

analysis, has continued. Here the most significant development has been an assessment of the accuracy of powder methods (NBS 1980).

A consequence of the introduction of high intensity sources and position-sensitive detectors is the possibility of time-resolved diffraction. The potential of this technique has yet to be fully realised and it is a field in which important advances of the future may well occur, particularly in the study of phase transitions involving order-disorder phenomena.

For many years, until the late 1960s, workers with single crystals held sway; powder diffraction was almost a fringe interest pursued by a select group of devotees in a handful of laboratories. Now the situation has changed. Single-crystal methods are largely a matter of routine and have been eclipsed by the renaissance of powder diffraction.

ML.22-A INTERACTIVE COMPUTER GRAPHICS IN STRUCTURE

ANALYSIS. By W V Wright, IBM United Kingdom Ltd., UK Scientific Centre, Winchester, Hampshire, UK.

Molecular graphics, the application of interactive computer graphics to molecular studies, is established as a useful tool for studying the structure of biological molecules. Scientific results being obtained with these systems are rapidly repaying the investments made for their development. For research which involves the iterative refinement of Fourier synthesis maps, molecular graphics is indispensable.

Mechanical models have always played a central role in the study of molecular structure. The substitution of computer graphics for these began when Levinthal (Scientific American (1966) 214, 42) built a system for folding proteins. This goal proved too difficult, but several members of his group continued the work and developed successful systems for other phases of molecular research.

In 1972 Barry and North (Cold Springs Harbor Symposium on Quantitative Biology, 36, 577) identified the requirements for a system to build molecular models into electron density maps. Successful systems for this application began to emerge about three years later. These systems have also proved useful for molecular refinement, for comparing structures, and for packing studies. Experience indicates that the greatest power of molecular graphics lies in the user's freedom to move easily between the thinking and computational phases of his work.

The development of molecular graphics systems continues, and the area of application is expanding. One emerging use is in the study of the geometry and dynamics of enzyme-substrate interactions.

ML.22-B USE OF LATTICE IMAGING IN THE STUDY OF MINERALS. N. MORIMOTO, Department of Geology and Mineralogy, Faculty of Science, Kyoto University, Kyoto 606, Japan.

The electron microscopic studies of minerals made before 1970 were confined to very special minerals such as clay-like minerals. Since the high resolution imaging technique was first applied on minerals, only several years ago, there has been great progress in the use of transmission electron microscopy for the study of minerals. The appearance of commercial ion-thinning machine has improved mineral specimen preparation techniques for transmission electron microscopy. High quality lattice images have been obtained of mineral oxides, sulfides and many groups of rock-forming silicates. The imaging technique has proved indispensable in elucidating the local arrangement which may not be readily detected using x-ray diffraction alone, such as short-range order, antiphase domain structures, topological transformation, coherent intergrowth, polytypism and stacking disorder.

Current electron microscopic resolution is still insufficient for determining the exact atomic arrangement of minerals. However, the combination of the lattice imaging and x-ray diffraction methods has proved successful in determining the superstructures of the nonstoichiometric and solid solution minerals such as pyrrhotite and plagioclase. The use of in-situ x-ray microanalysis of small structurally characterized area (~30 nm) has offered further invaluable means in the study of minerals. The localized structural perturbation and superstructure in minerals can be used to understand the mechanisms of solid state reactions, and to reveal the past geological conditions in which the mineral was formed.

ML.24-A CRYSTALLOGRAPHIC ENGINEERING, By Robert E. Newnham, Materials Research Laboratory, Pennsylvania State University, University Park, Pennsylvania, U.S.A.

Crystallographic engineering—the design and construction of non-equilibrium crystal structures—is now a reality. Ion implantation, micro-machining, molecular beam epitaxy, and a host of other techniques developed by the semiconductor industry make it possible to devise miniaturized multiphase composites with a wide variety of connectivity patterns. Some examples of controlled structure-property relations involving the manipulation of conduction paths, mechanical stress configurations, and electric field distributions will be discussed, along with applications to acoustics, electronics, optics and medicine. Scaling down leads to new quantum phenomena and surprisingly large physical effects such as hot electron behavior and composite product-properties. Biological systems often serve as models for devices incorporating self-repair, memory, and membrane effects. Present and future goals for crystallographic engineers will be described.