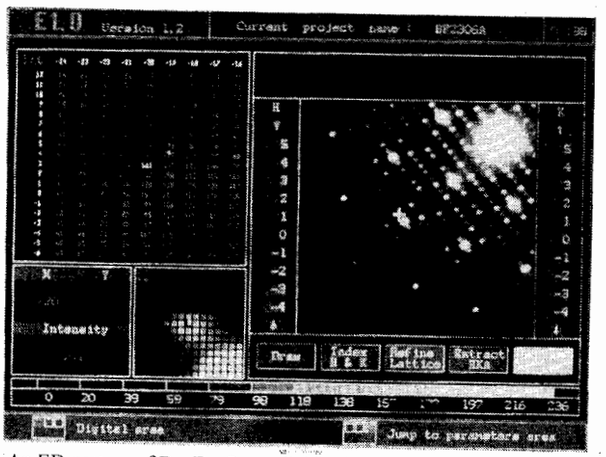
02-Methods for Structure Determination and Analysis, Computing and Graphics



An ED pattern of $Ba_2Fe_2O_5$ as digitized and displayed by ELD. The reflection at the cross is at 1.45 Å resolution.

PS–02.04.10 A NEW METHOD TO DETERMINE UNKNOWN CRYSTAL STRUCTURE BY ELECTRON DIFFRACTION. BY M. Han, Y. X. Cheng J. Q. Chen, Department of Materials Science and Engineering, Zhejiang University, Hangzhou, 310027, Y. R. Chen W. X. Liu, Analysis Center, Tianjin University, Tianjin, 300072, P. R. China.

To know the structure of crystal materials is important to investigate the mechanism of various phase transformations. In the general case, however, the determination processes are very difficult for unknown crystals. The principle of a new analysis method which could determine Bravais lattice of unknown crystals by means of three arbitary and different area-selected electron diffraction patterns is discribed in this paper. The intersections between two patterns are calculated and verified by computer. Considering two possible relationships, identical axis or different axes, a vector space corresponding a primitive cell of reciprocal lattice is built and reduced. By comparing the reduced result with Niggli reduced cells, the Bravais lattice type and parameters are finally determined. According to these main processes, a computer programme TEM has been already completed by C language. Applying this programme, a successful and convenient method to determine unknown crystal structure is realized. As an example, the structure of mullite has been determined.

02.05 – Diffuse Scattering

MS–02.05.01 MEASUREMENT AND INTERPRETATION OF X-RAY DIFFUSE SCATTERING FROM MACROMOLECULAR CRYSTALS, By D. S. Moss,* S. A. Butler, Birkbeck College, London, U.K., I. D. Glover, University of Keele, U.K., J. R. Helliwell, University of Manchester, U.K., and M. Adams, University of Oxford, U.K.

Crystals exhibit X-ray diffuse scattering when there is a temporary or permanent breakdown of space group symmetry. Such disorder is particularly prevalent in macromolecular crystals where the Bragg diffraction pattern may only extend to a limited resolution. The advent of area detectors, powerful X-ray sources such as synchrotrons, and high performance computing means that the measurement and interpretation of diffuse scattering from macromolecular crystals is now practicable.

We have modified conventional software for extracting Bragg reflections from scanned X-ray films so that diffuse intensities can be systematically measured.

From the diffuse intensities of 6-phosphogluconate dehydrogenase we have calculated vector correlation maps which show the direction and extent of correlated displacements within the crystals. They show highly anisotropic correlation extending up to about 30A.

We have also interpreted the diffuse scattering in terms of rigid body displacements of domains and secondary structural elements in proteins. We have shown that the diffuse scattering patterns cannot in general be uniquely determined by any one model of rigid body correlation.
Analysis of the components of diffuse scattering has shown that the so-called 'solvent ring' is due mainly to protein diffuse scattering (Acta Cryst. (1991) B47, 960-968).We have also measured the diffuse peaks under the Bragg reflections of ribonuclease-A and have shown that the profile is consistent with the one-phonon approximation.

MS–02.05.02 COMPUTATION OF DIFFUSE SCATTERING FROM SIMULATED DISORDERED CRYSTALS. By B. D. Butler*, Research School of Chemistry, Australian National University, Canberra A.C.T. 0200, Australia

A general computer program that can be used to efficiently calculate the diffuse diffraction intensities from large three dimensional (3D) simulated disordered crystals has been developed. The program is suited to crystals that contain both chemical *and displacement* disorder and was designed to be used with models that have an arbitrary number of distinct atomic species and disordered crystallographic sites per unit cell. The only restrictions on the simulation size are the available computer memory and CPU resources. Diffraction patterns from model systems containing several hundred thousand atoms have been successfully calculated with this program. It has been tested and used on several different computer architectures – ranging from desktop UNIX based workstations to the vector processing (Fujitsu VP2200) and parallel architecture (Thinking Machines CM5) supercomputers – and has been

