12.X-1 THE WHOLE PATTERN DATABASE - A NEW CONCEPT FOR POWDER DIFFRACTION. Deane K. Smith and Gerald G. Johnson, Jr., The Pennsylvania State University, University Park, Pennsylvania 16802, USA.

Powder diffraction patterns contain three types of information. The positions of the diffraction peaks yield the geometrical information on the periodicity of the crystal structure. The peak intensities provide the information on the positions and types of atoms in the unit cell. The peak profiles contain information on the perfection of the crystal. Storage of only two parts of this data set eliminates considerable information, so a new effort has been initiated to retrieve and store the full diffraction trace.

With both improvement in the convenience and accuracy of data collection and the reduced cost of manipulation and storage of information in computer readable form, it is now feasible to process and save the original raw data in a form which can be retrieved and processed by users other than the originator of the data. Computer-controlled instrumentation collects and processes diffraction traces as digitized information. A typical pattern collected over a 120^{o} 2θ range at an interval of 0.01^{o} would require around 12000 bytes of storage. With storage media now storing 500 megabytes on an optical disc, 50 thousand datasets on a single media are feasible.

Ideally, the data stored should be independent of the instrumental aberrations of the data collection system so that it truly represents the sample under study. Presently, the datasets are recorded with an accompanying trace from a standard sample such as silicon from which the instrumental profile can be extracted. Deconvolution algorithms are being developed to allow the users to compare data taken on different systems and to process raw data taken on their system for comparison with the database of patterns.

An early use of the whole pattern database has been quantitative analysis. The use of the whole trace improves the accuracy of the weight fraction estimates because it uses all the data in the diffraction patterns of the unknown and the reference datasets. The effects of random errors are minimized, and even the affects of systematic errors are reduced if the error varies in sign over the diffraction range.

The Pennsylvania State University initially developed a database for the analysis of clay minerals in sediments. The database has been extended to contain corrosion phases. Presently the JCPDS-International Centre for Diffraction Data is studying the feasibility of larger file based on compounds being examined by its Grant-in-Aid programs and is establishing guidelines for the parameters to be used for the collection of the primary data.

12.X-2 RECENT ADVANCES IN POWDER DIFFRACTION TECHNIQUES WITH SYNCHROTRON RADIATION. By D.E.Cox, Brookhaven National Laboratory, Upton, NY 11973, U.S.A.

In the past three years, considerable progress has been made in the application of synchrotron radiation to x-ray powder diffraction techniques. The high resolution and low background which can be obtained at synchrotron sources are being actively exploited by many groups for structure solution and refinement by the Rietveld profile technique, while white-beam energy-dispersive diffraction techniques involving diamond-anvil cells have evolved to the point where experiments can now be performed with incident beams as small as 10 μm square at pressures approaching 2 Mbar.

An overview will be given of some of the techniques being developed at various synchrotron centers, with particular emphasis on the different kinds of diffraction geometry which can be used with monochromatic radiation, how these compare to conventional techniques, and the applications for which they are best-suited. In the latter context, an important consideration is the inevitable trade-off between intensity and resolution, and this will be discussed in some detail. The different techniques include the use of film cameras, position sensitive detectors, Soller slit systems and perfect or narrow-mosaic analyzer (diffracted-beam) crystals, which serve as angular receiving slits of high resolution. The latter provide a very convenient and simple means of adjusting the angular position of the focussing minimum (typically about 0.02^{o} full-width at half-maximum on the 2θ scale) as appropriate for different applications, such as indexing of unknown phases, investigation of small unit cell distortions, ab-initio structure solution or Rietveld refinement. In addition to the normal type of extended flat-plate geometry, it is often possible to use capillary specimens (sometimes 1mm in diameter) with no loss of resolution, and thereby eliminate troublesome preferred orientation effects. A brief description will also be given of energy-dispersive diffraction techniques with semiconductor detectors and scanning monochromators, and some applications discussed.

The discussion will be illustrated with some examples of recent work at various synchrotron centers.

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