Si/SiGe Layers on Patterned Substrates for MODFET Applications

Y. Zhuang, P. Mikulik, V. Holý, G. Bauer

Institut für Halbleiterphysik, Johannes Kepler Universität Linz, Austria

R. Hammond, T. E. Whall, E. H. C. Parker

Department of Physics, University of Warwick, Coventry, England

We present a systematic study on the strain status of Si channel in Si/SiGe MODFET structures grown on mesa structures with lateral dimensions ranging from 3 to 20 µm, as well of its surface morphology. With decreasing mesa size, the surface undulations flatten and the in-plane strain of the Si channel is decreased.

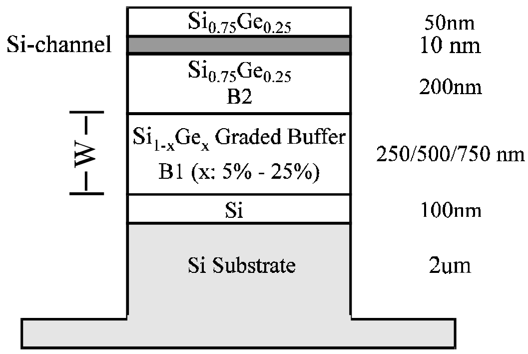
1. Introduction

In Si-channel n-MODFET structures, a two dimensional electron gas is confined in a strained about 100 Å thick Si layer [1]. For tensile strain, the six-fold degenerate conduction band of Si is split into a two-fold Δ2 and a fourfold Δ4 state. The confining potential for the electrons in this Si-channel layer is determined by the conduction band offset between the SiGe barrier and the Δ2 states of strained Si. In order to achieve the desired strain status, usually a graded SiGe buffer layer is deposited on (001) Si, on top of which a constant composition SiGe layer is deposited, followed by the Si channel and finally a modulation doped SiGe layer on top. The grading rate of the Ge content, the thickness of the graded layer (B1) and of the constant composition buffer (B2, see Fig.1) determine the amount of strain relaxation and thus the in-plane lattice constant of the top B2 SiGe layer. The subsequently grown Si channel is pseudomorphic, i.e. biaxially tensily strained with respect to buffer B2. The plastic relaxation of the SiGe buffer layer is through misfit dislocations, the stress fields of which give rise to the roughening of the epilayer and consequently also of the interface to the strained Si layer [1], [2] . The resulting cross-hatch surface or interface morphology has a lateral periodicity of typically 1 µm in the two orthogonal <110> directions, with rms heights of about 20 – 50 Å [2]. Too high values of this surface roughening might be not fully compatible with planar integrated circuit technology.

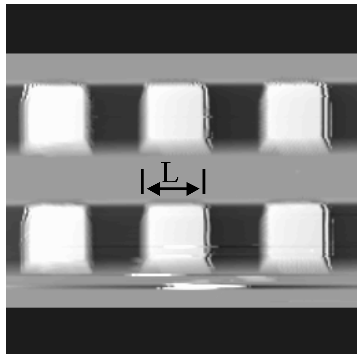
A concept for Si-based heterostructure devices has been developed, in which such devices could be integrated with conventional Si MOS technology on the same wafer (chip) by growing the layer sequence for heterostructure in selected areas. However, the quality of these devices always suffered from the high density of defects induced by the large lattice mismatch between Si and Ge. It has been found that reducing the lateral dimensions of the growth zone results to a dramatic decrease in the defect densities [3]. In this paper we describe a systematic study both of the strain status of the Si layer containing the 2D electron gas and of the surface morphology as a function of the lateral dimensions.

2. Experimental

The layer sequence as shown in Fig. 1 was grown on arrays of square Si (001) mesa pillars, oriented along the <110> directions, with lateral dimensions of 3, 4, 6, 10, 20 µm and for comparison also on an unpatterened region. The mesas were etched to a depth of 2 µm. By molecular beam epitaxy a Si buffer layer was deposited, followed by the graded SiGe buffer region (5 – 25%, with thicknesses ranging in three sample series from 250, 500 and 750 nm). A 200 nm thick SiGe buffer layer with constant Ge composition was followed by the 10 nm thick strained Si channel and a 50 nm thick SiGe layer for the n-type dopant Sb followed by a Si cap layer. The growth temperature was 550°.



(a)



(b)

Fig. 1: (a) Sketch of a MODFET grown on lateral patterned sample; (b) Top view on the sample with (10 * 10) μm^2 mesa size by AFM.

From x-ray reciprocal space maps we have determined the in-plane lattice constant of the top SiGe buffer layer and thus strain status of the Si channel. The data for series of mesas with the 750 nm thick B1 buffer layer are shown in Fig. 2.

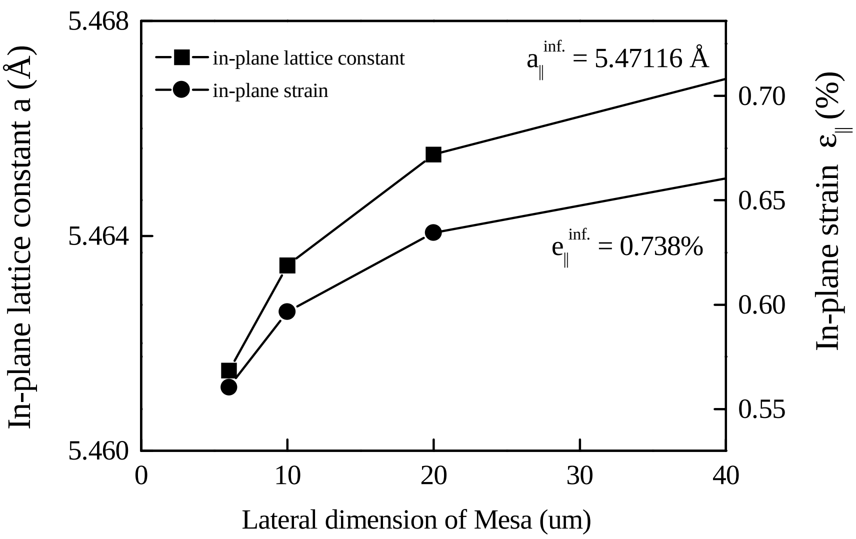
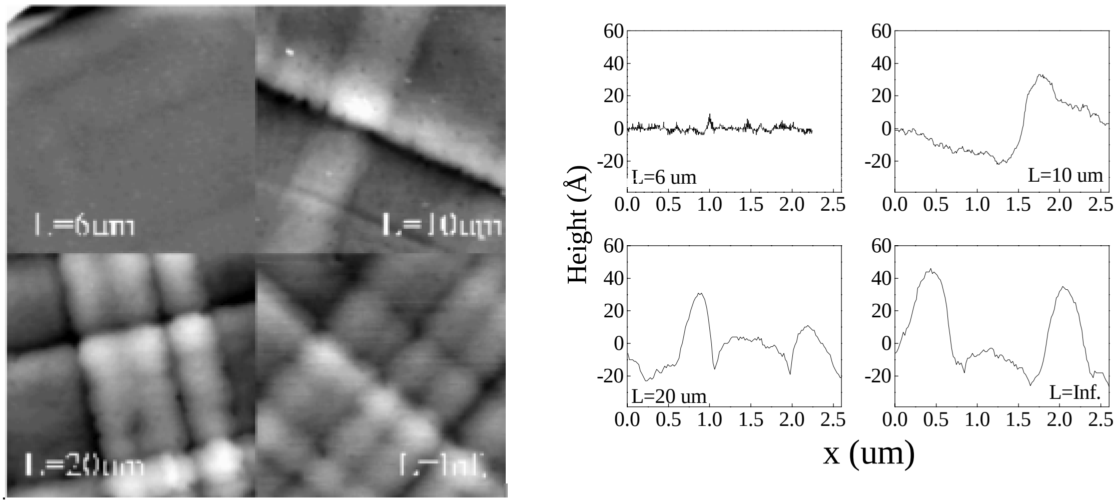


Fig. 2: In plane lattice constant ($a_\parallel$) and strain($\varepsilon_\parallel$) of Si-channel vs. mesa size. $\varepsilon_\parallel = (a_\parallel - a_{si})/a_{si}$. a_{si} is the cubic Si lattice constant.

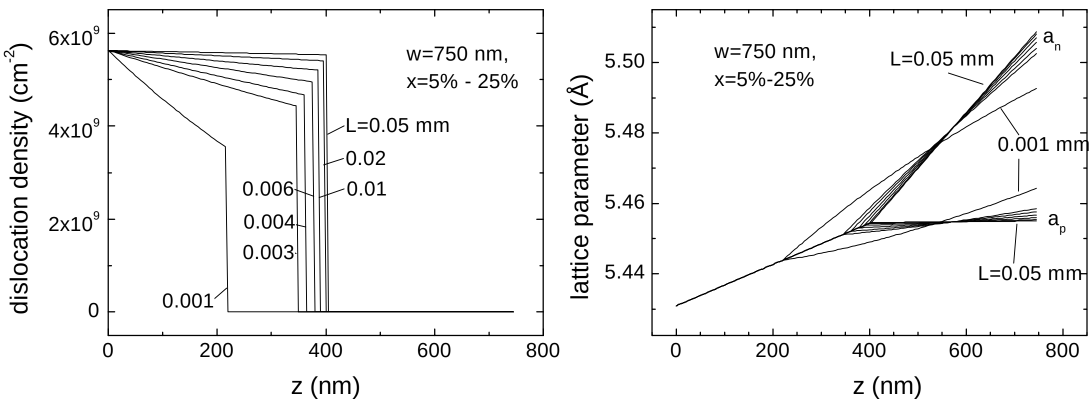
With decreasing mesa size the in-plane lattice constant and thus the in-plane strain in the Si channel decreases, causing a decrease of the confining potential. Below 6 µm mesa size, due to the simultaneous SiGe growth on the Si substrate beneath the etched pillars, the data cannot be reliably interpreted. In Fig. 3 the surface morphology from atomic force microscopy is shown for a samples sequence with mesa sizes from 6 µm to 20 µm and for layers grown on the unpatterned substrate. The line scans exhibit remarkable differences: For the smallest mesa size of 6 µm, in an area of 2.6 x 2.6 μm^2 no cross hatch pattern is visible and the line scan shows a quite smooth surface morphology. With increasing mesa size the troughs and hills due to the cross hatch formation cause the observed surface undulations. However, the smoother surface morphology for mesa size below 10 µm is accompanied with less SiGe relaxation of the SiGe buffer layers, and thus a decreased tensile strain of the Si channel.



(a) (b)

Fig. 3: (a) Surface morphology of samples with different mesa size from 6, 10, 20 µm and for growth on unpatterned substrate (B1: 750 nm thick). (b) Line scans (height modulation) for these samples.

In principle for the strain relaxation in the SiGe buffers grown on mesas two mechanisms have to be considered which mainly affect the strain in the upper Si layer, namely the elastic strain relaxation due to the limited mesa size, and at the same time the decrease of the misfit dislocation density with shrinking lateral dimension. The first mechanism increases the lateral strain in the Si layer, while the second one decreases it. In order to model these trends we have calculated the dislocation density profile by minimizing the total deformation energy (the elastic energy and the energy due to the line tension of dislocation) on the basis of a phenomenological assumption of the elastic relaxation (degree of relaxation decreases exponentially from the bottom towards the free surface of the mesa). According to Tersoff [4], we obtained this profile as shown in Fig. 4 (a). Limiting the lateral mesa size, we decrease the dislocation density in the relaxed part of the buffer. In Fig. 4 (b) the lattice constant as a function of the z-coordinate in the graded buffer B1 above the Si substrate is plotted for different mesa sizes. One can distinguish regions for which the elastic relaxation dominates (for $z > 550$ nm, for the 750 nm thick graded B1 layer) from regions where the decrease of the dislocation density with decreasing lateral mesa size dominates (for $z < 500$ nm). From the experimental data it follows that actually the second mechanism dominates in the samples studied. This is actually unfavorable for the total biaxial strain in the Si channel. Apparently for achieving a better correspondence between the calculations and the experimental data a more detailed finite element calculation of the strain status has to be performed.



(a) (b)

Fig. 4: (a) Dislocation density profile vs. depth in the graded buffer B1 for various mesa sizes L. (b) Lattice constants of B1(in plane: a_p and vertical: a_n) vs. z-coordinate. Origin of z-coordinate lies in the interface between Si buffer layer and B1 layer.

3. Conclusion

From the series of experiments on the strain status of Si/SiGe MODFET structures grown on mesa like pillars we draw the following conclusions: For mesa sizes below about 10 µm, the lateral period of the cross hatch pattern is substantially enlarged. The surface undulations are decreased. However, the reduction of dislocation density is accompanied by a decrease of the absolute value of the in-plane strain in the Si channel. In the samples studied, elastic relaxation might alter these conclusions for sufficient small mesa size does not yet play an important role.

Acknowledgements

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References

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