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Asymmetric strain relaxation in patterned SiGe layers: A means to enhance carrier mobilities in Si cap layers

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Strain relaxation in patterned $Si_{0.77}Ge_{0.23}$ stripes grown on Si(001) by chemical vapour deposition was investigated after He^+ ion implantation and annealing. Ion channeling measurements indicate asymmetric strain relaxation with a significantly higher residual strain parallel to the stripes than perpendicular to the stripes. These results are confirmed by plan view transmission electron microscopy showing a much higher density of misfit dislocations running along the stripes than across the stripes. Estimates based on a piezoresistivity model indicate significant enhancements of electron and hole mobilities for asymmetrically strained Si cap layers on such SiGe stripes. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2431702]

Application of stress is an efficient method to enhance carrier mobilities in semiconductors. Epitaxially grown Si on a relaxed SiGe buffer layer shows symmetric (two-dimensionally isotropic) biaxial stress and a substantially larger electron mobility[1] which increases with increasing stress. On the other hand, stressor layers on transistors produce uniaxial stress and enhance the hole mobility.[2] When biaxially stressed silicon on SiO_2 is patterned into small structures, strain relaxation preferentially along the shorter dimensions is observed.[3] Asymmetric stress relaxation via plastic flow was also observed for patterned Si/SiGe stripes on viscoelastic glass.[4] In this letter we will present a method to fabricate strongly asymmetrically strained silicon with improved mobilities for electrons and holes.

We have recently shown that in thin Si layers on SiGe/Si heterostructures, high biaxial tensile stresses can be generated by "strain transfer" from the relaxing SiGe layer to the Si layer.[5] The efficiency of this process was studied as a function of the Si layer thickness. The strain induced in the Si layer upon relaxation of the SiGe layer was described by

$$\varepsilon_{Si} = \eta R x f_{Ge,Si}. \quad (1)$$

Here $f_{Ge,Si}=4.2\%$ is the lattice mismatch between Ge and Si, R is the degree of relaxation of the $Si_{1-x}Ge_x$ epilayer, and η is the "strain transfer efficiency" which was shown to reach 100% for Si layer thicknesses below about 10 nm.

A key step in this strain transfer process is strain relaxation in the SiGe epilayers. We have recently shown that this can be efficiently achieved by He^+ ion implantation and subsequent thermal annealing.[5,6] In a model of this process,[6] we have assumed that the narrow defect band formed upon ion implantation underneath the SiGe/Si-substrate interface provides a high density of dislocation loops during annealing, part of which glides to the interface and evolves from there into dislocation arms consisting of segments of misfit dislocations (MDs) in the interface and threading dislocations (TDs) through the strained SiGe layer. The stress driven propagation of the TD segments through the SiGe layer along the [110] and [−110] directions is associated with an extension of the corresponding MD segments involving an increasing strain relaxation. Interaction and mutual annihilation of TD segments result in a reduction of the TD density to an acceptably low level.[7] In the final state, a long MD consists of the trails of many TDs. Accordingly, the final MD density and the corresponding level of strain relaxation are determined by the density of the loops contributing as dislocation sources and the average path length of the TDs before they annihilate or stop.

Since the probabilities for both the generation of loops with different but crystallographically equivalent Burgers vectors and the average path lengths of the resulting dislocations extending in the two in-plane ⟨110⟩ directions are equal, the relaxation of the SiGe layer is symmetric (isotropic), i.e., the SiGe crystal structure remains tetragonal during relaxation. Our model suggests that this symmetry can be broken by patterning the SiGe layer into micrometer narrow [110] stripes for which the average path length of TDs moving in the [−110] direction would be shortened by the two stripe boundaries, resulting in a reduction of the MD density in this direction and a corresponding reduction of the degree of relaxation in the [110] direction. This idea is illustrated in Fig. 1.

In the present letter, we report on a study of asymmetric stress relaxation in patterned SiGe stripe structures on Si(001) wafers. Epitaxial Si/$Si_{0.77}Ge_{0.23}$ (6 nm/180 nm) heterostructures were grown on Si(001) by chemical vapor deposition in an ASM Epsilon® production tool. The samples were implanted with 7×10^{15} He ions/cm^2 at an energy of 45 keV. Stripes along the [110] direction with widths varying between 0.8 and 10 μm were patterned using standard optical lithography and etching. Finally, the structures were annealed at 850 °C for 10 min in nitrogen to achieve strain relaxation.

The measurement of the strains in the stripe structures turned out to be difficult. Raman spectroscopy provides only an average strain and x-ray diffraction has been shown to

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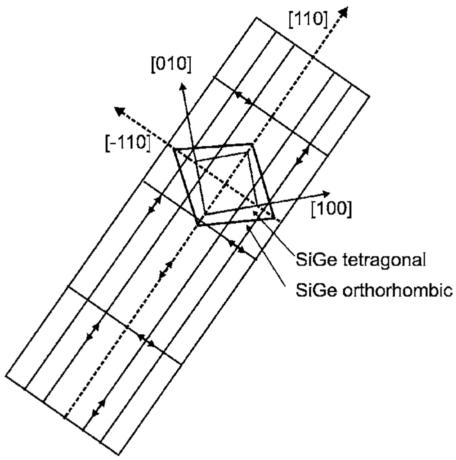

FIG. 1. Illustration of a misfit network after asymmetric strain relaxation in a SiGe stripe on (001) Si. The limitation of the paths of TDs in the [−110] direction by the stripe boundary results in a reduced MD density in this compared to the [110] direction and a correspondingly reduced degree of relaxation in the [110] direction. By this, the square basis of the tetragonal unit cell of the SiGe crystal is distorted to a rhombic basis of an orthorhombic unit cell in the [110]/[−110]/[001] coordinate system.

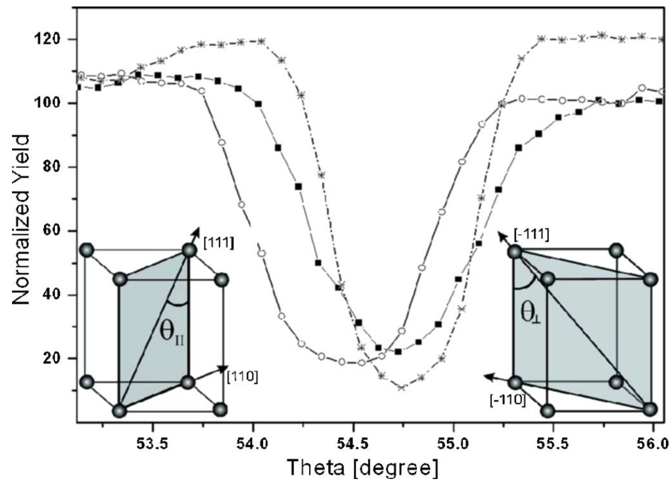

FIG. 2. (Color online) Channeling angular yield scans of the Ge backscattering signal from 0.8 μm stripes measured across (empty circles) and along the stripe (full squares), respectively. The corresponding scan of a cubic Si crystal with its midpoint at 54.74° is shown as reference (star symbols). The insets show the crystallographic directions of the two nonequivalent diagonals with the angles $\theta_\parallel$ and $\theta_\perp$ along the stripe and parallel to the stripes, respectively.

underestimate strain contributions of low MD densities and to overestimate by this the asymmetry.[8] In this work, we employ He ion channeling to measure strains. In detail, we perform ion channeling angular yield measurements of the Ge backscattering signal with a high-precision goniometer using 1.4 MeV He^+ ions at a scattering angle of 170°.

Ion channeling angular yield scans provide absolute angles between various crystal directions and by this the lattice strains.[9] For cubic lattices as unstrained Si or fully relaxed SiGe, the angle between [001] and [111], for instance, has a value of 54.736°. Compressive tetragonal strains in SiGe/Si lead to smaller angles $(54.736° - \Delta\theta)$ with $\Delta\theta < \Delta\theta_{ps}$ where $\Delta\theta_{ps}$ denotes the maximum angular shift realized by the unrelaxed symmetrically stressed, pseudomorphic SiGe layer. For symmetric (isotropic) biaxial relaxation, the degree of relaxation may be defined as $R = 1 - (\Delta\theta/\Delta\theta_{ps})$. We may directly extend this definition to asymmetrically relaxing [110] stripes if we assume the strain tensor to have the (110) and (−110) mirror symmetries of the stripes (as expected for two sets of MDs along [110] and [1−10], respectively). Then two different relaxation degrees, $R_\parallel$ and $R_\perp$, may be defined by the two different changes, $\Delta\theta_{1,2}$ of the angles shifts between [001] and [111], and [001] and [−111], respectively: $R_{\parallel,\perp} = 1 - \Delta\theta_{1,2}/\Delta\theta_{ps}$.

Accordingly, for asymmetrically relaxing [110] stripes, we performed angular scans along the (−110) plane through the [001] and the inclined [111] directions (along the patterned stripe, see Fig. 1) and along the (110) plane through the [001] and [−111] directions (across the patterned stripe). Figure 2 shows channeling angular yield scans of the Ge backscattering signal from a sample with a stripe width of 0.8 μm, both across and along the stripe. A corresponding scan for a cubic Si crystal is shown for reference. The midpoint of each scan represents the absolute angle between the [001] sample normal and the [−111] or the [111] directions, respectively (nonequivalent diagonals). The shift of the midpoint position provides direct evidence for the change of the tetragonal lattice to an orthorhombic lattice structure in the [110], [−110], [001] coordinate system.

The relaxation degrees of the SiGe stripes along, $R_\parallel$, and perpendicular, $R_\perp$, to the stripes are summarized in Table I. Obviously, the strain relaxation depends strongly on the width of the stripes. The very narrow stripes of 0.8 μm in width show nearly full relaxation (95%) perpendicular to the stripe direction but only small relaxation of about 34% along the stripes. The ratio of the two relaxation degrees, $R_\perp/R_\parallel$, has a value of approximately 2.8. For comparison we have

TABLE I. Relaxation degrees, $R_{\parallel,\perp}$, along and perpendicular to SiGe stripes of different widths, together with strains $\varepsilon_{\parallel,\perp}$ and stresses $\sigma_{\parallel,\perp}$ as well as resistivity changes, $\Delta_{\parallel,\perp}$, expected to occur in thin Si cap on the SiGe stripes. $\Delta_{\parallel,\perp}$ values are calculated on the basis of piezoelectric measurements on Si (Ref. 10).

SiGe stripes			Virtual Si top layers					
					Rel. res. change (%)			
Linewidth	Relaxation degree (%)		Strain (%)/stress (GPa)		*n*-Si		*p*-Si	
(μm)	$R_\parallel$	$R_\perp$	$\varepsilon_\parallel/\sigma_\parallel$	$\varepsilon_\perp/\sigma_\perp$	$\Delta_\parallel$	$\Delta_\perp$	$\Delta_\parallel$	$\Delta_\perp$
→∞	70	70	0.68/1.22	0.68/1.22	−59	−59	6.7	6.7
3.2	41	75	0.40/0.75	0.72/1.27	−46	−53	−31	43
2.8	35	77	0.34/0.65	0.74/1.30	−43	−52	−39	50
1.4	45	95	0.43/0.83	0.92/1.60	−54	−63	−46	60
0.8	34	95	0.33/0.65	0.92/1.60	−48	−61	−59	71

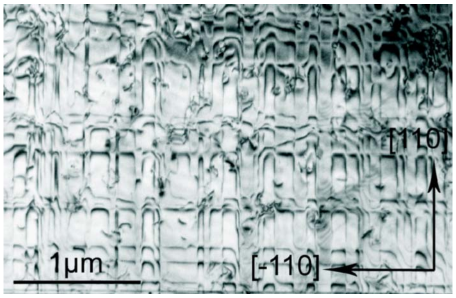

FIG. 3. (Color online) Plan view TEM micrograph of an asymmetric MD array in a 4 μm wide stripe, where the misfit dislocation density perpendicular to the direction of the stripes is about a factor of 2.4 larger than that parallel to the stripes.

included in Table I data for symmetrically relaxed blanket SiGe layers obtained previously.[5]

According to the physical picture described above, this asymmetry in strain relaxation is due to the different path lengths of the TDs propagating along the two in-plane ⟨110⟩ directions. If the TD path in the [−110] direction is limited by the stripe boundary, the density of MDs in this direction is reduced as illustrated by the thin line pattern in Fig. 1. This observation is also confirmed by plan view transmission electron microscopy (PV-TEM). Figure 3 shows a PV-TEM micrograph of a 4 μm wide stripe, where the misfit dislocation density perpendicular to the direction of the stripe is about a factor of 2.4 larger than parallel to the stripe which reflects the ratio of the corresponding relaxation degrees. The asymmetry decreases with increasing stripe width and vanishes when the stripe width becomes larger than the mean TD path length in the blanket layer. Our measurements indicate that this path length is of the order of a few micrometers.

Finally, we discuss the asymmetric strains and stresses and the electronic properties expected to occur in thin Si cap stripes on relaxed SiGe stripes. Assuming for thin Si cap stripes (<10 nm) perfect strain transfer efficiency, we calculate the asymmetric strains along and perpendicular to the stripes, $\varepsilon_{\|,\perp}$, by using $\eta=1$ and $R=R_{\|,\perp}$ in Eq. (1). For our stripe geometry, the asymmetric biaxial stresses $\sigma_{\|,\perp}$ are related to the asymmetrical strains by

$$\sigma_{\|,\perp} = [(C_{11}+2C_{12})(C_{11}-C_{12})/C_{11}](\varepsilon_\| + \varepsilon_\perp)/2 \pm (\varepsilon_\| - \varepsilon_\perp), \qquad (2)$$

where C_{11} and C_{12} denote elastic constants of Si. According to Table I, for our narrow stripes, values as high as $\varepsilon_\perp \approx 1\%$ corresponding to $\sigma_\perp \approx 1.6$ GPa are reached.

So far, no measurements of carrier mobilities in such asymmetrically stressed thin cap layers are available. To get an idea of trends we extrapolate previous piezoelectric measurements on Si (Ref. 10) for tensile stresses up to about 10 MPa to the two orders of magnitude higher stresses expected from our measurements. For our stripe geometry the anisotropic relative resistivity change in the [110] and [−110] directions, $\Delta_{\|,\perp}$, is given by

$$\Delta_{\|,\perp} = (\Pi_{11}+\Pi_{12}\pm\Pi_{11})\sigma_\|/2 + \Pi_{11}+\Pi_{12}\mp\Pi_{11})\sigma_\perp/2, \qquad (3)$$

where Π_{ij} are the piezoresistivity coefficients. The high values of $\Delta_{\|,\perp}$ given in Table I (even though beyond the limits of linear piezoelectricity) indicate significant changes in the carrier mobilities. The stress induced reduction of the relative resistivity change in *n*-Si is comparable for stripe and layer structures, whereas it is substantially larger in *p*-Si for narrow stripes than for layers. For comparison, we have included in Table I values for Si layers with symmetrical biaxial strain obtained previously.[5]

In summary, we have investigated strain relaxation of patterned SiGe stripes after He^+ ion implantation and annealing. Asymmetric relaxation of the SiGe stripes transforms biaxial stress into strongly asymmetric stress for very narrow stripes which should yield to significant improvements of the electron and hole mobilities (Table I). The effect is explained by the limitation of the paths of threading dislocations by the stripe boundary leading to an asymmetric misfit dislocation network.

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