

Title	X-ray scattering from crystalline SiO ₂ in the thermal oxide layers on vicinal Si(111) surfaces
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MS12.02.04 STRAIN INDUCED MACROSTEPS IN (GaIn)As/Ga(PAs) SUPERLATTICES GROWN ON OFF-ORIENTED GaAs SUBSTRATES. C. Giannini¹, Y. Zhuang¹, L. Tapfer¹, T. Marschner², W. Stolz², ¹Centro Nazionale Ricerca e Sviluppo Materiali (P.A.S.T.I.S.-C.N.R.S.M.), S. S. Appia Km. 712, Brindisi 172100, Italy, ²Wiss. Zentrum für Materialwissenschaften und Fachbereich Physik, Philipps-Universität, D-35032 Marburg, Germany

Symmetrically strained (GaIn)As/Ga(PAs) superlattices grown on off-oriented GaAs substrates by metalorganic vapour phase epitaxy were investigated by x-ray scattering techniques. High-resolution x-ray diffraction measurements and x-ray reciprocal space maps were performed for different off-orientation angles (0° – 4°) towards one of the nearest $\langle 110 \rangle$ directions. The substrate off-orientation and the strain were found to affect the structural properties of the superlattices inducing surface roughening and, consequently, the generation of laterally ordered macrosteps. The periodically ordered lateral microsteps give rise to a lateral modulation of the layer thickness (ordered interface roughness) and of the lattice strain. The x-ray diffraction measurements allowed us to determine the lateral and vertical periodicity of the superlattices as well as the strain modulation. The distribution and correlation of the roughness across the interfaces was investigated by the specular and non specular scattered intensity curves. Our results show that the morphology of the roughness on the growth surface is greatly influenced by the off-orientation angle. Evidence of anisotropy in the lateral and vertical correlation of the roughness is found.

MS12.02.05 WATER-INTERFACE STRUCTURES ON Cu(111) ELECTRODES. I. K. Robinson, Y. S. Chu and A. A. Gewirth, University of Illinois, Urbana IL 61801, USA

We have investigated the structure of Cu(111)/water interfaces using in-situ X-ray reflectivity and crystal-truncation-rod (CTR) diffraction. A thin-layer geometry and synchrotron radiation were used to obtain monolayer sensitivity. Careful electrochemical and contamination control were required to stabilize the interface structure during the time needed to complete the measurements.

We will first present the results of an experiment in which a monolayer of Pb was introduced on the electrode by underpotential deposition. This monolayer was found to be hexagonal, aligned with the substrate, but incommensurate. The Pb in-plane lattice parameter was found to change with potential, showing electro-compression. However the numerical value of the compressibility was different both from values observed on Ag(111) or Au(111) and from the value expected for an ideal 2D metal. The distance of the monolayer from the substrate was found to have little potential dependence.

Our second experiment looked at X-ray reflectivity data for the clean Cu(111) electrode in 0.1M perchloric acid at different potentials within its range of stability (between dissolution and hydrogen-evolution potentials). Substantially different curves were observed at -0.60V vs Ag/AgCl (within a narrow region close to the potential for hydrogen evolution), and at -0.05V vs Ag/AgCl, characteristic of most of the potential range. The change was well correlated with the cyclic voltammetry, which displayed a well-defined cathodic peak near the hydrogen evolution potential too. The difference in the reflectivity could be explained by fitting of these curves to simple layered models of the Cu/water interface, leading to the conclusion that oxygen becomes specifically bound to the electrode over most of the potential range. Since our experiments cannot detect the presence of H, it seems plausible that the bound species is OH, rather than just O.

MS12.02.06 X-RAY SCATTERING FROM CRYSTALLINE SiO₂ IN THE THERMAL OXIDE LAYERS ON VICINAL Si(111) SURFACES. T. Shimura, H. Misaki and M. Umeno, Department of Material and Life Science, Graduate School of Osaka University, 2-1 Yamadaoka, Suita 565, Japan.

Bragg reflections were observed from the crystalline SiO₂ in the thermal oxide layers on vicinal Si(111) surfaces, of which surfaces were tilted 4 degree from the $\langle 111 \rangle$ toward the $\langle 1\bar{1}2 \rangle$. The oxide layers were prepared by oxidizing the Si wafers at 950C in a dry oxygen atmosphere. The thicknesses of the oxide layers were 760Å, 340Å and 230Å. In the X-ray diffraction patterns from these samples, very weak peaks were observed on the lower angle sides of the CTR (crystal truncation rod) scatterings around the 111 Bragg points, of which position is nearly 0.42, 0.42, 0.51 in the reciprocal space. The intensity of the peak depends on the thickness of the oxide layer, and the peak is not observed in the etched sample. A high resolution measurement of the intensity around the peak using a synchrotron radiation source revealed that the profile had Laue-function-like oscillation fringe pattern, of which period corresponded to the inverse of the film thickness. From these results it was concluded that these peaks were Bragg peaks originated from the crystalline SiO₂, which coexisted in the amorphous SiO₂ film having an epitaxial relationship with the Si substrate.

Furthermore, another Bragg reflection from the crystalline SiO₂ was observed on the low angle side of the CTR scattering from the $1\bar{1}1$ Bragg point, of which position was nearly 0.74 0.74 -1.22 in the reciprocal space. With these two reflections the atomic structure model of the crystalline SiO₂ could be constructed.

MS12.02.07 INVESTIGATION OF THE ROUGHNESS REPLICATION IN MULTILAYERS BY DIFFUSE X-RAY REFLECTION V. Holy, Dept. of Solid State Phys., Masaryk University, Kotlarska 2, 611 37 Brno, Czech Republic, G. Bauer, A. Darhuber, J. Stangl, and S. Zerlauth, Inst. of Semiconductor Physics, Kepler University, Altenbergerstr. 69, 4040 Linz, Austria.

The correlation properties of the interface roughness in a multilayer can be investigated by measuring the diffuse (off-specular) component of the reflected x-ray intensity. From the distribution of the diffuse scattering in reciprocal plane, the correlation function of a rough interface (in-plane correlation) as well as the correlation function of a pair of interfaces (inter-plane correlation) can be deduced. The in-plane correlation is decisive for the intensity distribution along the axis parallel to the surface, the inter-plane correlation affects the intensity distribution in the perpendicular direction. Inter-plane correlations give rise to distinct sheet-like maxima in reciprocal space oriented perpendicular to the direction of maximum correlation. From the width of the maxima, the inter-plane correlation length can be stated. In the case of single crystalline multilayers grown on misoriented substrates, the miscut of the vicinal surface affects the diffuse scattering introducing an asymmetry of the intensity distribution with respect to the surface normal. All these features have been demonstrated by measurements of diffuse x-ray reflection from SiGe/Si superlattices. We have found a well pronounced inter-plane correlation, whose direction differs substantially from the growth direction. The in-plane correlation function could be modelled by means of the Markov random chains using either two-level or many-level models.