Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

<table>
<tr><td>ESRF</td><td>Experiment title:
Influence of the Si overgrowth on the structure of self-assembled Ge quantum dots</td><td>Experiment number:
HS-1583</td></tr>
<tr><td>Beamline:
ID-10B</td><td>Date of experiment:
from: January 25, 2002 to: January 31, 2002</td><td rowspan="2">Date of report:
22. 2. 2002
Received at ESRF:</td></tr>
<tr><td>Shifts:
15</td><td>Local contact(s):
Dr. Nicoleta Galatanu</td></tr>
<tr><td colspan="3">Names and affiliations of applicants (* indicates experimentalists):
V. Holy, Z. Bochnicek*, P. Klang* , Masaryk University Brno, Czech Republic,
G. Bauer, . Stangl*, Z. Zhong*, Kepler University Linz, Austria</td></tr>
</table>

Report:

The fabrication of semiconductor nanostructures represents a vivid field, as it promises new devices due to broad possibilities of band engineering. In particular, self-organized nanostructures are appealing due to their high density and virtually vanishing defect concentration.

Here we present a study of structure of buried self-organized Ge islands in Si/Ge/Si layer structures, since a capping Si layer above the array of the Ge islands is necessary for optoelectronic applications. The crucial point in the growth of capped Ge islands are their structural changes during the overgrowth by the Si layer. During the overgrowth, the changes both in the island shape and the chemical composition are expected. From a preliminary investigation using cross-sectional transmission electron microscopy (TEM) it follows that during overgrowth an interdiffusion between the island lattice and its neighbourhood takes place. Consequently, the width of the island base increases and the height decreases, so that the aspect ratio of the island decreases.

For the investigation of buried Ge islands we have used coplanar high-resolution x-ray diffraction (XRD). In comparison with TEM, the diffraction method is non-destructive and it probes a larger sample area, so that the island parameters have higher statistical relevance. The XRD is also sensitive to the strain in the lattice around and in the islands, from which the chemical composition of the islands can be deduced. The measurements have been carried out at the beamline ID10B at a wavelength of $\lambda = 1.55$ Å. The diffracted wave was analysed by means of an one-dimensional position sensitive detector. We have investigated a series of three Si/Ge/Si samples. In all of them, a nominally 5 monolayer thick Ge layer was deposited by molecular beam epitaxy on a thick (001) Si buffer. Then, a 150 nm thick Si capping layer was grown, at temperatures of 460^{o}C, 540^{o}C and 630^{o}C. We have measured asymmetric coplanar diffractions 224 and 404, the resulting intensity reciprocal space maps are plotted in Fig 1. We we can resolve distinct peaks caused by the islands (denoted "I") in addition to sharp substrate peaks ("S") in reciprocal Si lattice points and the coherent crystal truncation rods. The position of the peak I depends on the strain in the island lattice and in the neighboring Si matrix and it corresponds to the mean elastic relaxation of the island lattice. The shape of the peak depends on the island shape; the larger the island dimension, the narrower is the peak width in the corresponding direction. It is obvious that with increasing temperature of the overgrowth the elastic relaxation of the islands decreases, which corresponds to a transition from a high narrow island with large aspect ration and relatively large elastic relaxation to a broad and flat islands with negligible relaxation. The strcutre of the islands overgrown at higher temperatures is therefore similar to a two-dimensional strained layer.

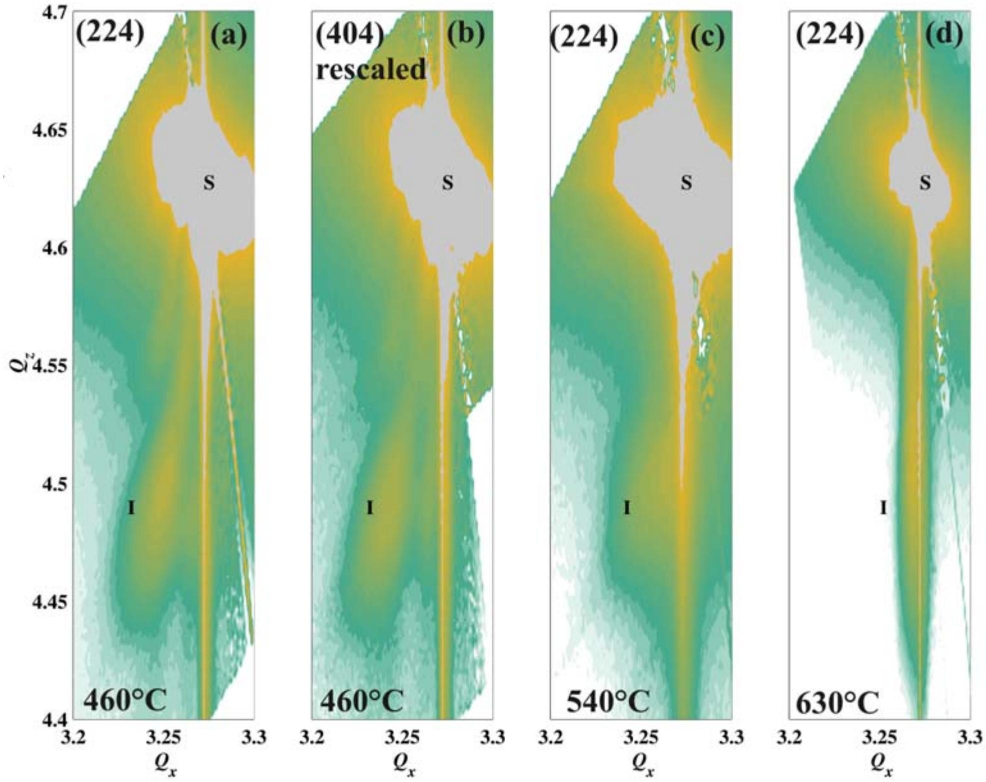

Figure 1. The reciprocal space maps obtained in coplanar diffractions 224 (a,c,d), and in diffraction 404 (b) for samples with various overgrowth temperatures. I and S denote the island and substrate peaks, respectively. In order to compare the positions of the I peaks in 224 and 404 diffractions, the values of Q_x in the panel 2 were divided by $\sqrt{2}$.

A detailed information on the island shape and chemical composition can be obtained by a comparison of the measured reciprocal space map with numerical simulations. We have performed these calculations using kinemtical diffraction and continuum elasticity [1,2]. From the comparison it follows that increasing the overgrowth temperature from 460°C to 630°C the diameter of the island base increases from 70 nm to 160 nm and the island height decreases from 15 nm to 6 nm. Due to interdiffusion during the overgrowth, a SiGe alloying in the islands takes place; the Ge concetration increases from the island bottom to the top. The bottom Ge concentrations range from 40% (for 630°C ovegrowth temperature) to 60% (460°C), the concentrations at the island top is between 50% (after 630°C overgrowth) and 85% (460°C).

In Fig. 1 we also compare the reciprocal space maps in diffractions 224 and 404, the azimuthal directions of the scattering planes of these maps differ by 45°. The lateral distance of the island and substrate peaks is proportional to the length of the lateral component $\mathbf{h}_{||}$ of the diffraction vector $\mathbf{h}$. In order to visualize the azimuthal dependendence of the lateral elastic relaxation in the island lattice we have divided the in-plane component of the scattering vector $\mathbf{Q}$ by $\sqrt{2}$ in the 404 map, since $|\mathbf{h}_{||}(404)| = \sqrt{2}|\mathbf{h}_{||}(224)|$. From the figure it is obvious that the strain distribution around the island is nearly cylindrically symmetric, since the corrected position of the I-peak does not depend on the azimuth. Numerical calculations performed for islands with pyramid-like and paraboloid-like shapes showed that the actual shape of the overgrown islands lies between a pyramid and a rotationally symmetric shape, i.e., the overgrowth causes a rounding of the originally flat crystallographic facets.

In summary, we have found that an overgrowth of self-organized Ge islands by a Si capping layer changes substantially both the island shape and its chemical composition. If, however, the overgrowth temperature is kept sufficiently low, a strain status of the overgrown islands similar to uncapped ones can be preserved.

[1] T. Wiebach, M. Schmidbauer, M. Hanke, H. Raidt, R. Koehler, H. Wawra, Phys. Rev. B 61, 5571 (2000).
[2] A. Hesse, J. Stangl, V. Holy, T. Roch, G. Bauer, O. G. Schmidt, U. Denker, Phys. Rev. B, submitted.