

PS12.02.29 AN ENHANCED TECHNIQUE FOR THE MODEL-INDEPENDENT RECONSTRUCTION OF STRAIN DISTRIBUTIONS IN CRYSTALS WITH NANOMETRE SPATIAL RESOLUTION. Andrei Nikulin, School of Physics, University of Melbourne, Parkville, Vic. 3052, Australia.

A new method for unique reconstruction of crystal-lattice strains in epitaxially grown layers from high-resolution x-ray diffraction data is discussed. The technique is based on the analysis of diffraction intensity profiles collected for two different radiation wavelengths.

The model-independent method for recovering one- (1D) and two-dimensional (2D) strain profiles in near-surface region of crystals has been recently developed [1-3]. The method relies on the high-resolution x-ray diffractometry. Spatial resolution is determined by the range of angles over which the data is collected. A logarithmic-dispersive relation is applied to retrieve the phases corresponding to the crystal truncation rod profiles. The method has been successfully applied to silicon crystals with ions implanted through a periodic oxide mask pattern and to SiGe/Si superlattices. However, the method did not give a unique solution because the measured intensity does not carry information about the phase of the scattered wave.

Present work reports the enhancement of the theory and recent experimental results in the practical implementation of the method: a unique solution for the phase-retrieval technique [4]; a practical procedure for the numerical regularisation of a displacement profile directly reconstructed from the x-ray diffraction data to improve the method precision [5].

The technique is applied to determine thicknesses and alloy composition in SiGe/Si superstructures. The recent x-ray high-resolution diffraction experiments which had been performed at the Photon Factory and ESRF synchrotron sources demonstrate a 1-2 nm depth resolution in the structures under analysis.

1. Nikulin, A. Yu. et al., *J. Appl. Cryst.* 27, 338 (1994).
2. Nikulin, A. Yu. et al., *J. Appl. Cryst.* 28, 803 (1995).
3. Nikulin, A. Yu. et al., *Phys. Rev. B.* 53, (1996) (in press).
4. Nikulin, A. Yu. et al., *Acta Cryst.* (1996) (submitted).
5. Nikulin, A. Yu. & Zaumseil, P., *Acta Cryst.* (1996) (submitted).

PR12.02.30 THIN FILMS STRUCTURE OF THE FLUORINE CONTAINING OLYGOMERS. German A.E., Struk V.A., Ovchinnikov E.V., Sen'ko A.F., Troichanskaya P.E., Grodno State University, Grodno 230023, Belarus.

The structure of the fluorine containing oligomers (FCO) on the metal substrates was studied by the electron paramagnetic resonance (EPR), infrared spectroscopy (IRS) and atomic force microscopy (AFM). It is determined that the strong chemisorption bonds with the substrate are founded at the deposition of the FCO on the metal. The "Sandwich" type structure occurs when the thickness of layer increases. In this case there are the ordering crystal structure covered by amorphous phase. The effect of the energetic (X-ray, thermotreatment) factors results in the formation of the "scales" type crystalline structure. The morphology of the founded structures depends on the type and time of the energetic influence.

PS12.02.31 STRUCTURE OF SiC FILMS GROWN ON Si(111) AND (110) SUBSTRATES BY SOLID-SOURCE MOLECULAR BEAM EPITAXIE. U. Kaiser, A. Fissel, W. Richter, S. B. Newcomb*, W. M. Stobbs*, Institut für Festkörperphysik, Friedrich-Schiller-Universität Max-Wien-Platz 1, D-07745 Jena, *Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge, CB2 3QZ

TEM and AFM studies have been carried out to demonstrate the influence of growth parameters and substrate orientation on the structure of SiC films deposited simultaneously and alternately from two sources by solid-source molecular beam epitaxy at low substrate temperatures (750 C-900 C). At 750 C and high growth rates (>2nm/min)

polycrystalline columnar films were grown which show a weak orientation relationship to the substrate. While growing the films under conditions for Si stabilization at the surface and over the substrate temperature range of 800 C to 850 C at high rates, the films are strongly textured but still grow with a columnar morphology. Clear evidence for the outdiffusion of Si from the substrate is found, leading to porous regions in the substrate at temperatures up to 800 C and to voids above 800 C. At growth rates below 1nm/min and a certain adatom ratio the nucleation mode changes from 3 to 2 dimensional and single crystalline epitaxial cubic films were grown. The influence of the adatom ratio Si:C on the growth and on the defect formation is discussed at 3 different Si:C adatom ratios (0.95, 1.05, 1.20). When the layer is deposited under slow and less kinetically controlled conditions using an alternating supply of Si and C controlled to the atomic plane level, single crystalline cubic SiC films with very flat surfaces are formed which tend to establish the hexagonal polytype. Differences in the growth on (111) and (110) substrates might be expected and are discussed as result of the differing crystallographies at the interface.

Surfaces III X-Ray & Neutron Reflectivity

MS12.03.01 GRAZING INCIDENCE X-RAY DIFFUSE SCATTERING FROM SURFACES AND INTERFACES. B. K. Tanner, I. Pape, T. P. A. Hase and M. Wormington*, Physics Department, Durham University, Durham DH1 3LE, U.K., *Bede Scientific, Lindsey Park, Bowburn, Durham, DH6 5PF, U.K., +Dept of Engineering, University of Warwick, Coventry, CV4 7AL, UK

Grazing incidence specular and diffuse X-ray scattering measurements from surfaces and interfaces are described. Conventional source and synchrotron radiation techniques are contrasted and the application of anomalous dispersion to highlight interfaces between materials close in the periodic table is described. The data are interpreted using novel computer simulation code, running on a PC, based on the distorted wave Born approximation theory of scattering from fractal interfaces.

Analysis of the scatter from polished surfaces of the glass ceramic Zerodur™ shows that the diffuse scatter is much less than that predicted from the surface roughness deduced from the specular reflectivity. Inclusion of a gradient in electron density at the surface gives excellent agreement between simulated and experimental data for all scattering vectors used. Studies of surfaces of GaAs polished using different chemical and mechanical techniques showed similar surface composition grading, with significant electron density variation over a period of months after polishing. Roughness σ , lateral correlation length ξ and fractal parameter h of the interfaces in Co-Cu multilayers have been measured and correlated with giant magnetoresistance (GMR) data. A linear fall in correlated roughness with GMR is found in multilayers grown on sapphire by MBE. Multilayers grown on copper silicide buffers on silicon show large ξ values and stepped interfaces which result in characteristic diffuse scatter. Simulation and experiment are in excellent agreement over a wide range of X-ray optical conditions. Sputtered multilayers grown on silicon show markedly less conformality in the roughness than MBE-grown layers.

MS12.03.02 Goebel