12.2-1 THE EFFECT OF CRYSTALLITE SIZE ON POWDER PATTERN RESOLUTION AND PHASE IDENTIFICATION -Deane K. Smith, The Pennsylvania State University University Park, Pennsylvania 16802, USA and Helein D. Bennett, National Aeronautics and Space Administration, John F. Kennedy Space Center, Florida 32899, USA

The inclusion of the crystallite size broadening in the calculation of powder diffraction patterns illustrates the problem of peak resolution and its effect on phase identification using standard search procedures. Patterns of low resolution due to the method of recording the data or poor crystallinity are often difficult to match with patterns of high resolution, even for materials which are otherwise identical in all respects. This problem is common even with modern diffractometers when trying to identify corrosion products which are often poorly crystalline.

A program, SIMUL, has been prepared to use the d-I data sets of the Powder Diffraction File and simulate the diffractometer trace from which the data was originally extracted. A Cauchy or modified Cauchy profile is used with its alpha 1 peak corresponding to the I value. The envelope of all the peaks is used as the final trace. The initial calculation uses half widths corresponding to a highly crystalline sample on a well aligned diffractometer. A Gaussian profile whose half width corresponds to the Scherrer broadening for a specific crystallite size is convoluted with the calculated diffraction trace. The resulting trace can be compared with the experimental data obtained from a sample with crystallite size broadening.

The series of hydrated copper chlorides illustrates the problems of identification when the pattern qualities are different. In this case there are several well defined reference patterns in the Powder Diffraction File. The well resolved pattern of $Cu_2Cl(OH)_3$, atacamite PDF-25-269, has its strongest three lines at 5.48A(100), 5.03(70) and 2.278(70). Using the broadening calculation for 200A crystallites, the three lines at 2.836(50), 2.779(50) and 2.759(55) coalesce and become the strongest line in the pattern. The other copper chlorides show similar effects. Whether using manual or computer searching, this identification would be a very difficult one to achieve.

SIMUL provides a means for the comparison of well- and poorly-resolved patterns. A cursory examination of patterns in the PDF show that many are modified significantly by broadening. The problem is most common when the pattern contains clusters of closely spaced lines of medium intensity. Similar calculations could be applied to comparing Debye-Scherrer and diffractometer data except that the problem is due to camera resolution in the case of the Debye-Scherrer camera.

12.2-2 A PROGRAM FOR COMPARING AND SELECTING OF X-RAY POWDER PATTERNS OF SUBSTANCES WITH SIMILAR STRUCTURES. By S.D.Kirik, S.A.Kovyazin, A.M.Fedotov, Institute of Chemistry and Chemical Engineering, 42, K.Marx St.,Krasnoyarsk, 660049,U.S.S.R.; Computer Centre Siberian Branch of USSR Academy of Sciences, Krasnoyarsk, 660036,U.S.S.R.

A computer program has been written for selectin X-ray powder patterns from automatic data base with a visual similarity to the certain pattern. Four criteria were tested as a quantitative measure of a visual similarity of patterns. Before comparison patterns are normalised. A powder pattern is considered as a discrete probability distribution of intensities. The distribution (pattern) is linearly transformed to a distribution with zero mathematical expectation and unit variance. As a result of the normalisation correspondig elements of visually similar patterns become geometrically close. Two criteria are the area between distribution functions and Levy's distance. The third criterion is a sum of distances between the nearest lines in compared normalized patterns, where the distances include difference of intensities. In the fourth criterion lines are compared succesively. The differnces in ratio of a distances between neighbouring lines and differences in ratio of line's intensities are summarized. The use of suggested criteria leads to the reasonable list of substances selected with the program. Structures of substances can be considered as a constructive hypothesis to solve different problems of X-ray structure analysis.

12.2-3 NBS CRYSTAL DATA: COMPOUND IDENTIFICATION BY LATTICE MATCHING USING ELECTRON, X-RAY, OR NEUTRON DIFFRACTION DATA. By V.L. Himes and A.D. Mighell, Reactor Radiation Division, National Bureau of Standards, Gaithersburg, MD 20899.

The NBS Crystal Data Center maintains a database that contains evaluated crystallographic and chemical data on ~120,000 materials. The data fall into the following categories: metals, intermetallics, organometallics, minerals, inorganics and organics. As a source of critically evaluated data, the database can be used as a basis for scientific research or as an aid to research (e.g. to locate compounds with a given Pearson's code, to obtain bibliographic data, and to identify unknown compounds). Using lattice-formula matching techniques, unknown compounds can be identified against entries in NBS CRYSTAL DATA. The technique can be used once any cell defining the lattice has been determined. Cell parameters may be measured by electron, neutron, or x-ray diffraction using single-crystal or powder diffraction methods. Highlights of the method include: fast and highly automated; highly selective even when large tolerances are used for the cell parameters; identification possible in spite of typical errors made by experimentalists; excellent method for all classes of solid-state materials. NBS*SEARCH has been written to provide all the required software for lattice matching against NBS CRYSTAL DATA. The program is written in standard FORTRAN and is designed to be used in any analytical laboratory. The NBS*SEARCH software is multifunctional in design, and it is planned to incorporate additional search functions in forthcoming versions of this program. Both the software and the database are available from the JCPDS-International Centre for Diffraction Data.