

14.X-4 ELECTRON DIFFRACTION PHENOMENA FOR VERY LOW ENERGY ELECTRONS. By D.F. Lynch, CSIRO Division of Materials Science and Technology, Norraanby Rd., Clayton, Victoria 3168, Australia and A.E. Smith, Department of Physics, Monash University, Clayton, Victoria 3168, Australia.

For most simple crystals of small unit cell size, i.e., axes about 5 Å, and for incident electron energies less than 15 eV, there exists only the specularly reflected beam and the incident beam outside the crystal. Thus, for simple arguments, the Ewald sphere only intersects one rod and so the observed intensity is influenced by the structure in the crystal in the direction of the surface normal (the (001) reflections). This simple argument is not supported by experimental result. In practice the effect of the inner potential ensures that the Ewald sphere can intersect other reciprocal lattice rods. The strong dynamic coupling that occurs in low energy electron diffraction ensures that the observed variation of the intensity of the reflected electron beam is strongly dependent on the intersections of the Ewald sphere with these other rods.

The structure observed in the CID experiment of B.H. Nall, A.N. Jette and C.B. Bergeron (1982, Phys. Rev. Letters, **49**, 882) is a graphic demonstration of this phenomenon. In the CID experiment the incident electron energy is kept constant and the reflected intensity, as measured by the specimen current, is displayed as a function of angle of incidence.

Calculations using dynamic theory (A.E. Smith and D.F. Lynch, 1985, Surf. Sci., **164**, 464-478) show quite good agreement with the reported experiments on Al when the incident energy is very small. Further measurements and calculations have been done for MoS₂ (A.E. Smith and D.F. Lynch, 1986, Surf. Sci. to be published). These also show good agreement as can be seen in Figs 1 and 2.

It is probable that this phenomenon is also of some importance in the interpretation of the contrast observed in the scanning tunnelling microscope, although, in that case, the problem must be considered in terms of a coherent spherical wave source.

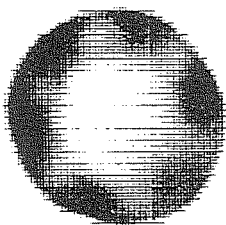


Fig.1 CID pattern from MoS₂. Incident energy 5eV.

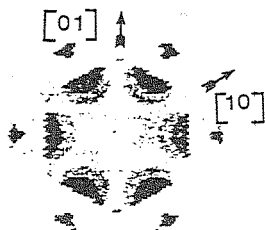


Fig.2 Calculated CID pattern for MoS₂. Incident energy 5eV.

14.X-5 RECENT EXAMINATIONS OF THE N-BEAM-DYNAMICAL METHOD IN MATERIALS ANALYSIS. By S. Amelynckx and D. Van Dijk, RUCA (University of Antwerp), 2018-Antwerpen, Belgium.

14.X-6 SURFACE STRUCTURE ANALYSIS OF Si(111)7x7-H BY RHEED. By S. Mizuno, A. Ichimiya, T. Fujii and K. Yamauchi, Department of Applied Physics, Nagoya University, Nagoya 464, Japan.

Rocking curves of RHEED intensities from Si(111)7x7-H surface were analyzed by a many-beam RHEED dynamical calculation (Ichimiya, Jpn. J. Appl. Phys., 1983, **22**, 176-180, and *ibid.*, 1985, **24**, 1365). Si(111)7x7 surface was exposed to hydrogen atoms, which were dissociated on a hot tungsten filament in pure hydrogen atmosphere. A RHEED pattern from Si(111)7x7-H surface is shown in Fig.1 in the [11 $\bar{2}$] direction of the incidence. The electron energy was 10 keV. The RHEED intensities were measured by a TV-camera with a micro computer system. The RHEED rocking curves on 00-rod (specular reflection) and 11-rod were compared with calculated rocking curves for two models of the surface structure based on the Dimer-Adatom-Stacking-fault (DAS) model (Takayanagi, Tanishiro, Takahashi and Takahashi, Surface Sci., 1985, **164**, 367-392) from the intensity distribution of the RHEED pattern in Fig.1: Model (a) shown in Fig.2a is Dimer-Stacking-fault (DS) model with twelve Si-H₂ molecules at random on-top sites and model (b) shown in Fig.2b DS model with hydrogen at on-top sites. Results of the calculations for the both models are shown in Figs.3 and 4 with the experimental results for 00- and 11-rods in the [11 $\bar{2}$] direction. The results for the model (a) are in very good agreements with the experimental rocking curves. For the [011] direction calculated rocking curves for the model (a) were also in good agreements with the experimental ones. It is considered that Si-Si bonds of the adatoms of the DAS structure are broken by hydrogen adsorption and SiH₂ is formed on the random on-top sites of the stacking-fault layer. No agreements between experimental and calculated results were obtained by breaking of the dimer bonds.

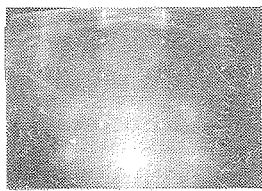


Fig. 1 RHEED pattern from Si(111)7x7-H in the [112] direction of the incidence.

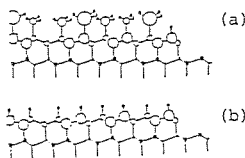


Fig. 2 Side views of Si(111) 7x7-H surface models. (a) SiH₃ at random on-top sites. (b) H at the on-top sites.

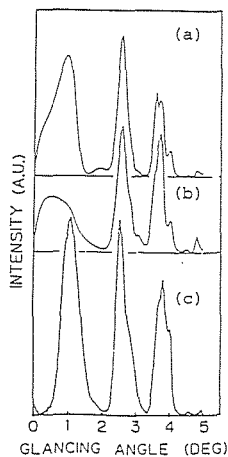


Fig. 3 00-rod rocking curves. (a) 5-beam calculation for the model(a). (b) The calculation for the model(b). (c) Experimental curve.

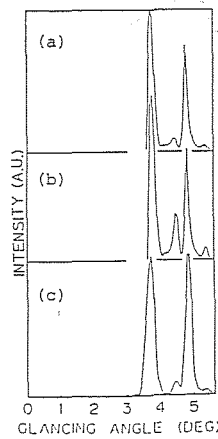


Fig. 4 11-rod rocking curves. (a) 5-beam calculation for the model(a). (b) The calculation for the model(b). (c) Experimental curve.

14.X-7 EXPLOITING DYNAMICAL HIGH ENERGY ELECTRON DIFFRACTION EFFECTS. By C.J. Humphreys and D.J. Eaglesham, Department of Materials Science and Engineering, University of Liverpool, P.O. Box 147, Liverpool, L69 3BX, U.K.

By exploiting dynamical high energy electron diffraction effects we can gain new insights into the structure of materials on an atomic scale. For example, conventional methods of microanalysis (e.g. Auger, EDX) often do not have the spatial resolution required for measuring composition changes in, say, quantum well structures. Microanalysis may, however, be performed using convergent beam electron diffraction (CBED) with a spatial resolution of the incident beam probe diameter, broadened only by elastic beam spreading (Eaglesham and Humphreys, Proc. XIth Int. Cong. on Electron Microscopy, Kyoto, 1986, 209). This technique utilises the fact that different fast electron Bloch wave states in a crystal are localised on different atomic strings (i.e. columns of atoms) for appropriate orientations of the incident electron beam. The wave vectors of these Bloch waves appear as different lines in higher order Laue zones of CBED patterns. Hence the separations of the lines are a direct measure of the potential of the atom strings, and hence the composition.

Similar exploitation of dynamical diffraction is utilised in ALCHEMI (Spence and Taftø) for atomic site location, the critical voltage effect for electron bonding location, and two-dimensional critical voltage effects for structure determination (Steeds and Vincent).

14.X-8 IMAGE DECONVOLUTION FOR PERFECT CRYSTAL IMAGES. By F.H.Li, Institute of Physics, Academia Sinica, Beijing, China.

High resolution electron microscopy is useful for determining structures of minute crystals. The disadvantage is in the close dependence of image contrast on defocus condition and specimen thickness. Even for weak phase objects the image intensity is expressed as a convolution of projected potential distribution function (PPDF) with the Fourier transform of contrast transfer function. To combine images from a through focus series is valid to obtain the so-called deconvoluted image where the phase shift of diffracted waves caused by the contrast transfer function is compensated (D.L. Misell and P.A. Child, J. Phys. D., 1972, 5, 1760; E.J. Kirkland and B.M. Siegel, Ultramicroscopy, 1984, 15, 151; E.J. Kirkland, B.M. Siegel, N. Uyeda and Y. Fujiyoshi, Ultramicroscopy, 1985, 17, 87; W.O. Saxton, Proc. 11th Intern. Congr. on Electron Microscopy, 1986, Post deadline paper one). For some specimens, especially most of organic materials, it is not allowed to record enough images with different defocus values for image deconvolution. Another problem is to tell the structure image from a series of micrographs taken under different imaging condition when the average structure of the examined crystal is still under determination. Hence, it is of interest to study how to restore the intuitive structure information from a single image of any defocus condition (N. Uyeda and K. Ishizuka, Proc. 8th Intern. Congr. on Electron Microscopy, 1974, Vol. 1, 322; F.H. Li and H.F. Fan, Acta Physica Sinica, 1979, 23, 276). It has been shown that for weak phase objects the image deconvolution can be made by use of the direct method well developed in X-ray crystallography on the basis of a combination of informations contained in a single electron micrograph and its corresponding electron diffraction pattern (F.S. Han, H.F. Fan and F.H. Li, Acta Cryst., 1986, A42, 353). In practice, crystal examined under a high resolution electron microscope are thicker than a weak phase object and generally can be treated as a pseudo weak phase object (F.H. Li and D. Tang, Acta Cryst., 1985, A41, 376). Its image intensity at the optimum defocus condition would be linear to a modified projected potential distribution function (MPPDF) depending upon the crystal thickness. Below a critical crystal thickness which depends on the heaviest atoms in the crystal and the electron wave length the MPPDF has its peaks at the same position as the PPDF and peak heights monotonically relate to those of the PPDF. Above the critical thickness the MPPDF would have negative peaks at the position of relative heavier atoms so that it would be no more similar to the PPDF (F.H. Li and D. Tang, Acta Cryst., A41, 376). This gives a possibility of reconstructing an image of any defocus value for pseudo weak phase objects to the optimum defocus one. A method of image deconvolution based on a single electron micrograph and its corresponding electron diffraction pattern has been proposed. The test result for simulated images of chlorinated-copper phthalocyanine with different crystal thickness and different defocus value is shown (D. Tang and F.H. Li, to be published).