14.1-04 THE TREATMENT OF INCLINED ILLUMINATION ON THE MULTISLICE METHOD. By K. Ishizuka, Department of Physics, Arizona State University, Tempe, Arizona. (On leave from Institute for Chemical Research, Kyoto University, Uji, Kyoto, Japan).

In the multislice method for calculating dynamical electron diffraction effects, the propagation function is usually used in the reciprocal space form (Goodman and Moodie, Acta Cryst (1974) A30, 280; Ishizuka and Uyeda, Acta Cryst (1977) A33, 740).

It was shown that the form of the reciprocal space propagation function is directly related to the excitation error when we take into account the boundary condition on an entrance surface. A generally valid form for the excitation error is applied to the inclined incidence of electrons such as occurs for tilted illumination and for convergent beam illumination. The parabolic approximation for the propagation function and the excitation error gives serious intensity differences especially for higher order reflections when the tilting angle becomes large.

14.1-05 SPACE GROUP AND STRUCTURE DETERMINATION OF $BaNd_2Ti_3O_{10}$ USING CBED AND HREM.

By A. Olsen[1], P. Goodman[2] and R.S. Roth[3], 1) Institute of Physics, University of Oslo, P.O.Box 1048, Oslo 3, Norway, 2) CSIRO, Division of Chemical Physics, P.O. Box 160, Clayton, Victoria, Australia 3168, 3) National Bureau of Standards, Washington, D.C. 20234, USA.

The crystal structure of $BaNd_2Ti_3O_{10}$ has been determined by combining high-resolution electron microscopy (HREM) and convergent beam electron diffraction (CBED). The structure has an orthorhombic pseudosymmetry Cmcm with lattice parameters: a_{ort}= 3.866 Å, b_{ort}= 28.16 Å, c_{ort}= 7.67 Å.

However, due to the small Nd^{3+} cations the Ti-octahedra are tilted and the structure is actually monoclinic. The relation between the monoclinic and orthorhombic lattice vectors are: $\underline{a}_m = 2\underline{a}_{ort}$, $\underline{b}_m = \frac{1}{2}(\underline{a}_{ort} + \underline{b}_{ort})$, $\underline{c}_m = \underline{c}_{ort}$.

The selected area electron diffraction patterns indicate either the space group $P2_1/m$ or Pm. The weak superlattice reflections generated by the oxygen displacements could not be examined directly with the normal CBED technique, because these reflections were lost beneath a high inelastic background. However, the CBED $[010]_{ort}$ zone-axis patterns, while only showing sublattice orders directly, showed an influence from the superlattice structure in the detailed intensity distributions from the strong reflections. From these details the space group of the $BaNd_2Ti_3O_{10}$ structure could be determined as Pm.

14.1-06 ELECTRON DIFFRACTION FROM VERY SMALL REGIONS OF CRYSTALS. By J. M. Cowley, Department of Physics, Arizona State University, Tempe, Arizona, USA

In a scanning transmission electron microscope using a field emission gun it is possible to obtain convergent beam diffraction patterns from regions of the specimen of diameter as small as 5Å. These can be recorded in a fraction of a second with a suitable two dimensional detector system. Because the incident convergent beam is almost perfectly coherent, the diffraction pattern intensities are sensitive to the relative phases of the diffracted beam amplitudes and many new diffraction effects are observed.

When the diameter of the main intensity maximum of the beam incident on a thin crystal specimen is smaller than the unit cell dimensions, the diffraction pattern intensities vary as the beam is moved within the unit cell. This may provide information concerning the structure and symmetry of localized atom configurations.

Diffraction patterns obtained from metal particles 20-30Å diameter show evidence of their multiply twinned structure. In such patterns any discontinuity of the structure, such as a crystal edge, gives rise to a splitting of the diffraction spots depending on the position of the discontinuity relative to the beam axis. Effects due to the potential fields at crystal surfaces are also clearly seen and can be used in conjunction with energy loss spectroscopy to investigate surface properties.

14.2-01 LEED STUDIES OF LEAD LAYERS ON COPPER (100). W. Hoesler, W. Moritz and D. Wolf, Institut für Kristallographie und Mineralogie der Universität München, München, BRD.

During the deposition of lead on copper (100) several different coverage-dependent superstructures can be observed. Two ordered superstructures are determined by comparing LEED intensity measurements with dynamical calculations.

At a well defined coverage of 0.5 an ordered c(2×2) superstructure has been discovered. By increasing the coverage to 0.6 , this structure transforms to the known $c(5\sqrt{2}\times\sqrt{2})$ R 45° structure (J. Henrion et al., Surf. Sci. 29 (1972) 20). Intensity versus energy measurements for 9, respectively 23, symmetrically non-equivalent beams have been compared with several structure models. The c(2×2) structure is formed by lead atoms adsorbed in the hollow sites of the (100) face. The layer spacing is approximately 2.4 Å and the Cu-Pb distance is 3.0 Å, which corresponds to nearly the sum of both metallic radii. Coverage and symmetry permit two models for the $c(5\sqrt{2}\times\sqrt{2})$ R 45° structure, a distorted hexagonal lead overlayer and a regular arrangement of compressed c(2×2) domains. Comparison with dynamical calculations have been done for both models, final results will be presented at the Conference.

Additional investigations have been performed to study the influence of random adsorbed atoms on intensity versus energy profiles. A lead coverage of 0.08 produces well observable changes in intensity profiles compared to that of clean copper. The changes in intensity profiles are in good agreement with dynamical calculations (W. Moritz, in: Surface Structure by LEED, Plenum Press 1981, in print).