ESRF	**Experiment title:** Interdiffusion studies in $Si_{1-x}Ge_x$ alloys with high Ge content by x-ray diffraction	**Experiment number:** SI-1617
Beamline: BM 20	**Date of experiment:** from: 30.8.2007 to: 5.9.2007	**Date of report:** 21.12.2007
Shifts: 18	**Local contact(s):** Carsten BAEHTZ (baehtz@esrf.fr)	*Received at ESRF:*

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Report:

The mechanism of interdiffusion and diffusion processes in SiGe alloys including self and impurity diffusion and interdiffusion coefficients are known with very low precision and only for low Ge content SiGe alloys. The situation is complicated mainly by the non-linearity of the diffusion process. The diffusion coefficient strongly depends on Ge content and also on strain. Since the diffusion coefficient can be written in the shape of Arrhenius equation, the problem reduces to the determination of activation energy and diffusion prefactor for certain Ge content and strain. In our recent experiments, we have reported the study of interdiffusion in $Si_{0.5}Ge_{0.5}$ and $Si_{0.75}Ge_{0.25}$ alloys but the data for the range from 50% to 100% of Ge were still missing in the literature. In this experiment, we have performed the in situ x-ray diffraction (XRD) measurements on SiGe multiple quantum wells (MQW) with average Ge content 70% and 90%. These studies will extend the knowledge about interdiffusion in Ge rich SiGe alloys and are very important for diffusion modeling of complicated SiGe electronic structures.

Two types of samples were investigated; 70% Ge samples contained MBE-grown (300°C) MQW's with 30 periods of $Si_{0.45}Ge_{0.55}$ (160Å)/Ge (80Å) bilayers grown on a $Si_{0.30}Ge_{0.70}$ constant composition relaxed pseudo-substrate and 90% Ge samples contained $Si_{0.15}Ge_{0.85}$ (160Å)/Ge (80Å) bilayers grown on $Si_{0.10}Ge_{0.90}$ pseudo-substrate. The superlattices were strain symmetrized in order to avoid the formation of misfit dislocations in the MQWs. We have performed a series of XRD measurement for the samples annealed *in-situ* at different temperatures in the range from 620°C up to 720°C. We have obtained the evolution of Ge content during annealing and found a temperature limit, at which the inter-diffusion started to affect these structures.

X-ray reflectivity and diffraction reciprocal space maps (RSM) have been obtained at room temperature and during annealing for different annealing periods, using a wavelength λ=1.5405 Å. We have used a small furnace with a Be dome available at BM20, in order to perform the *in-situ* annealing study. A position sensitive detector was used, to record the scattering signal intensity.

An example of XRD RSM around (224) diffraction point recorded at room temperature before annealing is shown in Fig. 1(a). XRD RSM of 90% Ge sample after annealing at temperature 710°C for 1.5 hour is shown in Fig. 1(b). In Figs. 1(c-d), the evolution of Bragg peaks during annealing of 70% sample at 710°C and 90% sample at 650°C are presented showing the difference in ***inter-diffusion velocity*** in these samples. It is evident that the interdiffusion process is much stronger in samples with the higher Ge content. The simulations of diffraction signal along Q_z cuts are plotted together with the measured ones also in Figs. 1(c-d) for both investigated structures. Results of these fits confirm the high quality of the samples and the fact the MQWs stay pseudomorphic during the annealing.

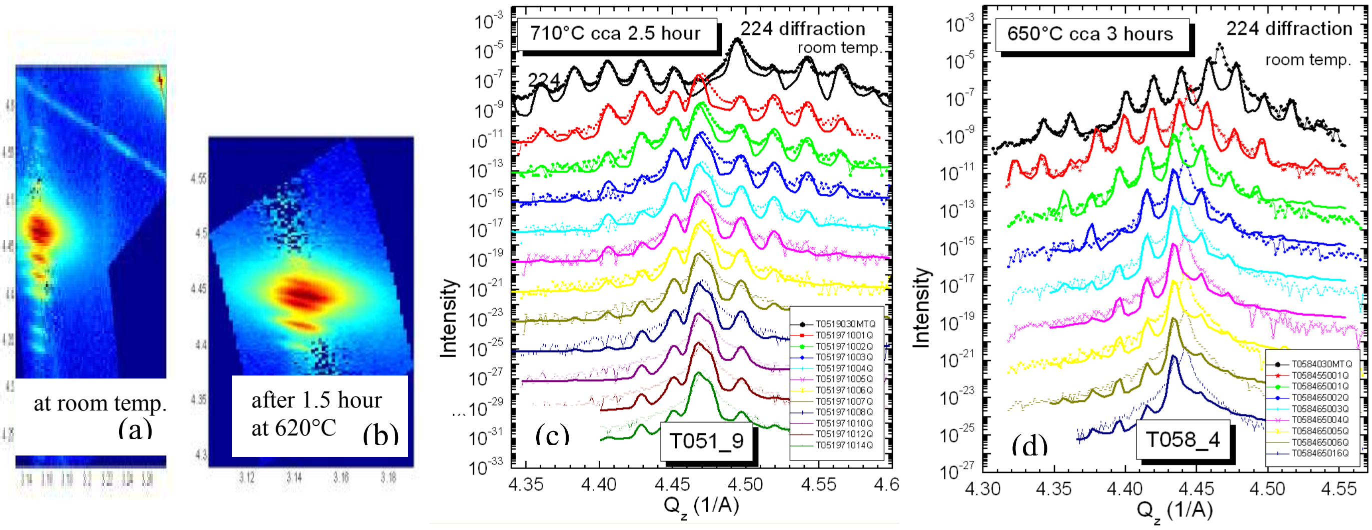

Fig. 1: XRD reciprocal space map around 224 diffraction of MQW sample with Ge content 90% (a) at room temperature and (b) after 1.5 hour of annealing at 620°C. (c)-(d) evolution of the diffraction pattern cuts in direction paralel to Q_z across the pseudosubstrate peak for 70% Ge (sample T051_9) and 90% Ge (sample T058_4) of Ge content. These figures show that the interdiffusion is definetely stronger in samples with higher Ge content.

From the simulations of XRD scans we have obtained the decay of maximum contrast of Ge content $\Delta\rho$ in the MQW. From the slope of exponential decay of $\Delta\rho$, we have determined the diffusion coefficients for all 6 various temperatures measured in the range 630°C - 720°C by 70% Ge samples and for 4 various temperatures measured in the range 620°C - 650°C by 90% Ge samples. The typical time of one measurement cycle was in the range from 5 to 25 min, nevertheless for slower diffusion processes only selection of measured maps was involved into analysis.

The series of obtained diffusion coefficients at different temperatures has allowed estimating the activation energy E_A and the diffusion pre-exponential factor D_0 for $Si_{0.3}Ge_{0.70}$ and $Si_{0.1}Ge_{0.90}$. Since the MQW was annealed up to a detection limit of diffraction satellites, we can assume that the structure was almost interdiffused at the last stage of annealing and only the Ge content of the pseudosubstrate (± 5%) was present inside the structure. The obtained values of activation energy E_A and the diffusion pre-exponential factor D_0 are shown in the Figs. 2(a-b) together with the results obtained in our previous experiments.

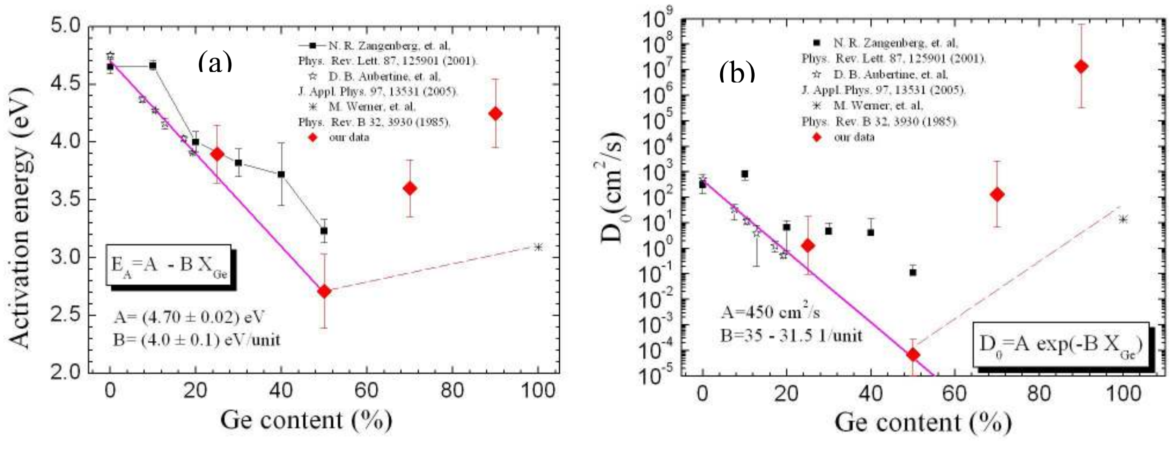

Fig. 2: (a) Activation energy E_A and (b) diffusion prefactor D_0 versus Ge content X_{Ge}. A comparison is made between values obtained in our experiments for X_{Ge}=25%, 50%, 70% and 90% (red diamond point) and recently published data determined for different Ge concentrations. The full line represents the extrapolation of data from Aubertine et al.. The dashed line represents just a guide for the eye from our data at 50% to data published for pure Ge. The data obtained in this experiment correspond to the points at 70% and 90% of Ge content.