14.X-01 HIGH RESOLUTION ELECTRON MICROSCOPY OF DISORDERED CRYSTALS. By Sumio Iijima, Center for Solid State Science, Arizona State University, Tempe, Arizona USA.

The high resolution electron microscope (HREM) can provide information on crystals in both reciprocal and direct space, and enables us to correlate between them directly. The technique therefore is suitable for investigation of two types of problems in crystal structure analysis which are associated with planar faults: (1) disordered states of crystals showing diffuse scattering in their diffraction patterns and (2) incommensurate phases of crystals.
As an example for the case of (1), a structure of sheet silicate mineral, manganpyrosmalite, will be considered. The structure and its related ones have been described previously as rhombohedral. Diffraction patterns {hk0} of this crystal show strongly diffused streaks parallel to c* due to stacking disorder on the basal planes. Examination of electron diffraction patterns and HREM images of many small local areas of the crystal disclosed a monoclinic structure. It was found that what appeared to be trigonal symmetry according to the diffraction data would have been simulated by frequent twinning and stacking disorder on the basal planes. For the case of (2), the HREM images of incommensurate lattice found in a hexagonal tungsten bronze, K_xWO_3 (Bando & Iijima, in this conference) and also 1T-TaS_2 will be discussed. In the former, its incommensuration results from the ordering of K ions in the WO_3 matrix lattice which would be distorted slightly. Purely displacive rearrangement of atoms results in incommensurate superlattices of TaS_2. In both instances, conventional HREM images of thin crystals fail to reveal the superstructures. However HREM images of thicker crystals where dynamical diffraction effects become significant were found to be useful for this purpose.

14.X-02 STRUCTURE ANALYSIS OF INORGANIC CRYSTALS BY HIGH-RESOLUTION ELECTRON MICROSCOPY. By L.A. Bursill, School of Physics, University of Melbourne, Parkville, 3052, Vic., AUSTRALIA.

Comparison of experimental and computer simulated images of crystal structures and of defects in crystals, provides a useful technique for the determination of structure in favorable cases.

In this paper criteria are developed which help to define the areas where the technique is most valuable. The validity of computer simulation techniques, including both the scattering theory and the treatment of instrumental electron optical parameters is first considered. Next the types of information available which are either complementary to that offered by neutron and X-ray diffraction, or which cannot, for fundamental reasons, be obtained by the other diffraction techniques, are then defined.

Such criteria will be illustrated by practical applications of the technique to study of new hollandite-related materials, rutile-type structures of SnO_2 and TiO_2, twinning and ferroelectric domains in $LiTaO_3$, framework structure and cation-ordering in zeolites, the study of voidites and platelets in diamond and the observation of heavy cations in apparently amorphous silicates.

14.X-03 REAL STRUCTURE OF ALLOYS STUDIED BY HIGH-VOLTAGE, HIGH-RESOLUTION ELECTRON MICROSCOPY. By M. Hirabayashi, K. Hiraga and D. Shindo, The Research Institute for Iron, Steel and Other Metals, Tohoku University, Sendai, Japan.

Taking advantage of the high spatial resolution, high voltage electron microscopy has been used for direct imaging of atoms in alloy crystals. High-voltage, high-resolution electron microscopy (HVHREM) is most useful in the study of real structures which cannot be determined by other indirect methods.

The direct determination of complicated structure was carried out on binary ordered alloys of Au-Cd, -Mn and others by using a 1 MV electron microscope. The high resolution images formed by a number of diffracted beams exhibit regular alignments of bright or dark spots corresponding to the solute atom-positions projected parallel to the incident beam direction. From the observed images, we may propose a structure model with the aid of computer simulation based on the many-beam dynamical diffraction theory.

The crystal structure of an alloy $Au_{31}Mn_9$ was directly proposed from the observation by HVHREM (Hiraga et al., Acta Cryst. B36 (1980) 2550). The one-to-one correspondence between the bright or dark spots in the observation and the Mn atom positions in the calculation is obtained, supporting the validity of the proposed model. The superstructure of $Au_{31}Mn_9$ is tetragonal (space group P4/m), and the cell dimension is $A = \sqrt{10}a$ and $C = a$ where $a = 4.0$ Å is the lattice constant of the fundamental fcc cell. The images of HVHREM which are interpretable in terms of the atomic arrangement in the superstructure are observed for the alloy foils as thick as several hundred Å, being named superstructure images. From the many-beam dynamical diffraction calculation, it turns out that the kinematical relationships are approximately held among some of the superlattice reflections which contribute dominantly to the superstructure images. The image contrast of atom-positions changes from bright to dark and vice versa depending on film thickness and defocus.

The superstructure images allow us to propose the atomic configurations in imperfectly ordered alloys as well as perfectly ordered ones. Valuable information is provided on the local randomness and the antiphase-domain boundaries. In the imperfectly ordered alloys, the substitution of wrong atoms to right atoms is estimated from the variation of brightness of the spots. Concentration density waves are seen as periodic changes in the image contrast. As to the antiphase domain structures, the mixing fashion of domains is observed in the atomic level, and the incommensurate periods are interpreted from the observed images.

The structural defect in intermetallic compounds is another interesting subject for the study of HVHREM. An example is the planar defect in the so-called tetrahedrally close-packed Frank-Kasper structures in alloy systems of transition metals. The defect structure is analyzed by observing the distribution of bright or dark dots which correspond to the coordination polyhedra rather than the atoms.