14.X-9 SIMULATING AN ELECTRON IMAGE AT HIGH RESOLUTION. By D. Van Dyck and W. Coene, University of Antwerp, RUCA, Groenenborgerlaan 171, B-2020 Antwerp, Belgium.

It is now quite well established that the interpretation of high resolution electron micrographs is more reliable if the experimental images are compared with computer simulations for plausible trial structures. Today most of the HREM laboratories have their own image simulation programs. However, as opposed to the gradual improvement in the resolution of the electron microscopes during the last decade, the simulation technique did not follow the same evolution. It is sometimes more used as a gadget than a tool and is seldom convincing. The comparison between experimental and simulated images is often done visually and the reliability of the simulation is restricted to thin objects. The situation bears some resemblance with the early days of X-ray diffraction when the power of the technique was recognised but the application were limited by interpretation problems. In this work the state of the art is critically surveyed. Some recent developments for increasing the speed of the calculation are examined such as the real-space method and the atom colum approximation. The reason for the unreliability of the simulation technique for thicker crystals is discussed in terms of effects that are not properly accounted for, such as absorption, inelastic scattering, upper layer line effects, thermal atom motion, beam convergence, etc. and some prospects are given for the future. A discussion is devoted to some particular systems for which the image characteristics can be interpreted without the need for simulation. A method is proposed in which two images taken with somewhat different imaging parameters (beam convergence e.a.) are substracted so as to reveal high resolution details that otherwise remain hidden in the images. The possibilities are discussed of a direct method (to compare with the direct methods of X-ray crystallography). A method is presented which allows to restore the wave function at the exit face of the object in a direct way without using a recursive scheme hereby eliminating the influence of the electron microscope and using every bit of information in the images over a relatively large focal range. Then the possibility is investigated for a retrieval of the object structure starting from the wave function at its exit face. Finally some speculations are presented about the "ideal" experimental set-up for the future and the ultimate resolution of the technique.

14.X-10 STRUCTURE DETERMINATION OF APERIODIC OBJECTS BY HIGH-RESOLUTION ELECTRON MICROSCOPY. By L.A.BURSILL, School of Physics, University of Melbourne, Parkville, 3052, Victoria, Australia.

The validity of structures deduced by use of high-resolution electron micrographs and computer-simulation techniques is discussed. Some advantages and limitations, as experienced presently, will be pointed out through illustration of a number of such studies. These may include (i) structure of isolated defects in transition metal oxides and semiconductors (including both small and extended defects); (ii) structure of incommensurate super-lattices in ferroelectric materials; (iii) structure of quasicrystalline alloys and (iv) structure and polarity of the surface of alumina (ruby and sapphire).

14.1-1 BLOCH WAVE DEGENERACIES AND NON-SYSTEMATIC CRITICAL EFFECTS IN CONVERGENT BEAM ELECTRON DIFFRACTION By J. Gjønnes and H. Matsuhata, Department of Ohysics, University of Oslo, Norway.

The systematic critical voltage (Watanabe, Uyeda & Kogiso, Acta Cryst. 1968, A24, 249) may be the most sensitive effect used for structure factor determination by dynamical electron diffraction. But its application is limited, since only a few low order reflections can be obtained, through determination of magnitudes of the type V_h^2/V_{2h} - to an accuracy of a few tenths of per cent.

The scope can be increased considerably by exploiting similar effects, i.e. accidental Bloch wave degeneracies in non-systematic cases (Gjønnes & Høier, Acta Cryst. 1972, A27, 313). The use of convergent beam patterns (instead of Kikuchi lines) and the flexibility offered by the continous voltage variation make modern intermediate voltage microscopes well suited for such measurements.

Mathematical procedures for determining the condition for such degeneracies have been extended to cover four and multiple beam cases. These are applied to a search for such cases in FCC, BCC, diamond, NaCl- and ZnS-type structures. Experimentally they are revealed in CBED disks as distinct features which are characterized by diffraction condition, i.e. position within the disk, and accelerating voltage.

Experimental patterns from different substances: Si, GaAs, ZnS, MgO are evaluated. In favourable cases sensitivity comparable with the systematic case can be obtained. Absorption effects are discussed.