X-Ray Diffraction Study of the Composition and Strain Fields in ordered arrays of SiGe Islands


Institute for Semiconductor Physics, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria
Max Planck Institute Stuttgart, Heisenbergstrasse 1, 70569 Stuttgart, Germany
Faculty of Mathematics and Physics, Charles University Prague, Ke Karlovu 5, Praha, 12116, Czech Republic
IWF Dresden, Heimholtzstrasse 20, 01069 Dresden, Germany
TU Delft, Stevinweg 1, 2628 Delft, The Netherlands

Silicon-Germanium (SiGe) islands are a model system for the investigation of Stranski-Krastanow growth [1]. For any application these islands have to be capped with Si, as an example such structures are of interest for the realization of field effect transistors with strained Si channels [2]. Already during Ge deposition, depending on the growth temperature, interdiffusion and segregation processes change the composition and thus the strain state of the islands. The strain state of the Si capping layer is determined by the size, shape and composition of the buried islands.

We have performed systematic studies of strain and composition of uncapped and capped SiGe islands grown by molecular beam epitaxy using High Resolution X-Ray Diffraction (HXRD) at the BW2 beamline of Hasylab, Hamburg as well as at the ID10B beamline of the ESRF [3,4]. In order to ensure a small size distribution of the islands not planar but prepatterned 4 inch (001) Si substrates were used. The Si wafers were patterned by optical lithography and reactive ion etching. The pits for island growth were ordered in regular 2D arrays with periods ranging from 600 to 1000 nm along two orthogonal <110> directions. After the growth of a Si buffer layer 5 to 9 monolayers of Ge were deposited at a temperature of 700°C, leading to the formation of islands with certain shapes (either dome- or barn shaped) corresponding to the number of monolayers deposited [5]. The capping of the islands was performed at low temperatures (300°C) to avoid intermixing and thus strain relaxation in the island which would also cause a loss of tensile strain in the Si capping layer. After Si capping the surface morphology was studied by Atomic Force Microscopy (AFM). This information was used to set up models for three-dimensional Finite Element Method (FEM) simulations of the capped islands which served as an input for calculating the diffracted intensities.

Reciprocal space maps around the vicinity of the symmetric (004) and several asymmetric Bragg Peaks, such as (113) and (224), were recorded in coplanar geometry. The X-ray simulations were based on kinematical scattering theory. Special attention was given to the non uniform distribution of the germanium within the island. The use of different germanium gradients (constant, 1D and 3D gradients) leads to strongly altered scattered intensity distribution of the X-ray signal of the SiGe islands and consequently information on this quantity was obtained for both dome and barn shaped islands. In the Figure an example of the procedures described above is represented for a sample containing uncapped dome-shaped islands, containing an AFM image, data on the corresponding FEM model and both experimental and calculated X-ray data. The importance of the performed simulations is given by the fact that up to now there is no method to determine the strain within the silicon capping layer itself, as features of this part of the structure cannot be seen in the X-ray measurements. Therefore the correct modeling of the island's properties is essential to get information on the strain state of the Si capping layer out of the simulations. During this work it turned out, that in the Si layer above such islands tensile strains up to 1% are achievable without introducing defects, i.e. much higher than on planar SiGe stressor structures [6].
Figure 1: In part a of this figure a detailed AFM image of a dome-shaped island is shown (part a) with the corresponding shape used for the FEM Simulation underneath (part b). As can be seen, special care was given to the exact shape of such an island using the facets known from various analyses of AFM data. The middle part shows the strain component $e_{xx}$ as result of a FEM simulation which is then the base for recalculating X-ray data. In the two panels to the right a comparison of experimental (d) and simulated (e) X-ray data is shown, in this case reciprocal space maps of the (113) Bragg peak. The strong feature labelled 'Si' is the Silicon substrate peak, the rather faint, elongated signal labelled 'SiGe' results from the SiGe islands. The strong streak at the substrate peak seen in the measurement is an artefact due to the absorbers used to avoid saturation of the CCD detector at the maximum of the Bragg peak.

We thank the staff at BW2 at Hasylab and the ID10 at the ESRF for their support and G. Vastola, A. Marzegalli, F. Montalenti and L. Miglio for discussions on the 3D FEM simulations. This work was supported by the FWF, Vienna (SFB025) and the EC d-dotFET project (012150-2).

References