ROBL-CRG	**Experiment title:** **X-ray diffraction and reflectivity studies of Si/SiGe based quantum cascade structures**	**Experiment number:** **20_02_610**
Beamline: BM 20	**Date of experiment**: from: 18.06.2003 to: 24.06.2003	**Date of report**: 20.08.2003 *Received at ROBL:* *20.08.03*
Shifts: 18	**Local contact(s)**: Dr. David Dekadjevi (e-mail: dekadjevi@esrf.fr)	

Names and affiliations of applicants (* indicates experimentalists):

G. Bauer, M. Meduna*, G. Chen*, *Institute of Semiconductor Physics, J.Kepler University, Linz, Austria*

C.V. Falub*, *Laboratory for Micro- and Nanotechnology, Paul Scherrer Institute, Villigen, Switzerland*

D. Dekadjevi*, N. Schell*, *ROBL beamline at ESRF, Grenoble, France*

Report:

High Ge composition $Si/Si_{1-x}Ge_x$ (x=80%) superlattices are important for design flexibility of SiGe based quantum cascade lasers. In this experiment, we focused on the **annealing behavior of strain compensated $Si/Si_{1-x}Ge_x$ multiple quantum well (MQW) structures with high Ge composition (x=80%), grown on $Si_{0.5}Ge_{0.5}$ pseudo-substrates**. These structures have been investigated by **x-ray small angle scattering** and high resolution x-ray diffraction (**XRD**) in a coplanar setup. XRD is sensitive mainly to the strain and x-ray small angle scattering, e.g. x-ray reflectivity (XRR) is only sensitive to the morphology of interfaces. Such superlattices which are originally designed for their photoluminescence and tunneling properties remain enormously highly strained, and are in a metastable regime. Thus, a study on the temperature dependence of the Ge inter-diffusion is desirable and XRR measurements are very suitable for the investigation of inter-diffusion.

The investigated samples contained MBE-grown (300°C) MQW's with 30 periods of $Si_{0.2}Ge_{0.8}$ (83.3Å)/Si (50Å) grown on a $Si_{0.5}Ge_{0.5}$ graded relaxed pseudo-substrate. The superlattices were strain symmetrized by the system of layers graded up to $Si_{0.2}Ge_{0.8}$ situated below the MQW and above the MQW in reversed order, in order to avoid the formation of misfit dislocations in the MQW. We have performed a series of XRR and XRD measurement for the samples *in-situ* annealed at different temperatures, in order to obtain the evolution of interfaces during annealing and to find a temperature limit, at which the strain and inter-diffusion start to affect the structure.

X-ray reflectivity and diffraction reciprocal space maps (**RSM**) have been obtained at room temperature and during annealing for temperatures ranging from 600°C up to 830°C for different annealing periods, using a wavelength λ=1.5405 Å. We have used a small furnace with a Be dome available at ROBL, to perform the *in-situ* annealing study. A **position sensitive detector** was used, in order to record the scattering signal intensity. We have found, that significant changes in reflectivity RSMs start to appear around a temperature of 790°C. At lower temperatures (<700°C), we did not observe any change in the reflectivity for 4 hours. However, the change in scattered intensity in RSM was so fast while the temperature was reaching 830°C, that only two maps could be measured. Fig. 1 shows a whole set of reflectivity RSMs corresponding to different annealing temperatures and time, i.e., room temperature (a), 800°C (b), 830°C (c), and 830°C for 35 minutes (d), where the MQW structure disappeared. In fig. 2, a series of specular reflectivity curves, obtained as cuts from RSMs, are plotted for temperatures 790°C (a) and 830°C (b). The notable difference in the velocity of structure evolution under the above two annealing temperatures could be seen clearly. At 790°C the structure disappeared after 330 min annealing, while at 830°C the structure disappeared after 35 min. We have also performed a series of XRD RSMs at different temperatures. The evolution of diffraction signals around (224) reciprocal space point is depicted in the fig. 3. It is evident that significant changes in the diffraction RSMs already start to appear at temperature 735°C. This means that the **changes in the strain**

status precede the inter-diffusion processes, considering the fact that, the structure has almost disappeared in diffraction after 2 hours at 780°C, while in XRR the signal from the periodical structure is still observable.

As a **conclusion**, the results of our experiment exhibit that the ***critical temperature for Ge inter-diffusion in $Si_{0.2}Ge_{0.8}$ is likely around 790°C*** although the strain status of the MQW already starts to change at 735°C.

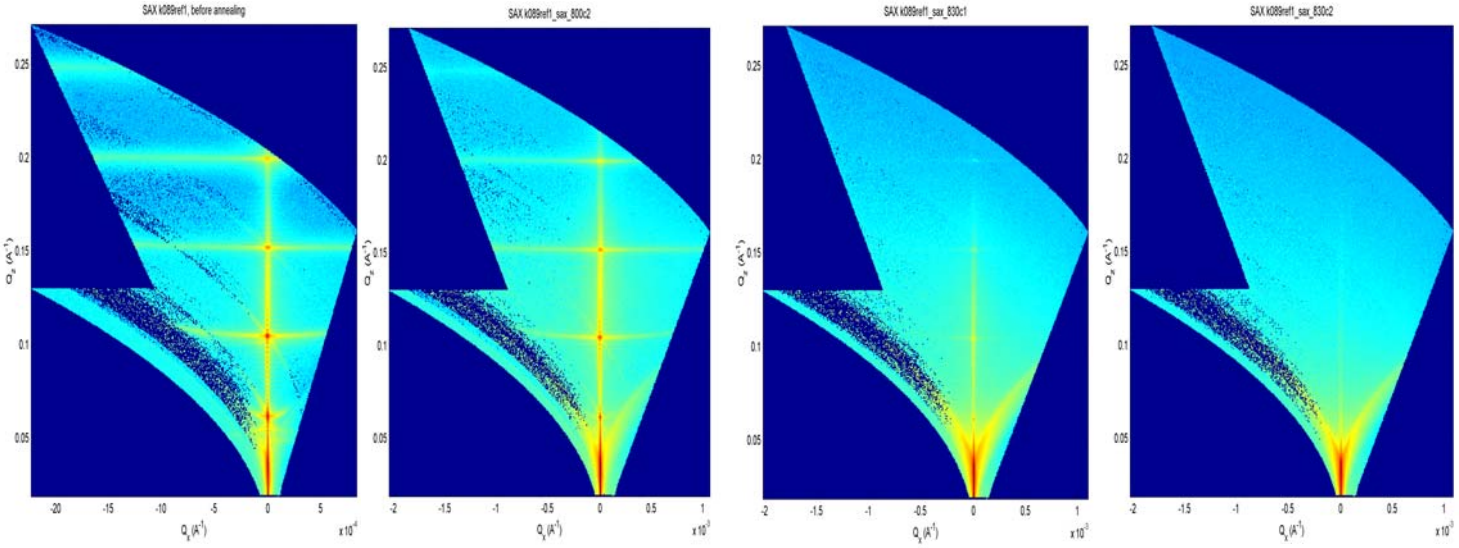

Fig. 1: Series of examples of XRR reciprocal space maps at room temperature (a), 800°C (b), 830°C (c) and 830°C after 35 min (c). The measurement interval between (b) and (c) was about 50 min.

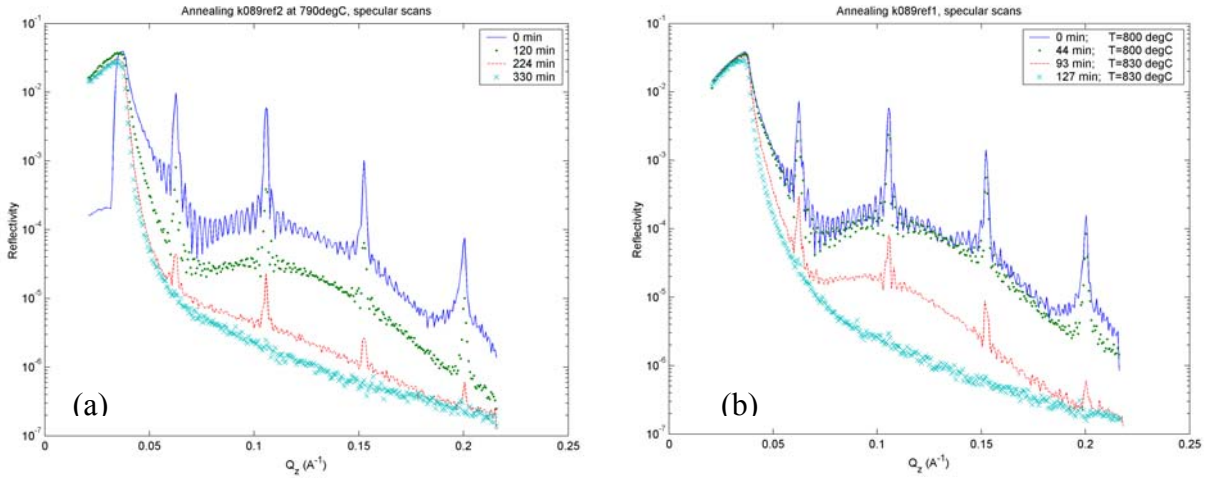

Fig. 2: Cuts of specular reflectivity from XRR reciprocal space maps at temperatures 790°C, 800°C and 830°C.

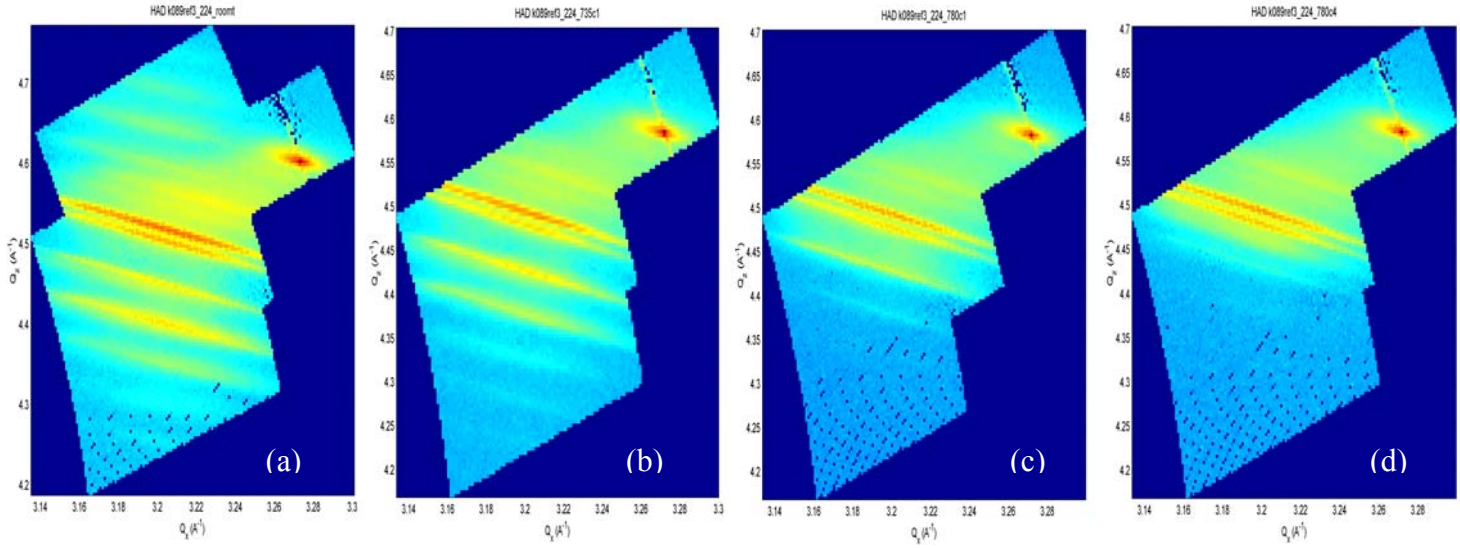

Fig. 3: Series of reciprocal space maps in asymmetrical (224) diffraction at room temperature (a), 735°C (b), 780°C (c) and 780°C after 125 min (d). The time interval between (b) and (c) was about 75 min.