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 Silfhout, EMBL, 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 most experimental surface 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. This integration of 2D 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 with the emphasis on (111) semi-conductor surfaces, which have been studied intensively.

MS-11.01.02 STRUCTURE DETERMINATION OF THE 3x3 SUPERSTRUCTURE OF THE (111)-B-SURFACE OF InSb BY THREE DIMENSIONAL X-RAY DATA. By J. Wever, H.L. Meyerheim, V. Jahns, W. Moritz and H. Schulz, Institut für Kristallographie, Universität München, Theresienstr. 41, 8000 München, Germany

Several attemps have been made to solve this structure by two-dimensional in-plane data, including our group. Up to now all attemps were successless. 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 5% and a GOF of 1.3. The InSb($\bar{1}\bar{1}\bar{1}$) surface was prepared in UHV by Ar^{+} ion bombardement and annealing at 673 K for ca. 1/2 h and subsequent slow cooling to room temperature at about 2K/min. X-ray measurements were performed at the wiggler beam line at the HASYLAB (Hamburg, 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 60° which allowed to measure reflections up to l = 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 mm^2. The data set consisted of 24 superstructure lattice rods measured in steps of l = 0.4. A total of 218 symmetrically independent reflections were used. The inplane data set consisted of 73 reflections. All vacancy and trimer models which had been proposed for the ($\bar{1}\bar{1}\bar{1}$) surfaces of compound semiconductors can be ruled out. Additionally all models based on relaxations and models preserving the 3m1 symmetry of the unreconstructed 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 trigonal shape occurs with two orientations [1]. The final structure model exhibits similarities to the model derived recently for the ($\sqrt{19}$x$\sqrt{19}$) reconstruction of the GaAs($\bar{1}\bar{1}\bar{1}$) surface from STM measurements [2].
These two types of atom rings are arranged above the top layer such that each ring saturates 6 dangling bonds. The rings are centered around an Sb atom.
The surface undergoes a reversible phase transition at about 600K. 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 $[h0]^*$ direction could be measured.

References

[1] Seehofer and R.L. Johnson, private communication.
[2] D. K. Biegelsen, R. D. Bringans, J. E.Northrup and L. E. Schwarz, Phys. Rev. Letters 65 (1990) 452.

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

Arsenic deposition on clean Si(111) surface removes the 7×7 reconstruction to give a simple 1×1 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 lone-pair orbital. X-ray standing-wave (XSW) work (Patel, Golovchenko *et al.*, Phys. Rev. B 1987, 36, 7715) shows As atoms lying at 0.17 Å 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-1×1 surface structure (Copel, Tromp & Koeller, Phys. Rev. B 1988, 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-1×1 samples in a utrahigh vacuum chamber using XSW's in the grazing-angle geometry (Jach & Bedzyk, Phys. Rev. B 1990, 42, 5399). XSW's created from the Si(2$\bar{2}$0) Bragg planes with 16.5 keV synchrotron X-rays had an intensity modulation parallel to the surface. Emission profiles were observed from monolayer As atoms at glancing incidence angles ϕ close to the critical angle for total external reflection, ϕ_c. Unlike in the ordinary geometries, emission profiles at $\phi < \phi_c$ in our geometry with an h vector nearly parallel to the surface show characteristic dependence on the degree of order of fluorescing 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 (2$\bar{2}$0) planes with a high order.

MS-11.01.04 A DYNAMICAL EFFECT OF CRYSTAL TRUNCATION ROD AND ITS APPLICATION TO X-RAY STUDY OF Cu_3Au (001) SURFACE. By H.-H. Hung*[1], S.L. Chang[1,2] and K.S. Liang[3], [1]Synchrotron Radiation Research Center and [2]Department of Physics, National Tsing-Hua University, Taiwan and [3]Exxon Corporate Research, NJ, USA.

