Structural Investigation of Si/SiGe Quantum Cascade Structures

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We have investigated the structural properties of Si/SiGe electroluminescent quantum-cascade structures, by means of x-ray reflectivity and diffraction. The cascade structures were grown at a comparatively low temperature of T = 350 °C to avoid misfit dislocation formation. Despite an overall thickness of the cascade structures of about 9000 Å and Ge contents of up to more than 40% in some of the SiGe wells, the as grown stack of layers is indeed pseudomorphic with respect to the Si substrate. The analysis of x-ray reflectivity data yields a rather small r.m.s. interface roughness below 3 Å throughout the cascade structures. An annealing study of the structures was performed in order to determine the allowable thermal budget during processing. It was found that the structures are highly metastable, and annealing at 600 °C for 10 minutes leads already to partial plastic relaxation.

1. Introduction

Recently it has been shown that the concept of quantum cascade structures (QC), which has first been demonstrated for InGaAs/InAlAs [1], can be extended to the Si/SiGe system [2]. In QC structures, the optically active transitions occur within one band, between subbands formed in a sequence of quantum wells, under applied bias. In strained Si/SiGe heterostructures grown pseudomorphically on Si, considerable band offsets exist only in the valence bands of light and heavy holes. Recently, Si/SiGe based QC emission structures exhibiting well-resolved electroluminescence in the 10 µm wavelength range and linewidths down to 22 meV have been demonstrated [2].

To achieve a high emission efficiency of such QC emission structures, all design parameters (quantum well thicknesses and Ge contents) have to be met very accurately and with rather precise layer to layer reproducibility. In QC emission devices, an active unit consists of an injector, the active quantum well, and a collector. These units are repeated several times, thus making up rather complex many-layer heterostructures.

Despite the lattice mismatch of 4.17% between Ge and Si and the large overall thickness of QC structures, plastic strain relaxation has to be avoided, because dislocations represent nonradiative recombination sites. Furthermore, any change of the strain state alters the band alignment, which is crucial for QC devices. To avoid dislocation formation, the growth temperature has to be kept rather low. The resulting structures are highly metastable, and thermal treatment, e.g., during subsequent processing steps, may lead to plastic relaxation as well. Hence the thermal budget allowable without degradation of the structures is an important parameter.

2. Experimental

The cascade structures were grown using molecular beam epitaxy at a substrate temperature of 350 °C on high resistivity Si (001) substrates with a very small miscut of about 0.1° and with a miscut azimuthal direction of 3° off the [100] direction. Details on growth and the electroluminescence can be found in Ref. [2].

The interface roughness in these sample has been investigated from reciprocal space maps in x-ray reflectivity (XRR) geometry (Fig. 1, left panel). The intensity is peaked into so-called resonant diffuse scattering (RDS) sheets. Their width along q_z is inversely proportional to the vertical correlation length, giving a measure of how far the interface morphology in the multi layer stack is replicated. Obviously, the width of these sheets depends on q_x. The right panel of Fig. 1 shows this dependence for several scans taken from the maps in the indicated position. The width follows very well a quadratic increase as a function of q_x [3]. From this analysis, we find that in the roughness spectrum, higher spatial frequencies are replicated to a lower extent than those with low spatial frequencies [4]. With interface roughnesses below 3 Å throughout the whole stack [4], the structural quality of the investigated sample is very high.

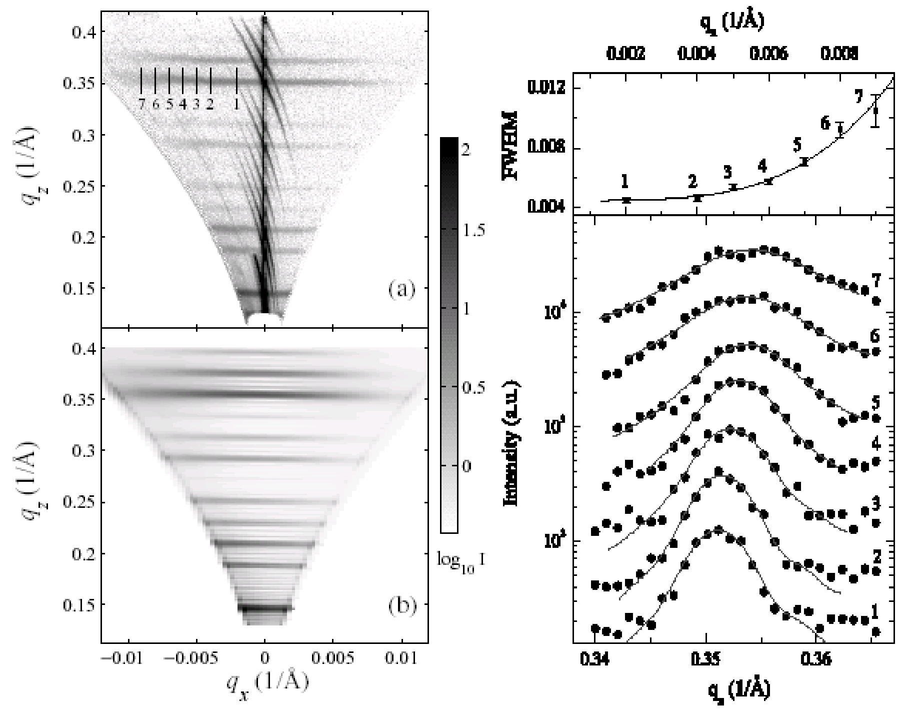

Fig. 1: Left panel: reciprocal space map in XRR geometry of the as grown cascade structure (a), and simulated diffuse intensity distribution (b). The correlated interface roughness leads to intensity sheets along q_x. Their width along q_z as a function of q_x is shown in the right panel for the selected positions as indicated. The increase indicates a decrease of correlation for decreasing roughness wavelengths.

In order to prove the pseudomorphic growth, high resolution x-ray diffraction (XRD) reciprocal space maps were recorded. We have used reciprocal space mapping around the symmetric (004) and asymmetric (224) reflection, shown in Fig. 2, left panel. The diffraction pattern due to the superlattice appears at the same q_x position as the Si substrate peak, and the width of the intensity distribution along q_x is rather small, i.e., with a similar FWHM as that of the Si substrate. These two facts indicate that the entire cascade structure is grown coherently with the in-plane lattice parameter being the same in all layers of the sample.

However, due to the large number of SiGe layers, the total strain is rather large, and the structure is highly metastable. Therefore we performed an annealing study, in order to determine the thermal budget allowable for such cascade samples during subsequent processing steps. We have annealed the sample in high vacuum conditions for 10 minutes at temperatures of 500 °C and 600 °C, respectively. In order to monitor a possible relaxation, we recorded reciprocal space maps around the (224) reflection in coplanar geometry (Fig. 2). The left panel shows the pseudomorphic as-grown structure. The center panel for the piece annealed at 500 °C already shows an increase in the diffuse scattering, but no significant shift of the superlattice peaks with respect to the Si substrate peak. In the right panel, plastic relaxation is clearly visible for the piece annealed at 600 °C: the superlattice peaks are broadened, and the whole pattern is shifted towards higher q_x (lower absolute value), indicating an increase in the in-plane lattice parameter in the multi layer stack. Hence for these cascade structures, annealing at 500 °C for several minutes is the limit of thermal budget in order to keep a pseudomorphic layer structure and avoid dislocation formation, which would be detrimental for the optoelectronic performance.

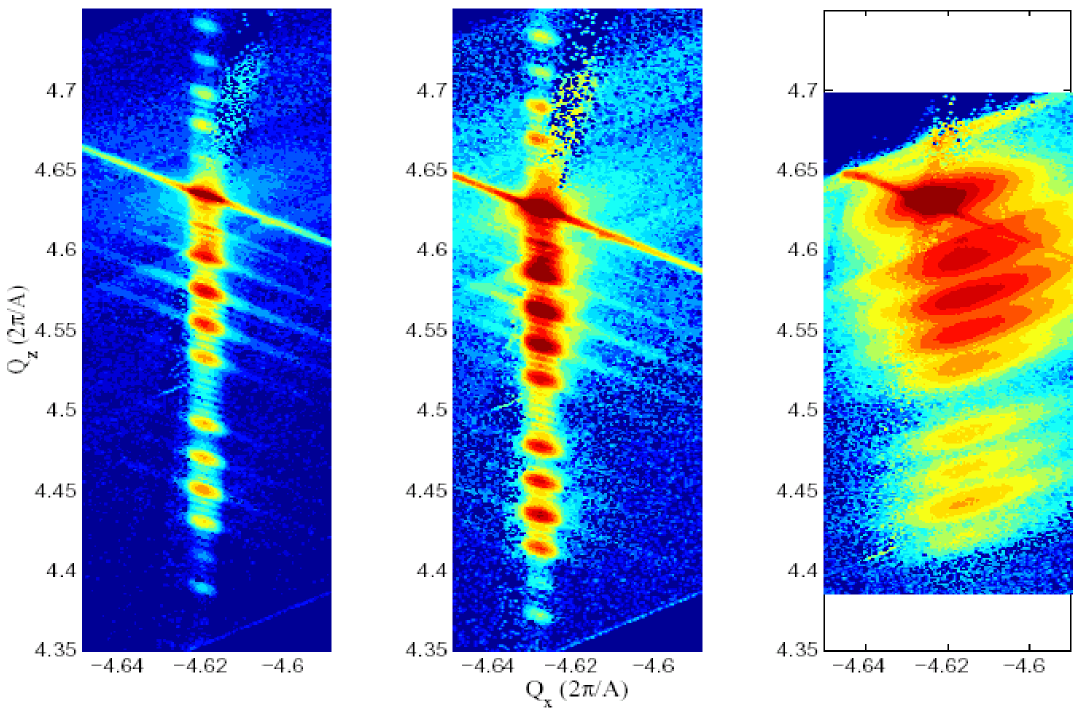

Fig. 2: Reciprocal space maps around the (224) reflection for the as-grown cascade structure (left), and after annealing for 10 minutes at 500 °C (center) and 600 °C (right).

3. Conclusion

The x-ray diffraction and reflectivity data investigations demonstrate a high degree of structural perfection of the Si/SiGe quantum cascade structures. The whole multilayer stack with a total thickness of more than 900 nm and an average Ge content of about 10% grows pseudomorphically on the (001) Si substrate. The Si/SiGe interfaces are rather smooth, with r.m.s. roughness values of about 2.5 Å. The vertical correlation length of the interface roughnesses is of the order of the thickness of two cascades (about 600 Å) for long range interface fluctuations (> 1500 Å) but corresponds only to one cascade, i.e., to 300 Å for short range lateral fluctuations (< 900 Å). Very smooth interfaces have been achieved despite a growth temperature of the Si/SiGe multilayers as low as 350 °C, and consequently the structures are well suited for observing intersub-band cascade emission. However, the structures are highly metastable against thermal treatment. An annealing study showed that a thermal budget in device processing up to about 10 min. at 500 °C is tolerable, before plastic relaxation leads to a degradation of the structures.

Acknowledgements

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