Conversion of strain state from biaxial to uniaxial in strained silicon

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The Raman shift of $\Delta \omega_i$ in (001) strained silicon is found to be independent of the azimuthal angle of the patterned structures but exhibits shape dependence in strain relaxation. The tensile strain is reduced from 0.85% in the unpatterned thin film to 0.16% in the cylindrical pillars showing 82% relaxation. It becomes more significant along the width direction of the patterned gratings due to Poisson’s effect and only a tensile strain of 0.07% remains. Consequently, the strain state changes from biaxial into uniaxial and is expected to enhance the carrier mobility. Finite element analysis is conducted to elucidate the mechanism. © 2011 American Institute of Physics.

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Strained silicon (s-Si) is used to enhance the carrier mobility in very large scale integrated circuits.1-3 Biaxial strain can usually be induced by epitaxial growth of silicon on SiGe.4 The enhancement in the carrier mobility and device performance induced by biaxial strain usually diminishes at high vertical electric fields but can be maintained in the case of uniaxial strain.5 Hence, conversion of the strain state from biaxial to uniaxial in strained silicon is found to be independent of the azimuthal angle of the patterned structures but exhibits shape dependence in strain relaxation. The enhanced carrier mobility and device performance often depend on the azimuthal angles of the patterning.6,7 Whereas patterning may redistribute the strain considerably thereby affecting device performance,8-11 the smaller the features, the stronger is strain relaxation. Symmetrical relaxation often occurs in square and cylindrical pillars, whereas asymmetrical relaxation is usually found in parallel gratings.9 In particular, the strain along the width direction of the gratings is relaxed significantly although that along the length direction changes only slightly in comparison. Hence, it is possible to utilize patterning to produce uniaxial strain in silicon. In this work, the strain relaxation in patterned cylindrical pillars and gratings in (001) s-Si is studied by Raman spectroscopy and finite element analysis. The results reveal that strain relaxation in the width direction of the gratings is larger than that in the cylindrical pillars but the strain in the length direction is almost unchanged. Uniaxial strain can be obtained if the patterned structures have a small width and large aspect ratio.

Owing to the anisotropic elastic properties of single-crystal silicon, the strain relaxation and accompanying Raman shifts may depend on the azimuthal angles of the patterned structures and this issue must first be tackled. With regard to the (001) oriented s-Si, the laboratory and crystal coordinates are the same in which the x, y, and z axes are along the [100], [010], and [001] directions, respectively. In the sample system, the x' and y' axes are parallel and perpendicular to the gratings, whereas the z' (z) axis is along the normal direction, as schematically shown in the inset of Fig. 1. The angle between x and x' or y and y' is the azimuthal angle, $\theta$. Strain induced breaking of the crystal symmetry will lead to the triply degenerate phonon frequency $w_0$ at 521 cm$^{-1}$ splitting into three shifts by $\Delta \omega_i$ ($i=1, 2, \text{and} 3$). The Raman shifts in $\Delta \omega_1$, $\Delta \omega_2$, and $\Delta \omega_3$ corresponding to the vibration eigenvectors along x (TO$_x$), y (TO$_y$), and z (LO$_z$) can be obtained by solving a secular equation if we know the strain components $\epsilon_{ij}$ in the crystal coordinates.12 In the patterned gratings, the strain component in the length direction ($\epsilon'_{zz}$) has almost the original value of $\epsilon_0$ in the s-Si thin film but the strain in the width direction ($\epsilon'_{yy}$) is changed substantially assuming $\epsilon'_{yy} = \alpha \cdot \epsilon_0$. The shear strain component diminishes in the middle of the gratings, that is, $\epsilon'_{ij} = 0$ for $i \neq j$. The stress component $\sigma'_{xx}$ is equal to zero as a result of the free surface condition. Accordingly, we can obtain all the strain components in the crystal system by solving Hooke’s equation and the results are presented in Eq. (1)

![FIG. 1. SEM images of (a) pillars 170 nm in diameter and (b) gratings 170 nm wide together with the schematic diagram of a patterned grating with the crystal and sample systems marked in the inset figure.](Image)
The calculated results indicate that although $\Delta \omega_1$ and $\Delta \omega_2$ depend on the azimuthal angles quite sensitively, $\Delta \omega_3$ is constant for given $\varepsilon_0$ and $\alpha$ and can be expressed as

$$\Delta \omega_3 = \frac{\omega_0 \varepsilon_0 \alpha}{2 (1 + \alpha)} \left( \frac{K_{12} - c_{12} \tilde{K}_{11}}{c_{11}} \right),$$

where $K_{11}$, $K_{12}$, and $K_{44}$ are the phonon deformation potentials and $c_{11}$ and $c_{12}$ are elastic constants and can be found in Refs. 13 and 14. It should be noted that only $\Delta \omega_3$ can be detected from (001) s-Si in the backscattering geometry. Hence, it is not necessary to consider the crystal orientation of the patterned gratings for the strain characterization by Raman spectroscopy. Assuming isotropic strain relaxation for the cylindrical pillars, that is, $\varepsilon_{xx}' = \varepsilon_{yy}' = \alpha \cdot \varepsilon_0$, we obtain the frequency shift in $\Delta \omega_3$ as follows:

$$\Delta \omega_3 = \omega_0 \varepsilon_0 \alpha \left( \frac{K_{12} - c_{12} \tilde{K}_{11}}{c_{11}} \right).$$

Equation (2) and (3) can be used directly to characterize the strain in the patterned structures.

Experimentally, 30 nm thick strained Si fabricated on relaxed Si/Si$_3$Ge$_{0.7}$ substrate was patterned into cylindrical pillars 170 nm in diameter with a spacing of 270 and 170 nm wide rectangular gratings with a spacing of 430 nm using electron-beam lithography and reactive ion etching. Figure 1 depicts the scanning electron microscopy (SEM) images (JEOL JSM-7000F) of the patterned structures. Raman measurements were performed at room temperature in the backscattering geometry on a JY LabRam HR800 spectrometer equipped with a 2400 lines/mm grating and a 325 nm He–Cd UV laser with a power of 30 mW was used. The irradiation time was set as 1 s to avoid overheating. A 15× objective was used to focus the laser spot to about 1 μm in diameter covering about 5 pillars. The final Raman spectra were obtained by averaging data acquired from 5 randomly chosen regions, that is, average of more than 25 circular pillars, so that the measurement uncertainty induced by an individual nonstandard shape could be minimized. The results are shown in Fig. 2. Relative to the Raman peak of bulk Si at 520.7 cm$^{-1}$, that of s-Si shifts to 513.6 cm$^{-1}$ by about 7.1 cm$^{-1}$ corresponding to a biaxial tensile strain of 0.85%. Compared to the unpatterned s-Si thin film [Fig. 2(a)], the Raman peaks of the patterned structures shift to higher frequencies [Figs. 2(b) and 2(c)], indicating that the strain is partially relaxed. The Raman peak of the cylindrical pillars is located at 519.4 cm$^{-1}$ corresponding to a biaxial strain of 0.16%. It means that the initial strain is relaxed by about 82%. The Raman peak of the patterned gratings is at 517.0 cm$^{-1}$ corresponding to a strain sum of $\varepsilon_{xx}' + \varepsilon_{yy}' = 0.92\%$ which is relaxed by about 46% on a whole. However, it should be noted that the strain relaxation along the length direction of the gratings can be neglected, as demonstrated by our finite element analysis to be described later. The remnant strain in the width direction can be calculated accordingly and it is indeed 0.07% corresponding to 92% relaxation. Therefore, the strain relaxation along the width direction of the gratings is more significant than that in the pillars. This can be ascribed to Poisson’s effect.9 This inhomogeneous strain redistribution can also be inferred from the broadened Raman peaks with the full-width at half-maximum values of the blanket s-Si thin film, circular pillars, and rectangular gratings being 6.33 cm$^{-1}$, 9.36 cm$^{-1}$, and 10.8 cm$^{-1}$, respectively. The final strain state should depend on the film thickness and stacking configuration as well.

Finite element analysis is performed to elaborate the mechanism. The strain in the Si capping layer on the SiGe substrate is initialized to be 0.85%. The patterned structures such as pillars and gratings are constructed by cutting surrounding materials and the strain distributions are recalculated. The results are shown in Fig. 3. In the cylindrical pillars, the remnant strain is isotropic, as indicated by the same distribution of the two in-plane components, $\varepsilon_{xx}'$ and $\varepsilon_{yy}'$ in Figs. 3(a) and 3(b). The strain in the center of the pillars is 0.18% to 0.32%. The average tensile strain on the top surface is about 0.2% and relaxed by 76% which is slightly smaller than the experimental value. As shown in Figs. 3(c) and 3(d), the remnant strain in the patterned gratings is anisotropic. The strain component along the width direction $\varepsilon_{yy}'$ is reduced greatly although it is nearly unchanged and homogeneously distributed along the length direction. It can also be observed from the strain profiles in the $y’z’$ and $x’z’$ planes in Figs. 3(e)–3(h), $\varepsilon_{yy}'$ in the center has the range of 0.18% to 0.32% and approaches zero near the edges or even induces a large area of compressive strain distribution due to Poisson’s effect. Hence, strain relaxation along the grating width is larger than that in the cylindrical pillars. As the grating width decreases, the strain should be further reduced on condition that the strain component along

![Graph showing Raman spectra of different structures](image_url)
backscattering geometry is found to be azimuthal angle independent for both the cylindrical pillars and rectangular gratings. In contrast to the symmetrical relaxation in the cylindrical pillars, it is asymmetrical in the patterned gratings. The strain along the width direction of the gratings is reduced from 0.85% in the original s-Si thin film to 0.07% by about 92%. The change along the length direction is comparatively small and the experimental results are consistent with simulation conducted by finite element analysis. The uniaxial strain state is expected to enhance carrier mobility as well as device performance.

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FIG. 3. (Color online) Finite element analysis results of the strain component distributions in the patterned structures: [(a) and (b)] $e'_{xx}$ and $e'_{yy}$ in the top surface of the pillars, [(c) and (d)] $e''_{xx}$ and $e''_{yy}$ in the top surface of the gratings, [(e) and (f)] profile distribution of $e'_{xx}$ as well as [(g) and (h)] $e'_{yy}$ in the planes of y'z' and x'z'.

the length direction is retained if the aspect ratio is large enough. This will change the strain state from biaxial to uniaxial. It can also be found that the side surface of the grating shrinks inwards slightly and the top surface is depressed to some extent, as shown in Figs. 3(e) and 3(g). Highly strained local regions appear near the edges of the exposed SiGe substrate and it can be inferred that strain relaxation proceeds via a mixed mechanism.\footnote{15}

In conclusion, Raman spectra are acquired from (001) s-Si to investigate the azimuthal angle dependence of the strain relaxation in the patterned nanostructures. The Raman shift in $\Delta \omega_3$ of the LO$_2$ vibration mode detected using the...