

## 11.X-12 SURFACE X-RAY DIFFRACTION.

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A single monolayer of atoms at a crystal surface or interface is itself a two-dimensional crystal with a characteristic diffraction pattern of streaks perpendicular to the plane. Sources of synchrotron radiation have now evolved to the point that these weak diffraction signals can be detected by conventional diffractometry; the experimental difficulties lie mainly with *in situ* surface preparation, characterization and containment. Two practical approaches to these experiments will be described: an ultra-high vacuum diffractometer operating at the National Synchrotron Light Source and a method of preparing samples 'off-line' by capping with inert material.

It will be shown how the abrupt termination of a bulk crystal gives rise to 'crystal truncation rods' which are similar to and overlap with the monolayer diffraction rods from the surface layer. It will be demonstrated with examples how the registry of the surface layer can be determined by considering the interference of these. A crystallographic analysis of the Si(111)7x7 structure will be presented which shows, through the pattern of displacements parallel to the surface, that it is the local strain fields surrounding the adatoms, and not the more general homoepitaxial strain, which drives the reconstruction. Finally, results for the Si(111)7x7/a-Si interface show the mechanism of the propagation of order from the crystal into the amorphous region.

11.1-1 CHARACTERIZATION OF CUBIC BORON NITRIDE SINGLE CRYSTALS USING X-RAY TOPOGRAPHY AND ION PROBE ANALYSIS TECHNIQUE. By Shanu Pratap Singh, National Physical Laboratory, New Delhi-110012, India.

In the present investigation perfection and purity of cubic boron nitride crystals were evaluated. Double crystal X-ray diffraction topographic technique has been used for assessment of crystal perfection. A monochromatic  $\text{CuK}\alpha$  beam obtained from an asymmetrically cut silicon single crystal was used as the exploring beam to record X-ray topographs from (111) diffracting planes of Cubo-octahedral specimens. X-ray topographs of the three investigated specimens revealed the presence of columns of lattice defects running parallel to  $\langle 110 \rangle$ . Also inclusions of varying sizes were observed in these specimens.

Purity of these crystals was evaluated by recording an in-depth profile using  $\text{O}^+$  ions as a probe. The resulting mass spectra revealed the presence of Cr, Fe and Ti as predominant impurities whose peak heights changed considerably with depth. Ca, Mg and Ni were detected as background impurities.

11.1-2 MEASUREMENT OF LATTICE PARAMETER DIFFERENCES WITHIN A MIXED-HABIT NATURAL DIAMOND BY SYNCHROTRON DOUBLE-CRYSTAL TOPOGRAPHY. By A. R. Lang, G. Kowalski, A. P. W. Makepeace, H. H. Wills Physics Laboratory, University of Bristol, U.K. and Moreton Moore, Physics Department, Royal Holloway and Bedford New College, University of London, Egham, Surrey, U.K.

Among natural diamonds which have had epochs of mixed-habit growth during which crystallization proceeded simultaneously both on normal {111} facets and on non-faceted 'cuboid' surfaces of mean {100} orientation there is evidence of a higher level of nitrogen incorporation in the {111} compared with the cuboid growth sectors, at least as far as nitrogen aggregation in 'A' defects (probably a pair of nitrogen atoms substituting for a pair of carbon atoms), 'B' defects (probably four substituted nitrogen atoms tetrahedrally surrounding a carbon vacancy), and platelet precipitates on diamond {100} planes is concerned. The increase of lattice constant,  $a$ , with increasing concentration of nitrogen in A-defect form is known,  $\Delta a/a = 10^{-5}$  for 200 ppm N (Kaiser & Bond, Phys. Rev. **115** (1959) 857-863). However, the effect on lattice constant of B defects, and of platelets of a given size and concentration, is unknown. Measurements have now been made of the ratio  $\Delta a/\bar{a} = [a(\text{octahedral}) - a(\text{cuboid})]/\bar{a}$  by means of double-crystal topography at the SRS, Daresbury, on a particularly interesting mixed-habit specimen whose growth morphological features have been described by Suzuki & Lang (J. Crystal Growth **34** (1976) 29-37). Its {111} growth sectors have stronger A and B infrared absorptions than the cuboid sectors, and much stronger infrared absorption attributable to platelets. On the basis of the excess A absorption alone,  $\Delta a/\bar{a} \approx 1\frac{1}{2} \times 10^{-5}$  is expected. The observed value was about three times greater, suggesting a strong contribution from platelets and possibly also from B defects.

11.1-3 X-RAY STUDY OF BRAZIL TWINS IN NATURAL AMETHYST. By Z. Baran, K. Godwod and T. Warminski, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland. \*on leave from Universidade Federal da Bahia, Salvador, Brazil.

The physical nature of the lamellar structure observed on an unprocessed natural rhombohedral growth face,  $r$ , (011) of Brazilian amethyst quartz was studied by X-ray divergent beam reflection topography and double crystal topography combined with polarized light optical microscopy. The lamellar structure which was formed during growth, was found to be due to polysynthetic Brazil twins and the stripes observed on X-ray topographs identified with the right and left handed individuals of the twins observed optically. Lattice spacing and lattice rotation fluctuations over the areas where the lamellae outcrop on the natural face were measured using double crystal topography. Detailed studies of the concentration of some impurities at the twin boundaries were performed using quantitative electron probe microanalysis. They indicated that the distortions of the lattice around twin boundaries were not caused by the impurities. The observed contrast at the twin boundaries shows a contraction of the lattice spacing equal to  $\Delta d/d = -2 \times 10^{-5}$  between the twin lamellae and the twin boundary layer which plays the role of an accommodation layer. Since the distortions of the lattice around the twin boundaries are not caused by impurities, they are to be associated with the atomic displacements necessary to minimize the accommodation energy.