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Report:

The detailed investigation of Si/SiGe multiple quantum wells (MQW) is important for the design of the more complicated SiGe based cascade emitter structures. Since such emitters are usually exposed to high temperatures during device operation, it is very important to determine the temperature stability and diffusion properties of this quantum cascade laser (QCL) structures, usually grown strain symmetrized on SiGe pseudosubstrates. At high temperatures, the metastable QCL structures can suffer strain relaxation through dislocation formation and the interface roughness can change as well. Thus the temporal evolution of Si/SiGe interfaces and Ge content at various temperatures as obtained by x-ray reflectivity (XRR) and diffraction (XRD) are desirable for determining of diffusion processes in these structures.

In this experiment, we focused on the annealing behavior of strain compensated $Si/Si_{1-x}Ge_x$ MQW structures (x=30%) with different multilayer periods, grown on $Si_{0.25}Ge_{0.25}$ pseudo-substrates. These structures have been investigated by XRR and XRD in a coplanar setup. XRD is sensitive mainly to the strain and x-ray small angle scattering, e.g. x-ray reflectivity is only sensitive to the morphology of interfaces. Thus we have performed a series of XRR measurements for the samples with different periods *in-situ* annealed at different temperatures, in order to obtain the evolution of interfaces during annealing depending also on layer thickness in the structure.

The two investigated samples contained MBE-grown (300°C) MQW's with 30 periods of $Si_{0.7}Ge_{0.3}$ (5nm)/Si (1nm) (sample K012) or $Si_{0.7}Ge_{0.3}$ (11nm)/Si (2.2nm) (sample K014), grown on a $Si_{0.25}Ge_{0.25}$ graded relaxed pseudo-substrate. The superlattices were strain-symmetrized by the system of layers graded up to $Si_{0.7}Ge_{0.3}$ situated below the MQW and above the MQW in reversed order, in order to avoid the formation of misfit dislocations in the MQW. The samples with such parameters were originally designed for investigations of intersubband transitions between the light hole 1 and the heavy hole 1 state (at *k*-vector values not equal to zero), which results in an emission in the 100 µm wavelength region.

X-ray reflectivity and diffraction reciprocal space maps (RSM) for both structures have been obtained at room temperature and during several isothermal annealing processes for temperatures ranging from 550°C up to 824°C, 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.

An example of XRR RSM recorded at room temperature before annealing is shown in Fig. 1(a). The simulations of specular reflectivity extracted from reflectivity RSMs are shown in Fig 1(b) for both investigated samples at room temperature. Results of these fits confirm the high quality of the samples with

the interface roughness up to 0.8 nm. In Figs. 1(c-e), the evolution of Bragg peaks during annealing of sample K012 at 711°C and sample K014 at 710°C and 784°C are presented showing the difference in ***critical temperature for Ge inter-diffusion*** in these samples. The selected Bragg peaks in Figs. 1(c-e) were zoomed from the series of specular scans extracted from RSMs obtained during annealing.

We have also recorded XRD RSMs of sample K012 before and after annealing and at temperatures 600°C and 690°C. An example for diffraction signals around (224) reciprocal space point before and after annealing K012 is depicted in the Fig. 1(f-g). It is evident from diffraction signal that the structure stays pseudomorphic during annealing.

From the series of isothermic *in-situ* annealing measurements we have observed, that significant change in reflectivity RSMs, corresponding to the inter-diffusion in $Si_{0.7}Ge_{0.3}$/Si layers, depend on the individual layer thickness. In sample K012 with the smaller period, the disappearance of the Bragg peaks starts to be observable much earlier, already at a temperature of 690°C and the diminishing of the multiplayer peaks continues at higher temperatures, see Fig.1(c).

During annealing of the sample K014, the complete diminishing of the Bragg peaks started to be significant above temperature 750°C. At lower temperatures (~700°C), we also observed changes in the reflectivity of the sample K014, but only in the envelope curve of Bragg peaks. The evolution of the envelope curve of Bragg peaks, corresponding most likely to the Si/SiGe interface shift, saturated after about 2hours at 700°C and next significant change appearing after 12hours when increasing the temperature to 784°C, see Fig. 1(e). As a conclusion, the results of our experiment exhibit that the ***critical temperature for Ge inter-diffusion in $Si_{0.7}Ge_{0.3}$ is depends most likely on the thickness*** of the individual layers in the structure and ***varies within the interval from 700°C to 800°C*** for samples with MQW periods 5.8 – 12.5 nm. The further analysis of the data and detailed description of the diffusion process is currently in the progress.

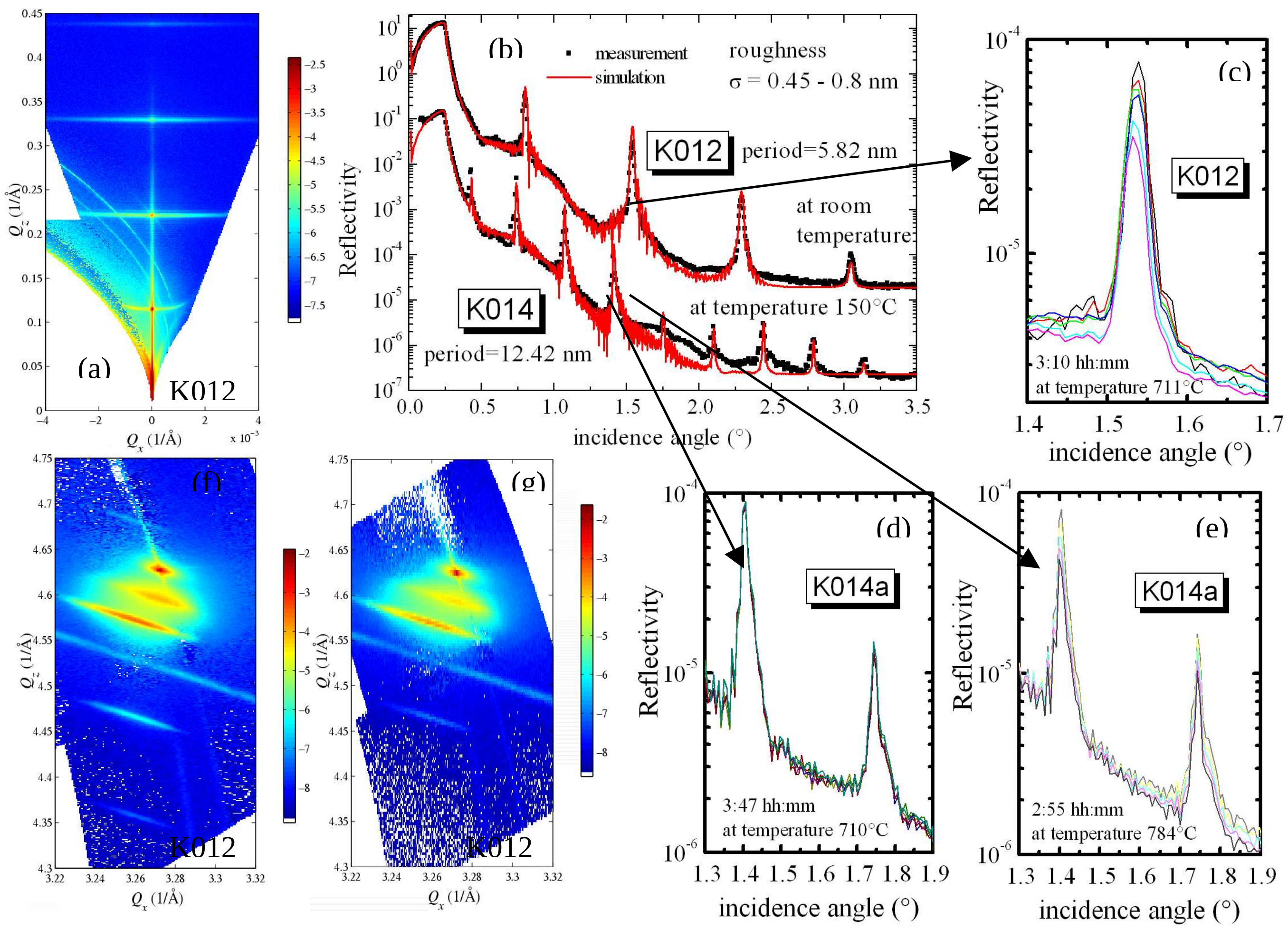

Fig. 1: (a) XRR reciprocal space map of sample K012 at room temperature; (b) simulations of specular reflectivity of measured samples at initial annealing temperatures; (c) evolution of the 2nd Bragg peak during annealing of the sample K012 at 711°C; (d)-(e) evolution of the 2nd and 3rd Bragg peaks during annealing of the sample K014 at 710°C and 784°C; (f) XRD (224) reciprocal space maps of the sample K012 after 5 hours annealing at 700°C. (g) XRD (224) reciprocal space maps of the sample K012 after total 14 hours of annealing at 700°C, 750°C and 780°C.