for crystallographic databases, role of participating organizations (National Institute of Standards and Technology, JCPDS-International Centre for Diffraction Data and Sandia National laboratory), historical development of these databases will be discussed.

WS-02.02 MAINTENANCE AND USE OF DATA BASES FOR POWDER DIFFRACTOMETRY By R. Jenkins, International Centre for Diffraction Data, Swarthmore, PA, U.S.A.

The Powder Diffraction File (PDF-2) is maintained and supplied by the International Centre for Diffraction Data (ICDD). The current version of the (PDF-2) contains about 60,000 unique single-phase, data sets, about 70% of which are from inorganic materials. About one third of the patterns are produced via a Grants-in-Aid program, sponsored by the ICDD, and most of the remainder are derived from the open literature. Over the past 50 years or so, the ICDD has developed a detailed but effective editorial process, whereby incoming patterns are screened, checked and classified.

Although the main use of these data are for qualitative phase analysis using the classic Search/Match/Identify process developed by Hanawalt, Rinn and Frevel in the 1930's, a number of special products have been derived by merging data from the PDF, with data from the NIST Crystal Data File (CDF). All of these data bases are now available in computer readable form, either on tape or CD-ROM. A somewhat reduced version of the full file is also available (PDF-1) for use with computer controlled diffractometers where storage space is limited.

Because of historical limitations of data storage, it has been the practice to reduce experimental powder patterns to a set of d-spacing and relative intensity data. More recently, there has been interest in producing a data base of calibrated, fully digitized experimental and calculated data (PDF-3). It is hoped that such a data base will provide the raw data needed for the application of full pattern matching methods. This paper briefly discusses the maintenance and use of these data bases. A short demonstration of the use of the data bases will follow the talk.

WS-02.03 NIST CRYSTAL DATA AND ELECTRON DIFFRACTION DATABASES FOR RESEARCH AND ANALYSIS. Alan D. Mighell* and Vicky Lynn Karen, Reactor Radiation Division, National Institute of Standards and Technology, Gaithersburg, MD 20899.

The NIST Crystal and Electron Diffraction Data Center has built a crystallographic and chemical database with information on approximately 183,000 materials including metals, intermetallics, organometallics, minerals, inorganics, and organics. As a source of critically evaluated data, this information can be used as a basis for scientific research or as an aid to research. For example, the data can be used to generate statistics, to evaluate symmetry of materials, to carry out bibliographic searches, to find compounds with specified compositions, to characterize materials, and in materials design.

From our central database, two distribution databases are generated: (1) NIST Crystal Data and (2) the NIST/Sandia/ICDD Electron Diffraction Database. The recently developed Electron Diffraction Database is especially designed to identify phases using elemental and d-spacing data obtained with an electron microscope. Recently, it has been integrated into a number of work stations associated with the analytical electron microscope. Likewise NIST Crystal Data can be used to identify materials using lattice-matching techniques. Thus as soon as any cell defining the lattice is known, this database should be checked to identify the material. When the database and search software are integrated into the single-crystal x-ray diffractometer, a powerful new analytical tool is created for materials analysis. Both NIST databases and search software are available to the scientific community on magnetic tape, CD-ROM, scientific instrument, and online and are supplied with search software.

WS-02.04 NEW ICDD METALS AND ALLOYS INDEXES, A POWERFUL MATERIALS RESEARCH TOOL. By L. D. Calvert, T. C. Huang*, M. H. Mueller, P. L. Wallace, and S. Weissmann, Metals and Alloys Subcommittee of the Technical Committee, International. Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, USA.

A new Metals and Alloys (M&A) Indexes has recently been developed and published by the International Centre for Diffraction data (ICDD). The objectives of these indexes are: (1) to make characterization of samples easier by providing a new Alphabetical Formula Index that allows systematical searches for chemical analog and greater use of partial chemical knowledge, (2) to make analysis of new materials more accurate by providing a new Pearson Symbol Code index, and (3) to aid in using and editing the M&A Subfile of the ICDD Powder Diffraction File (PDF), so that new and existing diffraction data can be properly analyzed using information from these indexes.

The indexes are designed to be used in conjunction with or independently of the PDF and contains the following four indexes: Alphabetical Formula Index (AFI), Pearson Symbol Code Index (PSCI), Common Name Index (CNI), and Strukturbericht Symbol Index (SSI).

The AFI contains all phases in the PDF M&A Subfile and has entries for an n-component material in n different locations according to their alphabetical order. The multiple listings assist the user in locating possible phases when partial chemical information is known.
The PSCI contains all phases in the PDF M&A Subfile, including those that have either partial Pearson Symbol Code or none at all. The index has entries arranged in Pearson Symbol order. Hence, one can find all the compounds with a given structure, and if desired, compare their atomic contents and lattice parameters. The latter are in the standard Crystal Data setting to aid in structural comparisons.

The CNI permits cross-referencing common metallurgical names such as austenite, cementite, etc. to the appropriate PDF data. It also has cross-references for all mineral names that have found their way into metallurgical usage.

The SSI provides cross-referencing between Strukturbericht Symbols and the corresponding prototype structures. This index includes those structures for which Strukturbericht Symbols have been assigned and which are likely to be found in metallurgical applications.

The indexes have been used successfully for prototype structure, Pearson Symbol Code, and/or (hkl) indexes assignments. An example of the applications is in analyzing unindexed or incorrectly indexed X-ray powder diffraction patterns. Another example of the application is in discovering two prototype structures, which has the same Pearson Symbol Code, are actually isostructural.