ML.15-2 QUASIPERIODIC CRYSTALS. By Dan Shechtman, Department of Materials Engineering, Technion, Haifa, Israel.

Quasiperiodic crystals are a new class of aperiodic atomic structures which have δ-functions in their Fourier transform but non-crystallographic point symmetries. The mathematical background for the formation of Bragg diffraction from quasiperiodic structures have been well established long before the announcement of the Icosahedral phase, the first quasiperiodic crystal, in late 1984. It was this discovery and the realization that crystals can be quasiperiodic that started the larger international interdisciplinary scientific activity to study and understand the structure and properties of quasicrystals. It is by now well established that crystals can have quasiperiodic order in addition to the periodic one. Also, it has been found that a large number of metallic systems form the icosahedral phase, and in some cases the decagonal phase (another quasiperiodic phase). The techniques to produce quasicrystalline phases include now among others rapid solidification, thin film deposition, single crystal growth from the melt and a large variety of properties have been theoretically predicted and experimentally measured. The crystallography of this new class of materials is probably the most intriguing property, and electron microscopy as well as X-rays and neutron diffraction play complementary roles in deciphering the code of its local atomic structure.

ML.17-1 LATTICE DEFECTS STUDIED BY HIGH RESOLUTION ELECTRON MICROSCOPY. BY M. Hirabayashi, The Research Institute for Iron, Steel and Other Metals (Renamed Institute for Materials Research), Tohoku University, Sendai 980, Japan.

The continual progress in the spatial resolution of electron microscopes is improving the reliability and accuracy of detail in the atomic scale structure investigations, and high resolution electron microscopy (HREM) is extending its applications to wide areas of solid state science. In surface science, as an example, dynamic motion of atoms in surface processes as well as static steps of monoatomic height are revealed by means of HREM. In-situ HREM observations of dynamic behavour at the atomic level are opening up unique applications in materials science.

Here we shall deal mostly with three subjects; (1) lattice fringe observations at elevated temperatures, (2) modulated block structures induced by shock wave, and (3) defects in quasicrystal structure.

(1) Combining with a video-recording system, lattice fringe imaging is utilized to investigate dynamic formation and growth processes of the one-dimensional long period antiphase structure of CuAuII at elevated temperatures. The growth of CuAuII occurs apparently like drawing of a maze pattern of the lattice fringes which correspond to the periodic antiphase boundaries with the spacing of 2nm. In-situ lattice fringe observations are also applied to the study of an incommensurate-commensurate phase transition of the one-dimensional long period antiphase structure of Ag_3Mg. Discommensuration lines disappear gradually with annealing time in forming the commensurate structure.

(2) Recently Kukuchi et al. (Jpn. J. Appl. Phys., 1985, 24, 1600) found by HREM that complete conversion of single crystal H-Nb_2O_5 (monoclinic) to single crystal T-Nb_2O_5 (orthorhombic) occurs under shock wave pressure in the range of 20-40 GPa. When single-crystal H-Nb_2O_5 is shocked perpendicular to the b-axis, a modulated structure is formed besides T-Nb_2O_5. This structure is a two-dimensionally disordered H-Nb_2O_5, which is probably realized in the shock-released process from T-Nb_2O_5. The high resolution image shows a bundle-like pattern consisting of various sizes of the columnar blocks of which the orientation is completely random keeping the longer or shorter edge of individual blocks apparently either parallel or perpendicular to each other.

(3) HREM may be only the way to elucidate structures of the quasicrystal with icosahedral symmetry found in the rapidly solidified alloys. The observed images are interpreted well with the projection of three-dimensional Penrose tiling with long-range quasiperiodic translational order (Hiraga, K. et al., J. Microscopy, 1987, in press). Deviations from the basic structure occur frequently in the quenched alloys. Lattice defects observed in the icosahedral quasicrystal are explained in terms of frozen phason strain and dislocation. Recovery processes to a stable crystalline phase are investigated by HREM. The appearance of two-dimensional quasicrystal having decagonal symmetry and of structure modulations associated with the quasicrystal to crystal transition will be discussed in some detail.

ML.17-2 THE STRUCTURE OF A BACTERIAL PHOTO-SYNTHETIC REACTION CENTER. By J. Deisenhofer and H. Michel, Max-Planck-Institut für Biochemie, Martinsried, FRG

The first step in photosynthesis is the absorption of a light quantum, followed by the transfer of an electron across a cell membrane. This light driven charge separation happens with high speed and a quantum efficiency of near unity within a membrane-bound complex of proteins and pigments, the photosynthetic reaction center (RC).
The RC from the purple bacterium *Rhodopseudomonas viridis* was one of the first membrane proteins for which well ordered 3-D crystals were obtained (Michel, J. Mol. Biol., 1982, 158, 567-572). The X-ray structure analysis of these crystals allowed the construction of an atomic model including the RC's protein subunits L, M, H, and cytochrome, and 4 bacteriochlorophyll-b (BChl-b), 2 bacteriopheophytin-b (BPh-b), 1 menaquinone, 1 non-heme iron, and 4 heme groups (Deisenhofer, Epp, Miki, Huber, and Michel, J. Mol. Biol., 1984, 180, 385-398; Deisenhofer, Epp, Miki, Huber, and Michel, Nature, 1985 318, 618-624; Michel, Epp, and Deisenhofer, EMBO J., 1986. 5, 2445-2451). BChl-bs, BPh-bs, non-heme iron, and quinone are associated with the subunits L and M in the central part of the RC complex. The arrangement of the pyrrole ring systems of the BChl-bs and BPh-bs shows approximate twofold symmetry. Near the symmetry axis two BChl-bs are in close contact and form the "special pair", the primary electron donor of the photosynthetic charge separation process. From the "special pair" two branches of pigments extend

through the membrane; however, only one of them is used for electron transfer. The folding of the subunits L and M is very similar with five membrane-spanning helices per subunit as the outstanding feature. The aminoterminal segment of the subunit H is folded into a membrane-spanning helix; the remainder of the subunit forms a globular domain which is bound to the cytoplasmic side of the L-M complex. The cytochrome subunit is attached to the L-M complex at the periplasmic side of the membrane and contains the four heme groups in a linear arrangement. This atomic model provides insight into the architecture of membrane proteins, and can serve as a basis for the explanation of functional properties of the RC.

ML.18-1 COMPUTER GRAPHICS IN STRUCTURE ANALYSIS. By T.A. Jones, Dept. of Molecular Biology, BMC, Box 590, S751-24 Uppsala Sweden.

Computer graphics allows one to present complex three dimensional data such that it can be more easily absorbed by the viewer. This data is often merely illustrative, or is constructed with the aim of allowing the viewer to make some kind of decision. The term "computer graphics" covers a multitude of equipment whose power varies by 5 orders of magnitude and of applications ranging from illustrating the results of a crystallographic investigation to designing a protein mutagenesis experiment.
My primary interest has been concerned with the protein crystallographers' problems first to construct a model then to improve it during refinement (Jones, 1978, J. Appl. Cryst. 11, 268-272). Our recent work (Jones and Thirup, 1986, 5, 812-822) was made possible by hardware developments resulting in affordable 32 bit computers and high performance colour displays. This work makes use of a skeletal representation of electron density (Greer, 1974, J. Mol. Biol. 82, 279-302) to present a much larger volume and colour to represent possible folding hypotheses. Taken together this helps the initial map interpretation. This aspect of the implementation has similarities to the Grinch system developed at the University of North Carolina. However, our skeleton can then be used as a framework to locate the best matching fragments from a data base of well refined proteins. Alternatively the fragments may be chosen from 170 five residue building blocks which are the result of a cluster analysis study (Jones and Levitt, in preparation). This technique Proleg, (PROtein LEGo) has affected our general attitude to molecular modelling which then becomes a problem of picking the best fragment to fit our observations (crystallographic, NMR or structurally related proteins).
Our future developments are aimed at a networked environment of work stations (of various capabilities) with cpu and data base servers. One of our goals is to produce a real space fitted protein model (Diamond, 1971, Acta Cryst. A27 436-452; Jones and Liljas, 1984, Acta Cryst. A40, 50-57) without manual intervention and to locate and correct the majority of conformational errors during refinement.

ML.18-2 X-RAY CHARACTERISATION OF SUPERLATTICES AND EPITAXIAL LAYERS. By M. Sauvage-Simkin, Laboratoire de Minéralogie-Cristallographie, F-75252, Paris-Cedex 05, and LURE, Bât. 209D, UPS, F-91405 Orsay.

Since about ten years, multilayer stacking of semiconducting materials has become a fundamental step in optoelectronic and hyperfrequency device elaboration. Molecular Beam epitaxy and Metal Organic Vapor Phase Epitaxy, both allow the preparation of tailored ultra-thin layer heterostructures. However, a perfect control and reproducibility of the individual layer thickness and composition, in the case of semiconductor alloys, cannot be guaranteed. Post-growth assessment of the actual heterostructure parameters is then still needed to predict or interprete the multilayer system optical and transport properties.

It is now well recognized that X-ray imaging and diffractometric methods are mostly suitable for this purpose, being non-destructive and accurate enough to provide the searched information. A review of the experimental and theoretical work performed in the various laboratories involved in the field will be presented and it is worth mentioning that among these, several are industrial research centers.

In order to fully characterise a heterostructure, the two approaches mentionned above should be combined :
X-RAY IMAGING : standard Lang topography in the transmission or reflexion geometries, Synchrotron Radiation (SR) White Beam or Plane-Wave topography are used to detect extended interface defects such as misfit dislocations and to qualify the lateral homogeneity of the sample. For example, SR topography on high order satellite reflexions enable to reveal lateral gradients in both the composition and period for superlattices.