X-Ray Investigation of Interface Broadening by Rapid Thermal Processing

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Quantum cascade lasers (QCLs) [1] – [3] can be tuned by post-growth rapid thermal processing. Interdiffusion at the barrier-well interfaces in the temperature range between 850 and 875 °C shifts the energy levels and thus the gain and emission wavelength of the structure in the range from 10.3 to 11.9 μ m [4]. The diffusion has been investigated quantitatively by high-resolution x-ray diffraction measurements. Rocking curves ($\omega - 2\theta$) measured on a thermally processed set of samples confirm Al-Ga intermixing at the interfaces.

Because of the complexity of QCL structures, the x-ray measurements were done on a periodic superlattice structure. The structure period of 35 nm GaAs ($n_{Si} = 5 \times 10^{15} \text{ cm}^{-3}$) and 5 nm Al_{0.4}Ga_{0.6}As ($n_{Si} = 3 \times 10^{15} \text{ cm}^{-3}$) is repeated 60 times and buried under 300 nm GaAs ($n_{Si} = 1 \times 10^{17} \text{ cm}^{-3}$). Prior to the RTP, all samples were covered with 200 nm SiO to prevent outdiffusion of As. Four different pieces were then heat-treated for 60 s at 850, 875, 900 and 950 °C in forming gas atmosphere. After heating the samples to 200 °C, the temperature was ramped to 650 °C with 37.5 °C/s and then to the target temperature with 20 °C/s.

X-ray diffraction $\omega - 2\theta$ spectra were measured using a high-resolution double crystal diffractometer. CuK α 1 radiation was used and a 0.2° receiving slit in front of detector served to increase the signal-to-background ratio. The data were recorded around the GaAs (002) substrate reflection where we can achieve suitable contrast due to larger difference between the scattering factors of Al and Ga.



Fig. 1: X-ray diffraction ω – 20 scans around the GaAs(002) reflection. The measured curves are shifted in y-direction for clarity. Due to a slight period inhomogeneity over the wafer, the satellites do not appear at the exactly the same angular positions.

Figure 1 shows series of measured data curves for as-grown and heat treated periodic superlattice structures. The main substrate peak at zero arcsec is accompanied by several of superlattice peaks at constant angular separation, which represent the reciprocal space picture of the superlattice in the growth direction. Higher order satellites, at larger angular distance from the substrate peak, provide information about the finer details of the interfaces. By increasing the order, the satellite heights decrease due to their broadening. Therefore, we have used integrated intensities of satellites for the analysis of the data. The measured data were fitted with a computer calculation using dynamical x-ray diffraction theory with the layer thicknesses and AI content as fit parameters (Fig. 2a). The envelope of the calculated pattern matches very well with the envelope curve of the integrated satellite intensities. The modulation of the envelope curves shows a systematic decrease with the RTP temperature. This effect corresponds to an increase of AI-Ga interdiffusion at the AIAs/GaAs and GaAs/AIAs interfaces. The AI concentration gradients at the interfaces were included into fitting model by simple linear gradients. Results of fitting of the envelope curves of the measured data are shown in Fig. 2 (b). The increase of the interface width (compared to the asgrown sample). Δw. is plotted vs. temperature. Already at 850 °C and 875 °C, the interface width has increased by about 1 nm (3.6 monolayers) and 2.5 nm (8.9 monolayers), respectively.



- Fig. 2: (a) X-ray ω 20 spectrum of as-grown sample. The integers indicate the order of the superlattice satellites. Dots are the integrated satellites intensities; dashed curve is the calculation.
 - (b) Change of the AlAs/GaAs interface width Δw due to RTP.

Si as a dopant as well as a constituent of the SiO layer that was applied for RTP is known to increase the Al-Ga interdiffusion.[5] – [7] Therefore, the interdiffusion width of the investigated superlattice is presumably somewhat higher than it would be for a sample without any Si. In the QCLs, on the other hand, the active region is separated by a 3.2 μ m thick layer from the highly doped (n_{Si} = 4 x 10¹⁸ cm⁻³) cap layer. Thus, the interdiffusion in QCLs should not be enhanced by Si. Therefore, the values obtained by x-ray diffraction measurements for the reference sample represent an upper limit for the interdiffusion.

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