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 Mighall, Materials Science and Engineering Laboratory, National Institute of Standards and 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 is 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, ICDD - 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 30 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 Hanawall, Rinn and Frelas in the 1970'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 databases 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.

WS-02.03 NIST CRYSTAL DATA AND ELECTRON DIFFRACTION DATABASES FOR RESEARCH AND DESIGN By Alan Mighall and Vicky Lynn Karen, Reactor Radiation Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, U.S.A.

The NIST Crystal and Electron Diffraction Data Center has built a crystallographic and chemical database with information on approximately 153,000 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 searchers, to find compounds with specific compositions, to characterize materials, and in materials design.

From our central database, two distribution databases are generated: (1) the 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 incorporated 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 routines are added 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 for the scientific community on magnetic tape, CD-ROM, scientific instrument, and online and are supplied with search software.


A new Metals and Alloys (M&A) Index 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 Alphabetic Formula Index that allows systematic searches for chemical analogs, 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 Metals and Alloys (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: Alphabetic Formula Index (AFI), Pearson Symbol Code Index (PSI), Common Name Index (CNI), and Strukturbericht Symbol Index (SSI).