Experiment title: The strain field in the proximity of SiGe nanoscale islands as measured by triple crystal grazing incidence x-ray diffraction	Experiment number: HS 1735

Beamline:	Date of experiment:	Date of report:
ID10 B	from: 19 June 2002 to: 24 June 2002	07 April 2004
Shifts:	Local contact(s):	*Received at ESRF:*
15	O. Konovalov	

Names and affiliations of applicants (* indicates experimentalists):

Martin Schmidbauer* schmidbauer@physik.hu-berlin.de

Peter Schäfer*

Michael Hanke*

Humboldt-Universität zu Berlin
Institut für Physik, AG Röntgenbeugung
Newtonstr. 15
D-12489 Berlin

Report:

Triple crystal grazing incidence x-ray diffraction from nanoscale islands have been carried out at ID10B beamline. In this report we will explicitly demonstrate the impact of the reflected wave on the scattered diffuse intensity distribution. In order to visualize this influence the model system SiGe islands grown on Si(001) by means of liquid phase epitaxy (LPE) has been chosen. These islands are especially suitable, owing to their high perfection regarding uniform shape and size (Fig.1). Moreover, they are large enough to give a sufficiently high scattering signal. Corresponding theoretical simulations based on the distorted-wave Born approximation (DWBA) have been carried out. The strain field inside and in the vicinity of the SiGe islands that is used in the scattering simulation was calculated in the framework of linear elasticity theory using the numerical finite element method.

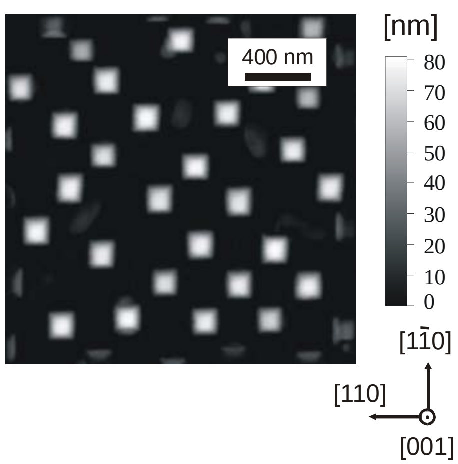

Figure 1: Atomic force micrograph of SiGe nanoscale islands grown on (001)Si by LPE.

Results of out of-plane diffuse intensity in the vicinity of the 220 reciprocal lattice point are presented in Fig.2. The diffuse intensity pattern in reciprocal space reveals a well resolved fine structure with prominent maxima and a complicated fringe pattern. The distribution of diffuse intensity in reciprocal space strongly depends on the angle of incidence with respect to the sample surface. Experimental and theoretical results are in excellent agreement. This substantiates the important role of basically four scattering channels that have to be considered for a complete understanding of the scattering scenario.

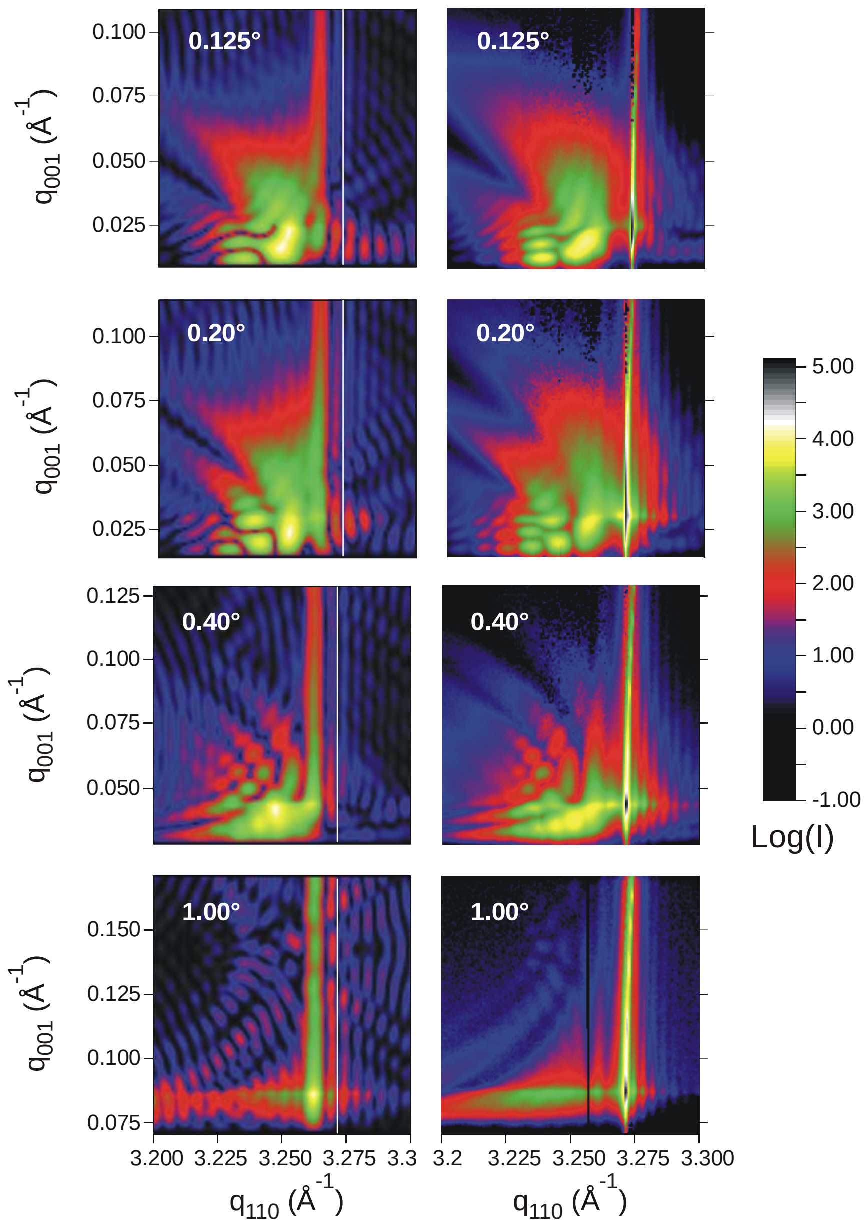

Figure 2: Experimental out-of-plane measurements (left) and corresponding theoretical simulations (right) of the diffuse intensity (GID,220) of $Si_{0.7}Ge_{0.3}$ islands at different angles of incidence. The scattering plane contains the <110> direction. The simulations were carried out in the framework of the distorted-wave Born approximation. The positions of the substrate peak and crystal truncation rod are marked by vertical white lines.

From a set of measurements as shown in Fig.2 a refined island model concerning shape, size and Ge composition was elaborated. For more details see [1].

It is interesting to investigate the role of the diffuse scattering from the strain field inside the substrate. For that purpose, simulations have been carried out for the in-plane diffuse intensity by either (i) neglecting scattering from the substrate and (ii) taking into account scattering from the substrate. Results are shown in

Fig.3 (b) and (c) along with experimental data (Fig.3(a)). These calculations clearly show that the diffuse intensity from the substrate can be separated from the diffuse intensity from the islands. The pronounced fringe pattern in the vicinty of the Si 220 substrate reflection is not directly connected with the island size (130 nm base width) but it is related to the extended strain field inside the substrate which is created by the island.

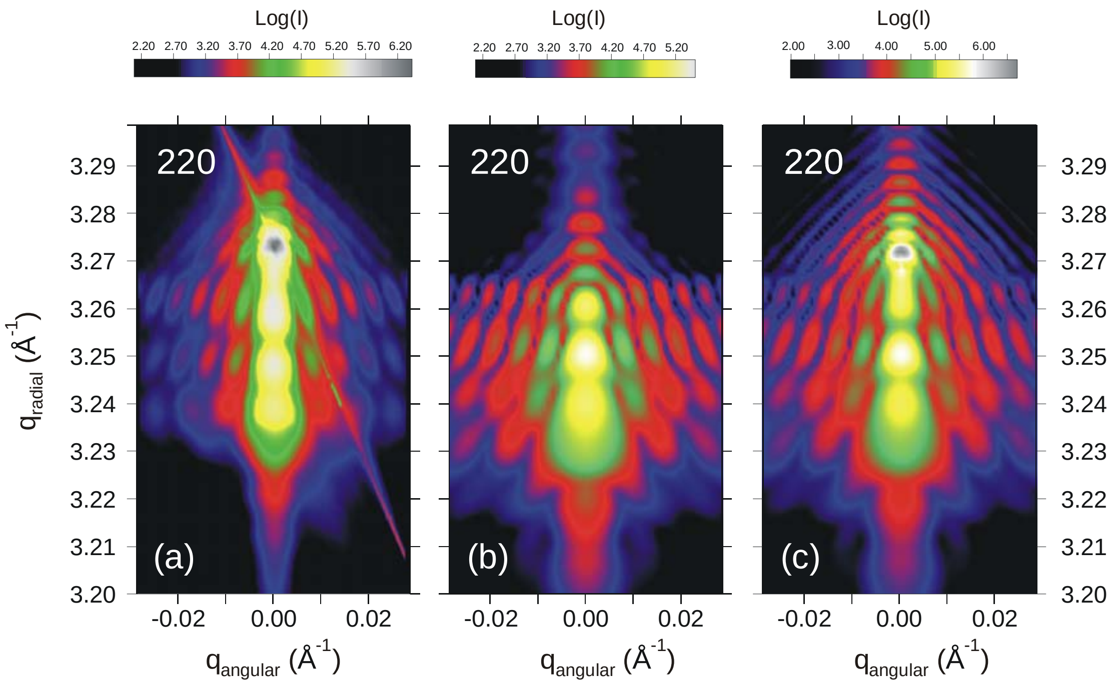

Figure 3: Diffuse intensity in the vicinity of the 220 in-plane reciprocal lattice point: (a) experiment, (b) simulation (island only), (c) simulation (island and substrate). The angle of incidence $\alpha = 0.25°$ was chosen to be slightly above the critical angle of total external reflection (for Si, $\alpha = 0.22°$ at $\lambda = 1.542$Å). The simulations were based on the DWBA. The simulated intensity was integrated vertically over $\Delta q_z = 0.02$ Å^{-1}.

References:

[1] D. Grigoriev, M. Hanke, M. Schmidbauer, P. Schäfer, O. Konovalov, and R. Köhler, J. Phys. D **36**, A225 (2003)