

## 1.2 Microstructure

This department conducts fundamental and applied research on the structural, chemical, and mechanical properties of low-dimensional semiconductor systems, heterostructures, metastable materials, and ferromagnet-semiconductor hybrid structures. X-ray and electron diffraction, electron microscopy imaging and spectroscopy techniques as well as scanning tunneling microscopy are applied with high spatial resolution and sensitivity to analyze material systems on different length scales down to atomic resolution. Experimental results on interface structures, phase stabilities, strain relaxation processes, and the formation of extended defects are compared with computer simulations and supported by theoretical modeling.

Interfaces of epitaxial III-V compound semiconductor heterostructures are generally not atomically sharp, but reflect a transition region in the chemical composition. We found by transmission electron microscopy (TEM) analysis that the functional dependence of the change in composition across the interface is sigmoidal and can thus be expressed by an analytical function that enables a quantitative determination of the interface width by comparing the simulated and experimental TEM contrast. The model describes perfectly the distribution profiles of several material systems, including the interfaces of As-based compounds and those of InAs/GaSb short-period superlattices with uncommon interface atoms [E. Luna *et al.*, *J. Cryst. Growth* **311**, 1739 (2009)].

The growth mode and the interface roughness of Fe<sub>3</sub>Si/GaAs heterostructures have been investigated by grazing-incidence x-ray diffraction at the synchrotron BESSY of the Helmholtz Center Berlin for Materials and Energy [B. Jenichen *et al.*, *Phys. Status Solidi A* **206**, 1740 (2009)]. The x-ray intensity oscillations during the initial phase of lattice-matched Fe<sub>3</sub>Si growth reveal a roughening of the surface due to the formation of small three-dimensional islands. Two-dimensional layer-by-layer growth arises in a later stage of growth after coalescence of the islands. The surface energy increase due to three-dimensional nucleation is confirmed by ab-initio calculations allowing to identify the growth as a strain-free Volmer-Weber transient. Kinetic Monte Carlo simulations, which correctly incorporate this energy increase, reproduce the characteristic x-ray intensity oscillations found in the experiment [V. Kaganer *et al.*, *Phys. Rev. Lett.* **102**, 016103 (2009)]. Furthermore, the interface roughness has been determined by a detailed analysis of the crystal truncation rods (CTRs). We have found that thin Fe<sub>3</sub>Si epilayers grown on GaAs(001) exhibit a cube-on-cube orientation and do not result in additional roughness at the film surface in agreement with simulations of the CTRs based on the  $\beta$ -model, where  $\beta$  denotes a factor describing the probability of the terrace height [V. Kaganer *et al.*, *Phys. Status Solidi A* **206**, 1744 (2009)].

The strain relaxation in epitaxial films with large lattice mismatch may generate line defects at the interface as well as in the film. We have introduced a Monte Carlo technique to calculate the x-ray diffraction profiles from epitaxial films with arbitrarily correlated dislocation distributions [V. Kaganer *et al.*, *Phys. Rev. B* **80**, 033306 (2009)]. The coexistence of misfit

and threading dislocation ensembles is considered explicitly. Using this technique, the experimental line shapes have been quantitatively reproduced for thin (100 nm) and thick (1000 nm) GaN epitaxial films on SiC (0001). In both cases, the line shape is caused by the correlated distribution of misfit dislocations.

Strain relaxation mechanisms occurring during self-induced growth of free-standing group-III-nitride nanowires have been studied by both, in-situ reflection high-energy electron diffraction and ex-situ high-resolution TEM. The GaN nanowires nucleate on an AlN buffer layer grown on Si(111) with the initial formation of coherently strained, three-dimensional islands. The epitaxial strain is firstly relieved elastically via island shape transitions — from spherical caps through truncated pyramids to full pyramids. A strong correlation is observed between the subsequent process of plastic relaxation and the final shape transition to the nanowire morphology. The experimental critical radius, at which misfit dislocations nucleate, is in agreement with the theoretical description of misfit dislocation formation in full-pyramid-shaped islands, but smaller than the theoretical value predicted for cylinder-shaped nanowires. Such a critical radius corresponds to the initial radius of the nanowires at nucleation. This answers the long-standing question about the mechanism that determines the nanowire radius in catalyst-free growth.

The research of the atomic scale includes the manufacturing and characterization of individual nanostructures by low-temperature scanning tunneling microscopy (LTSTM). In addition to assembling structures by atom manipulation, this technique provides local spectroscopic information and gives direct access to quantum phenomena at the nanometer and subnanometer-scale. We succeeded in the reversible repositioning of individual In atoms on the InAs(111)A surface allowing to construct one-atom-wide indium chains. Tunneling spectroscopy revealed that these chains form quantum states deriving from an adatom-induced electronic state and substantial substrate-mediated coupling [S. Fölsch *et al.*, Phys. Rev. Lett. **103**, 096104 (2009)]. Furthermore, we continued in studying the conformational switching of single organic molecules covalently linked to semiconductor surfaces. The biconformational switching of single 1,5-cyclooctadiene molecules chemisorbed on a Si(001) surface was explored by quantum chemical and quantum dynamical calculations and LTSTM experiments [Ch. Nacci *et al.*, Nano Lett. **9**, 2996 (2009)]. The calculations explain the experimentally observed switching driven by inelastic electron tunneling at 5 K. At higher temperatures, they predict a controllable crossover behavior between switching driven by inelastic electron tunneling and a thermally activated behavior, which is fully confirmed by experiment.