MS43-O3 Interplay of microstructure defects in GaN layers

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Because of its large energy gap, gallium nitride is regarded as prospective electronic material for LEDs emitting in the ultra-violet spectral range. Due to the lack of appropriate native substrates, GaN is typically grown on foreign wafers. Consequently, the production of large perfect GaN crystal is impeded by the lattice misfit between the substrate material and GaN, which is nearly 15 % for GaN grown on sapphire with the surface orientation (0001). Due to the slightly different thermal expansion coefficients of GaN and Al2O3, the lattice misfit is reduced at the growth temperature, but the reduction of the lattice misfit is only 0.1 %. As the corresponding interatomic distances, i.e. the distances between Ga atoms in GaN and between Al atoms in Al2O3, are larger in GaN than in Al2O3, compressive stress in GaN is expected, but not always observed. The lattice misfit and the resulting lattice strain are compensated by misfit dislocations in GaN. The dislocations act as recombination centres for charge carriers, thus they are unwanted in the GaN crystals. Still, many deposition techniques facilitate dislocation bunching during the growth of GaN and consequently the formation of GaN domains with a greatly reduced local dislocation density.In this contribution, the effect of the dislocation bunching is illustrated on the correlation between the residual stress and the density of threading dislocations in GaN layers grown by hydride vapour phase epitaxy. The residual stresses were determined by using two complementary methods – X-ray diffraction and micro-Raman spectroscopy. The later method revealed not only the average residual stress but also its depth gradient. The dislocation densities were concluded from the broadening of X-ray diffraction lines, the dislocation bunching from the transmission electron micrographs. In this context, the reliability of two competing X-ray diffraction methods were compared, which are alternatively utilized for determination of the density of threading dislocations. The first method is based on the analysis of the dislocation-controlled crystal mosaicity from the azimuthal scans in the reciprocal space, the second one on the analysis of the local strain fields around the threading dislocations from the two-dimensional mapping of the reciprocal space. Finally, the effect of the dislocation bunching on the dislocation density determined by using the respective method is discussed.

Keywords: Gallium nitride, X-ray diffraction, micro-Raman spectroscopy, residual stress, dislocation density, dislocation bunching

MS43-O4 Unravelling the mechanisms of and controlling molecular thin film growth

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Molecular, crystalline thin films are relevant in many technological applications but their thin film morphology is complicated to quantify as growth inherently is a non-equilibrium process. This means that the route to the final film structure is determined not simply by a minimization of the free energy, but by a non-trivial competition between thermodynamics and kinetics. For a quantitative understanding one therefore needs information on the nanoscopic surface processes such as molecular binding as well as surface diffusion and step-edge crossing. *In situ* real-time X-ray scattering is ideally suited for such measurements as it can be used to monitor temporal changes on the atomic scale.

We show how two types X-ray growth oscillations can be used to unravel growth of the molecule C60. Real-time Grazing Incidence Small Angle Scattering (GISAXS) can be combined with simultaneous X-ray reflectivity measurements to characterize both in-plane and out-of-plane film structure as a function of time. From this we determine diffusion barrier, step edge barrier and binding energy for C60 for a detailed, quantitative description of the thin film growth in dependence of growth rate and temperature. Beyond those two control parameters of rate and temperature, we report that light can act as a third, distinct parameter to control growth. We show that even at moderate intensities of ~1 W/cm^2 a direct influence of light on the molecular crystal structure in thin films is visible. For the example of alpha-sexithiophene (6T) bimodal growth with two coexisting crystal phases can be suppressed and phase purity increased.

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L. Pithan, S. Kowarik, et al. *"Light control of polymorphism in thin films of Sexithiophene"*, Crystal Growth and Design, **15 (3)**, 1319-1324, (2015)

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