

1.2 Microstructure

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

Interfaces in low-dimensional compound semiconductor heterostructures grown by molecular beam epitaxy have been explored with monolayer resolution by a combination of dark-field and high-resolution transmission electron microscopy (TEM). The indium distribution across (Ga,In)(N,As)/GaAs quantum wells has been determined experimentally and analyzed quantitatively using a sigmoidal law with the interface width as the main fitting parameter [E. Luna *et al.* Appl. Phys. Lett. **92**, 141913 (2008)]. The thermal stability of the interfaces and their interplay with indium segregation effects have been discussed in the framework of the inherent thermodynamic miscibility gap of the quaternary alloy.

Composition fluctuations and clustering in metastable (In,Ga)(N,As)/GaAs and (Al,In)N/GaN heterostructures such as quantum wells have been investigated using analytical electron microscopy including spatially resolved electron energy loss spectroscopy. In the quaternary (Ga,In)(N,As) alloys containing In and N concentrations above 20% and 2%, respectively, nanometer-sized fluctuations have been identified as areas with preferred Ga-N and In-As bond configurations. These nearest-neighbor configurations are driven by maximizing the cohesive bond energy despite increasing local strain. Surface roughening is initiated if sufficient strain is accumulated in the layer. Lowering the growth temperature reduces the level of fluctuations and results in more homogenous quantum well structures [X. Kong *et al.*, J. Phys. Chem. Solids **69**, 335 (2008)]. In case of the (Al,In)N/GaN system, the microstructure including the local chemical composition has been determined and used to clarify the cracking behavior in the layers with tensile strain [T. Ive *et al.*, Phys. Rev. B **78**, 035311 (2008)].

Ferromagnetic Heusler alloys are candidates for spin injectors in ferromagnet-semiconductor hybrid structures. Besides the basic requirement of structurally perfect interfaces, these intermetallic alloys have to exhibit long-range order. The atomic order and interface structure of Fe₃Si films grown on GaAs(001) have been studied in-situ by grazing incidence x-ray diffraction at BESSY [V. Kaganer *et al.*, Phys. Rev. B **77**, 125325 (2008)]. The experimentally observed crystal truncation rods have been analyzed by dynamic electron diffraction theory. The results demonstrate that the films are fully ordered in the Fe and Si sublattices, with the exception of one or two monolayers at the surface. Furthermore, two types of interface configuration have been found, with the first film layer on top of the last As layer of GaAs containing

either only Fe atoms or both Fe and Si atoms. The Si atoms in the first FeSi layer are located in between the top Ga-As atomic chains. Therefore, it is concluded that the actual interface configuration depends the residual arsenic at the surface.

The research of this department also includes the characterization of individual nanostructures by low-temperature scanning tunneling microscopy and spectroscopy (LT-STM/STS). In addition to nanostructure fabrication by atom manipulation, this technique provides local spectroscopic information and gives direct access to quantum phenomena at the nanometer and subnanometer-scale. Our research on quantum confinement in monatomic chains has been extended from metal-based to semiconductor-based systems. Concerning metal surface-supported atom chains, it has been shown that a Cu/Cu(111) quantum wire can guide a one-dimensional electron flux over a short distance and thus can be considered as a possible component in nanoelectronic devices [S. Díaz-Tendero *et al.*, *Nano Lett.* **8**, 2712 (2008)]. With respect to semiconductor-based systems, we have succeeded to extend the technique of atom manipulation to III-V semiconductor surfaces and demonstrated the feasibility of versatile nanostructure assembly by using adatoms as building blocks. Complementary to the LT-STM/STS activities on atom manipulation and atomic-scale quantum structures, we have continued to study functional organic molecules linked to Si surfaces. For single cyclooctadiene molecules on Si(001), the switching in the molecular tunneling conductance has been analyzed and ascribed to reversible conformational changes induced by inelastic electron tunneling [Ch. Nacci *et al.*, *Phys. Rev. B* **77**, 121405(R) (2008)]. Depending on the adsorption state of the alkene molecule, both binary and three-level switching of the tunneling conductance can be realized.