11. Surfaces, Interfaces and Thin Films

11.01 – Surface/Interface Structures

MS-11.01.01 3D SURFACE STRUCTURE DETERMINATION BY X-RAY DIFFRACTION. By R.G. van Slilfhout, EML, c/o DESY, Hamburg, Germany.

For many years X-ray diffraction has been a standard technique to determine the atomic structure of bulk crystals. Its application to the study of surfaces is more recent and became possible with the availability of synchrotron radiation sources. The object of our small-angle X-ray diffraction work performed so far was to figure out the in-plane (2D) structure of surfaces using a grazing incidence geometry.

A new development is to include measurements along crystal truncation rods (CTR's) in the analysis. The integration of crystallography with CTR analysis enables a full 3D structural determination.

We review the basic principles of CTR analysis, 3D structural determinations and show examples of recent accomplishments in the field. CTR measurements to the epitaxial silicon and semiconductor surfaces, which have been studied intensively.

MS-11.01.02 STRUCTURE DETERMINATION OF THE 3x3 SUPERSTRUCTURE OF THE (111)-SURFACE OF 40B BY THREE DIMENSIONAL X-RAY DATA. By J. Weyer, H.H. Meyerheim, V. Jahn, W. Monz and H. Scholz, Institut für Kristallographie, Universität München, Theresienstr. 41, 8000 Munich, Germany.

Several attempts have been made to solve this structure by two-dimensional in-plane data, including our group. To now all attempts were successles. We combined now the in-plane data with the intensities along of the superstructure reflections perpendicular to the surface. We used these data for the first time to calculate a so called periodic-nonperiodic Patterson function. The structure could be solved by interpretation of a section through this Patterson-density at w=0. This density showed main features which did not appear in the Patterson density calculated with the in-plane data only which represents a projection of the three dimensioned Patterson-density on the (uv) plane. This demonstrates clearly, that the whole three-dimensional information is needed for solving more complicated surface structures. The structure refinements gave an excellent weighted R-value of 3.2% and a GOF of 1.3. The InSb(111) surface was prepared in UHV by Ar+ ion bombardment and annealing at 673 K for ca. 1 h and subsequent slow cooling to room temperature at about 2K/min. X-ray measurements were performed at the wiggler beam line at HASYLAB (Hambrg, Germany) and in the laboratory using a rotating anode source. An incidence angle of 0.7° was chosen. The maximum X-ray exit angle was 69° which allowed to measure reflections up to 1 = 7.2. The angular resolution was limited by Soller slits to 0.4° in-plane and 0.8° out of plane. The sample size was 12x8 mm². The data set consisted of 24 superstructure lattice rods measured in steps of 1 = 0.4. A total of 2816 inplane-independent reflections were used. The inplane data set consisted of 27 reflections. All vacancy and trimer models which had been proposed for the (111) surfaces of compound semiconductors can be ruled out. Additionally all models based on relaxations and models preserving the 3mm symmetry of the unconstructed surface could be ruled out as well. This is in agreement with recent STM measurements which showed the existence of two types of rings of atoms above the top layer, one type of elliptic shape occurs with three orientations and a second type of ellipsoidal shape occurs with two orientations. The final surface model exhibits similarities to the model derived recently for the (19x19) reconstruction of the GaAs(111) surface from STM measurements.

These two types of atom rings are arranged above the top layer such that each ring saturates 5 dangling bonds. The rings are centered around an Sb atom.

The surface undergoes a reversible phase transition at about 400K. No hysteresis could be detected indicating an order-disorder transition. However, the possible existence of an ordered high temperature phase cannot be ruled out because only the disappearance of the reflections in [40°] direction could be measured.

References

MS-11.01.03 IN-PLANE STRUCTURE OF Si(111):As–1x1 SURFACE STUDIED BY GLAZING-ANGLE X-RAY STANDING-WAVE MEASUREMENTS. By Osaani Sakata and Kihou Hashizume, Res. Lab. of Engineering Materials, Tokyo Institute of Technology, Nagatsuta, Midori, Yokohama 227, Japan.

Arsenic deposition on clean Si(111) surface removes the 7x7 reconstruction on give a simple 1x1 LEED pattern. There is a great deal of data supporting As atoms substituting for the top half of the silicon (111) double plane to terminate the surface with a nonreactive three-atom orbital. X-ray standing-wave (XSW) work (Patel, Golovchenko et al., Phys. Rev. B 1987, 36, 7179) shows As atoms lying at 0.17 A above the unrelaxed bulk terminated (111) top-layer Si atoms with a nearly perfect crystalline order in the vertical direction, but ion scattering data suggests some disorder in the Si(111)As–1x1 surface structure (Cepel, Tromp & Koehler, Phys. Rev. B 1986, 37, 10756). We will show here that the As atoms actually occupy the high-symmetry sites on Si(111) surface with little disorder in the in-plane direction. An As K emission signal was observed from Si(111):As–1x1 samples in a high vacuum chamber using XSW's in the grazing-angle geometry (Jaco & Hedges, Phys. Rev. B 1990, 42, 5399). XSW's created from the Si(220) Bragg planes with 14.5 keV synchrotron X-rays had an intensity modulation parallel to the surface. Emission profiles were observed from monolayer As atoms at glancing incidence angles close to the critical angle for total external reflection. Unlike in the ordinary geometry, emission profiles at x > ka in our geometry with an h vector nearly parallel to the surface show characteristic dependence on the degree of order of finessing surface atoms in the in-plane direction. A very good agreement was found in the observed and calculated profiles assuming As atoms lying on the (2x2) planes with a high order.

MS-11.01.04 A DYNAMICAL EFFECT OF CRYSTAL TRUNCATION ROD AND ITS APPLICATION TO X-RAY STUDY OF Cu5Au (001) SURFACE. By H-H. Huang, S.L. Chang and K.S. Liang, Synchrotron Radiation Research Center and Physics, National Tsing-Hua University, Taiwan and 3M Corporate Research, NJ, USA.