ESRF

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:**

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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.

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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.

ESRF	**Experiment title:** Determiantion of strain and composition in the wetting layer between self-assembled SiGe islands on Si(001)	**Experiment number**: SI1055
Beamline:	**Date of experiment**: from: 28.01.2005 to: 04.02.2005	**Date of report**: 17.02.2005
Shifts: 18	**Local contact(s)**: Dr. Baerbel Krause	*Received at ESRF:*

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Report:

Standard surface-sensitive x-ray scattering methods such as grazing-incidence small angle scattering (GISAXS) and grazing-incidence diffraction (GID) are frequently used for the structure investigations of self-assembled semiconductor quantum dots (see [1] for a review). Using these methods, the shape and elastic strain in the dots can be determined. Measuring GID at two different energies (close to and far from the absorption edge of a chosen element), the local chemical composition of the dots can be obtained [2] (anomalous x-ray scattering). These methods, however, are not sufficient for a study of the microscopic atomic structure of the dot lattice, for which x-ray absorption spectroscopy methods (EXAFS or XANES) are more appropriate. In order to study the local atomic structure in a given position in the dot, a combination of the spectroscopy with diffraction must be used – diffraction anomalous fine structure method (DAFS) [3,4]. In this method, the intensity of the radiation diffracted in a given point in reciprocal space is measured as a function of energy in a vicinity of the absorption edge. From the measured data, the local arrangement of the atoms can be determined in a volume of the dot, having a given strain (iso-strain volume). Especially, one can distinguish the spectroscopy signal stemming from the dot itself from that of the wetting layer.

The purpose of the measurement SI1055 was to measure DAFS of a series of samples with Ge self-assembled quantum dots grown by molecular beam epitaxy (MBE) on a Si(001) substrate under various growth temperatures. From the DAFS spectra, we have expected to determine the local Ge content in the dots and in the wetting layer and its dependence on the growth conditions, as well as the atomic ordering in various positions in the dot lattice. The samples have already been investigated by anomalous x-ray scattering [5], from which we have determined both the shape and the vertical profile of the Ge content.

The DAFS measurements have been performed in GID geometry in the vicinity of the in-plane diffraction 220. In order to prevent the oxidation, the sample was kept in He atmosphere during the measurement. We have used a low-resolution analyser crystal (graphite) behind the sample to suppress the fluorescence background. The DAFS signal was measured by a scintillation counter, the detector slit was open in the direction perpendicular to the sample surface, so that the measured signal was integrated over a broad range of the exit angles α_f. The incidence angle α_i of the primary radiation was kept constant during the DAFS scans, its value was close to the critical angle of total external reflection for the energy of the GeK absorption edge. X-ray fluorescence was measured simultaneously by a solid-state detector. The DAFS data were normalized to the primary intensity using a beam monitor (ionization chamber) in front of the sample. The DAFS measurements were carried out around the GeK absorption edge (11.1 keV) in the energy range from 11.0 to 11.4 keV, with

angular positions of the sample and the analyzer were changed simultaneously with the change of energy.
In Fig. 1 we show the DAFS spectra of two samples. Both samples were grown by MBE at MPI Stuttgart (dr. M. Stoffel) with the growth rate of 0.04 monolayers/s and they consist of a single Ge layer on Si(001). In sample s1896, the Ge layer is nominally 9 monolayers thick, the growth temperature was 650°C; in sample s2322 the thickness of the Ge layer is 10 monolayers and the growth temperature is 740°C. In both samples, Ge domes grew at the sample surface; due to the different growth temperature, we expected different local Ge concentrations in the domes.

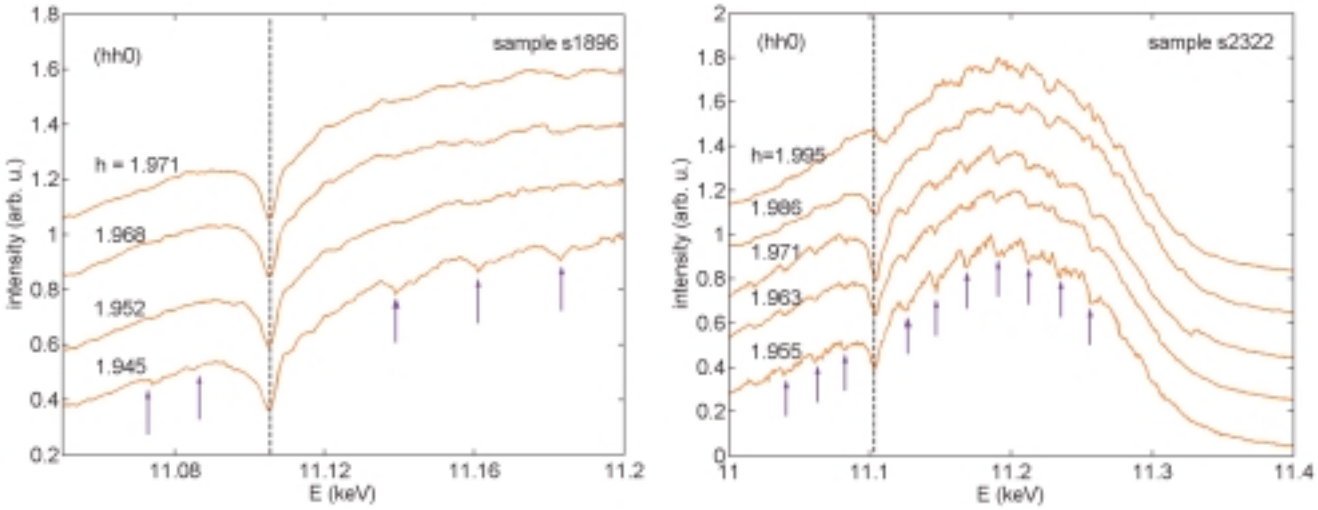

Fig. 1 DAFS spectra measured in the vicinity of in-plane 220 diffraction in two samples. The spectra are shifted vertically for clarity. The vertical dashed line represents the GeK absorption edge; the blue arrows denote the instrumental oscillations

From Fig. 1 it follows that, in sample s2322, the energy of the GeK absorption edge changes with the radial position in reciprocal space. This change can be ascribed to the chemical shift caused by different Ge concentrations in the dot base (h = 1.995) and in the remaining dot volume. The dot base is laterally strained so that the corresponding diffracted intensity occurs close to the substrate peak, and the Ge concentration there is rather low [5], while the dot volume (with larger Ge content) is laterally relaxed so that the corresponding intensity maximum appears for lower h. The dependence of the chemical shift on the local Ge content can be obtained theoretically by an ab-inito calculation of the photoelectron density of states or by comparing the measured position of the edge with the measurements on concentrations standards. This will be the subject of the next measurements.
The local neighborhood of Ge atoms in a given iso-strain volume could be determined from EXAFS oscillations in the DAFS spectra above the absorption edge. We have indeed observed intensity oscillations in the measured spectra (the blue arrows in Fig. 1); however, these oscillations are probably caused by an instrumental instability, since they are present also below the edge. Unfortunately, these instrumental oscillations did not allow to analyze the EXAFS oscillations. We expect to repeat the DAFS measurements as soon as this device instability is removed.

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