Quantitative High-Resolution TEM/STEM and Diffraction

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Quantitative HAADF-studies of GaP/Si-heterostructures

A. Beyer[1], K. Werner[1], B. Haas[1], K.I. Gries[1], K. Volz[1]

[1]Philipps Universität, Material sciences centre and faculty of physics, Marburg, Germany

andreas.beyer@physik.uni-marburg.de

The growth of III/V-material on silicon (Si) opens the possibility of new devices like high efficient solar cells, high mobility channel layers [1] or a laser on Si substrate [2]. Nevertheless, the growth of the polar III/V-material on the non polar Si holds several challenges, as anti-phase domains (APDs) may occur at monoatomic steps on the substrate. Moreover, the structure of the interface is not trivial because it is not necessarily charge neutral. We investigate galliumphosphide (GaP) grown on Si as a model system for the heteroepitaxy of polar material on nonpolar substrate because GaP is nearly lattice matched to Si.

GaP-layers were grown via metal organic vapour phase epitaxy on Si substrates with a small intentional offcut of 0.1 ° into one of the <110> directions in an Aixtron 200 GFR reactor. Special growth conditions were applied which result in optimum layer quality and minimum amount of residual APDs [3] as well as modified conditions to intentionally change the interface configuration. Electron transparent foils were prepared using conventional mechanical thinning followed by final argon ion-milling. For the investigation of the GaP/Si-interface high angle annular dark field (HAADF)-measurements were carried out in a JEOL JEM2200 FS, operating at 200 kV. It is equipped with a corrector for spherical aberration of the condensor lens system providing probe sizes below one Angstroem. For the quantification of the chemical composition at the GaP/Si-interface HAADF-intensities were simulated using a FFT-multislice [4] algorithm in an absorptive potential approximation [5]. Additionally, electron energy loss spectroscopy (EELS) was used to determine local thickness of the TEM foil.

Thickness dependent simulations and low resolution HAADF-measurements of wedge shaped samples show that the intensity ratio of Si and GaP is a function of TEM specimen thickness and microscope parameters as convergence angle and detection angle. Therefore, for known microscope parameters the thickness of an investigated sample region can be determined by this ratio.

Figure 1 depicts a representative HAADF-image of the GaP/Si-interface. The comparison to simulated intensities leads to a thickness of 30 nm. This value is in good agreement with the thickness derived from EELS measurements. Moreover, also the absolute HAADF-intensity of GaP and Si, which can be gained by normalizing the measured intensity with the intensity of the impinging beam [6] fits very well to this value. Further simulations at fixed thicknesses allow the investigation of the influence of chemical composition on the HAADF-intensity. With this knowledge it is possible to map the amount of Si on each atomic column. The map derived from the HAADF-image in Figure 1 is shown in Figure 2. It is observable, that the interface is not atomically smooth but an intermixing of 7 monolayers. The same intermixing behavior can be found for a wide range of different samples, irrespective of the Si-orientation and GaP-polarity. In contrast to that, increasing the growth temperature significantly results in different interface configurations.

In this contribution we will show how high resolution HAADF-measurements in conjunction with adequate simulation can be used to determine the thickness of TEM-sample very accurate. At known thicknesses the intermixing behavior of GaP and Si can be quantified on an atomic scale and correlated to the applied growth conditions.

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Figure 1. Representative HAADF-image of the GaP/Si-interface (The width of the scalebar is 1 nm).

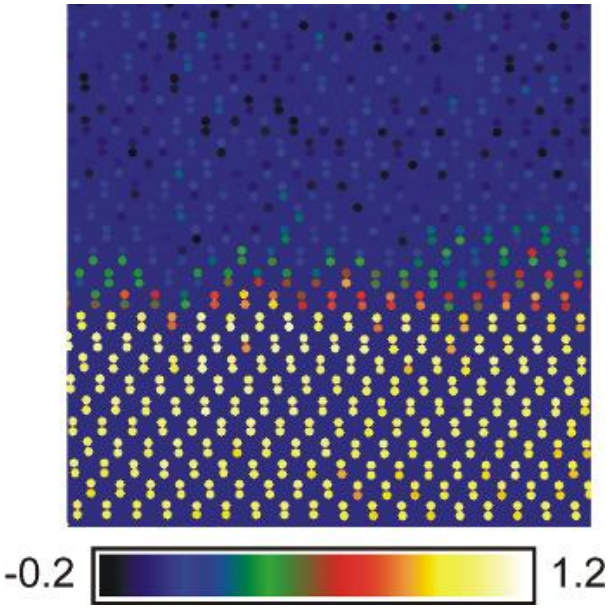

Figure 2. Atomically resolved Si-map, derived from the sample region depicted in Figure 1.