Study of Relaxation of Strain in Patterned Structures using X-Ray Diffraction Technique

Aaliya Rehman Khan, J. Stangl, G. Bauer, D. Buca[1], B. Holländer[1], H. Trinkaus[1], S. Mantl[1], R. Loo[2], M. Caymax[2]

Inst. for Semiconductor Physics, Johannes Kepler University Linz, Altenbergerstr. 69, A-4040 Linz, Austria
[1]Institut für Schichten und Grenzflächen (ISG1) and cni – Center of Nanoelectronic Systems for Information Technology, Forschungzentrum Jülich GmbH, D-52425 Jülich, Germany
[2] IMEC, Kapeldreef 75, B-3001 Leuven, Belgium

$Si/Si_{1-x}Ge_x$ heterostructures on Si substrates are of great interest for device applications. The lattice mismatch of 4.2% between Si and Ge is interlinked with strain in the $Si/Si_{1-x}Ge_x$ layers grown on Si (100) substrates, hence such layers may be used as virtual substrates for the growth of. strained silicon. Biaxial, tensile strained Si on such virtual substrates shows a large enhancement of the electron mobility, due to tensile strain and a resulting type II band alignment. Record electron mobility has been measured in Si channels on SiGe buffer layers[1,2]. On the other hand, improvement of the hole mobility is observed for uniaxially, compressively strained silicon [3].

In many cases, graded SiGe buffer layers with constant composition buffers on top are used as such psuedosubstrates. Using rather elaborate preparation techniques, low threading dislocation densities as small as 2×10^6 cm^{-2} have been achieved [4], but buffers fabricated by this approach suffer from very long growth times, mechanical stresses due to thermal strain (see below) and wafer bending. Furthermore, these layers exhibit a strong so-called cross-hatch pattern with amplitudes up to 100 nm, which is incompatible with the fabrication of integrated circuits.

On the other hand, varying the Ge concentration and/or the strain conditions between epitaxial over layers and the substrate also provides a means to adjust valence and conduction band offsets, because strain modifies the electronic band structure. It has been seen that He^+ ion implantation and annealing of pseudomorphic Si/SiGe/Si can be successfully used to relieve strain [5]. Cavities induced by the He^+ ions act as sources of dislocations spreading out through the SiGe layer upon annealing and forming a strain relieving network of misfit dislocations.

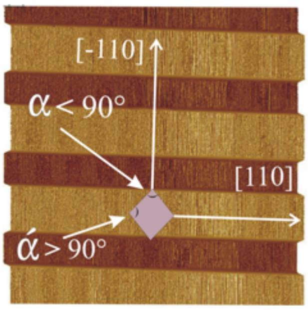

Figure 1: AFM image of a patterned sample with stripe width 2.9 µm. The inset shows the deformation of the unit cell within the stripe.

The aim of the presented work is to characterize patterned $Si/Si_{1-x}Ge_x$ samples with respect to the residual strain, and identify the strain conditions wherein the asymmetric relaxation of the patterned lines transforms the biaxial stress into nearly uniaxial stress for very narrow lines. In order to initiate the reverse strain relaxation process a He^+ implantation into the Si(100) substrate is conducted followed by an annealing step. During this process a narrow defect band is generated underneath the SiGe/Si substrate interface. It provides a high density of dislocations loops as sources for misfit dislocations (MDs) yielding efficient strain relaxation during annealing with low densities of threading dislocations (TDs) [6].

We employed high-resolution x-ray diffraction to study the relaxation of strain and to assess the structural quality of a series of SiGe striped samples with varying stripe widths from 0.82 to 100 µm, patterned in [110] direction on the (001) substrate using standard optical lithography and etching. We see that the strain in the stripes in the two orthogonal directions is different, i.e., the crystal structure of the stripes is orthorhombic. En route, we also determine precisely the Ge content in the SiGe layers.

We recorded reciprocal space maps in coplanar XRD geometry around the (004) and (224) Bragg reflection in two orthogonal [110] azimuths. Precise measurements of the momentum transfer **Q** corresponding to the individual layers are made from the RSMs. We calculate the lattice parameters of the different layers, as listed below. The measurements show that strain relaxation in the SiGe stripes with line width smaller than approx. 20 µm becomes asymmetric between [110] directions parallel and perpendicular to the stripes, leading to a transition from the tetragonal to an orthorhombic unit cell. Thus, one can envision a new concept of enhancing the hole mobility based on an asymmetry of the stress in patterned pseudosubstrates.

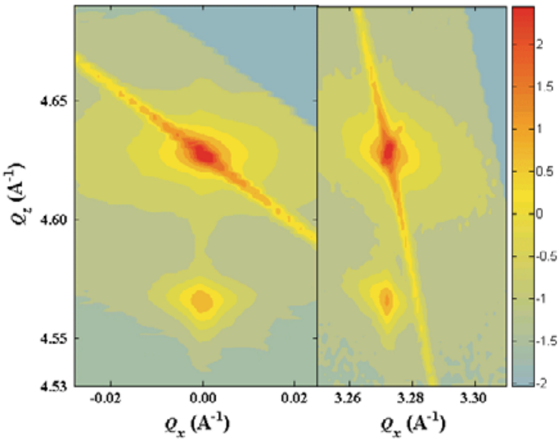

Figure 2: Reciprocal Space Map around 004 and 224 Bragg peaks for sample with stripe width 2.9 µm.

Table I. Lattice parameters and degree of relaxation of SiGe stripes of various widths

Stripe Width (µm)	$\overline{a}_{\parallel}$ (Å) [-110]	$\overline{a}_{\parallel}$ (Å) [110]	$\overline{a}_{\perp}$ (Å)	R% [-110]	R% [110]
0.82	5.457	5.432	5.506	52	2.3
1.4	5.449	5.433	5.507	39	5.2
2.9	5.459	5.431	5.505	57	0.9
3.2	5.462	5.449	5.505	61	36
10	5.460	5.447	5.498	61	33
20	5.458	5.455	5.496	57	52
100	5.466	5.464	5.489	70	70
None	5.466	5.468	5.488	75	78

[1] K. Ismail, M Arafa, K.L. Saenger, J.O. Chu, B.S. Meyerson, Appl. Phys. Lett. **66**, 1077 (1995).
[2] G. Höck, M. Cück, T. Hackbarth, H.J. Herzog, E. Kohn, Thin Solid Films **336**, 141 (1998).
[3] S.E. Thompson, *et al.*, IEEE EDL **25**, 191 (2004).
[4] M.E. Groenert, *et al.*, J. Appl. Phys. **93**, 362 (2003).
[5] D. Buca, B. Holländer, *et al.*, App. Phys.Lett. **85**, 2499 (2004).
[6] H. Trinkaus, *et al.*, Appl. Phys. Lett. **76**, 3552 (2000).