

The complex evolution of strain during nanoscale patterning of 60 nm-thick strained silicon layer directly on insulator

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Abstract,

The strain behavior in nanoscale patterned biaxial tensile strained Si layer on insulator is investigated in 60-nm-thick nanostructures with dimensions in the 80 - 400 nm range. The in-plane strain is evaluated by using UV micro-Raman. We found that less than 30 % of the biaxial strain is maintained in the 200 nm \times 200 nm nanostructures. This relaxation, due to the formation of free surfaces, becomes more important in smaller nanostructures. The strain is completely relieved at 80 nm. This phenomenon is described based on detailed 3D finite element simulations. The anisotropic relaxation in rectangular nanostructures is also discussed.

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Strain is omnipresent in semiconductor science and technology. In addition to its role in several nanofabrication processes, strain is regarded as a key factor for enhancing and tailoring the optical and electronic properties of thin films and nanostructures. In particular, the introduction of strain in the fabrication of Si-based transistors is the subject of increasing interest as one of the promising possibilities to respond to the relentless demand of higher performance ICs.¹ Indeed, recent models suggest that a strained Si lattice can give hole mobilities of up to 4× the unstrained value, and electron mobilities up to 1.8× the unstrained value.² Further improvement of device performance can be achieved by combining the benefits of strained layers with the advantages of silicon-on-insulator (SOI) in the same substrate of strained Si thin layer directly on insulator – commonly known as strained silicon-on-insulator (SSOI).³

The introduction of SSOI in device fabrication raises fundamental questions about the evolution and stability of the strain during different processing steps. It was demonstrated that the strain in SSOI can be maintained during high temperature annealing.⁴ However, the shrinkage of the dimensions upon sub-micro- and nanoscale patterning of strained thin films can affect the amount and distribution of the strain.^{5,6} Indeed, in a recent report, Himcinschi *et al.* demonstrated a pronounced relaxation in patterned strained Si on Si_{0.78}Ge_{0.22} virtual substrates.⁶ The extent of the relaxation was found to be size-dependent. Investigating this phenomenon for SSOI substrates is technology highly relevant. In their early study, Lei *et al.* have touched on this subject and found that the geometry of the patterned SSOI structures impact significantly the relaxation process.⁵ In that work, a large fraction of the strain is maintained in 90 nm wide stripes, whereas 80 nm × 170 nm SSOI pillars display a full relaxation. However,

the low spectral resolution (2.5 cm^{-1}) of their Raman setup limits the sensitivity to the small variations in the strain. Apart from these two extreme cases, studies on the evolution of the strain in structures with intermediate dimensions are still missing. In this letter, we address this issue and investigate the influence of the lateral dimensions of SSOI nanostructures on the relaxation and redistribution of the strain. This process is described by detailed 3D finite element simulations. The understanding of this phenomenon is necessary to develop a quantitative and predictive model of the performance of SSOI-based devices.

8-inch SSOI wafers were used in this study. The biaxial strain was generated by the heteroepitaxial growth of Si thin layers on $\text{Si}_{0.84}\text{Ge}_{0.16}$. This tensile strained thin layer was then transferred to a SiO_2/Si handle wafer by combining wafer bonding, hydrogen ion-induced thin layer transfer, and etch-back methods.^{7,8} The initial thickness of the transferred layer is 20 nm under a biaxial strain of 0.64%. Thicker layers (up to 60 nm) were obtained by an additional homoepitaxy. The strain in the 60 nm-thick layer decreases slightly to $\sim 0.6\%$. Extended ($400 \times 400 \text{ }\mu\text{m}^2$) ordered arrays of rectangular pillars with a width in the range of 80 to 200 nm and a length of 200 or 400 nm, separated by about 500 nm, were patterned on a negative resist using electron-beam lithography. Reactive ion etching (RIE) was applied to transfer the pattern to the strained layer leading to ordered arrays of rectangular strained Si nanostructures directly on SiO_2 (nanoSSOI). Figure 1 displays selected scanning electron microscopy micrographs of the arrays of nanoSSOI studied in this work. Note that outside the patterned region the strained Si layer was completely etched away.

UV micro-Raman was employed to characterize the strain states in different samples before and after patterning. The measurements were performed in backscattering geometry by a LabRam HR800 UV spectrometer with a 325 nm He-Cd laser line corresponding to a penetration depth of ~ 10 nm in Si. A $40\times$ objective was used to focus the laser beam to a spot of ~ 800 nm in diameter. About one to two nanostructures are exposed to the laser beam under this configuration. To avoid local heating effects, the laser power was kept below 2 mW. The backscattered Raman light is diffracted by a 2400 g/mm grating and detected by a charged coupled device camera. The spectral distance between adjacent channels is ~ 0.5 cm^{-1} . This setup enables the determination of Raman shift with an accuracy of 0.1 cm^{-1} allowing the detection of faint changes in Si-Si phonons wavenumber. The He-Cd plasma line at 854.7 cm^{-1} was used for the calibration of Raman spectra. It is important to note that the SiO_2 layer is transparent to the UV laser which reaches the underlying Si substrate. This source of background must be subtracted in the analysis of the different spectra. The strain values are calculated from the measured wavenumber of Si-Si phonons using:⁹

$$\omega_{\text{Si-Si}}^{\text{strained}} = \omega_{\text{Si-Si}}^{\text{bulk}} + \frac{\omega_{\text{Si-Si}}^{\text{bulk}}}{2} \left(q + \frac{s_{12}}{s_{11} + s_{12}} p \right) \times (\varepsilon_{xx} + \varepsilon_{yy}) \quad (1)$$

where $\omega_{\text{Si-Si}}^{\text{bulk}}$ and $\omega_{\text{Si-Si}}^{\text{strained}}$ are Si-Si Raman shift frequency (in cm^{-1}) of bulk and strained Si, respectively, ε_{xx} and ε_{yy} represent the strain in the two in-plane directions, s_{11} and s_{12} are the anisotropic elastic compliance tensor elements, p and q are the phonon deformation potentials. p , q , s_{11} , and s_{12} for Si are given in Refs. 9 and 10. Figure 2 displays the Si-Si intrinsic Raman spectra of different nanoSSOI structures. The peak position is determined by a *Voigt* function fit and the sum of the in-plane strains is evaluated using

(1). We note that all the spectra are shifted up compared to the Si-Si peak position of the strained film. These observations suggest that the patterning process induces a relaxation of the tensile strain. This shift is about 2.2 cm^{-1} for the largest structure $400 \text{ nm} \times 200 \text{ nm}$. The more the size shrinks the more the intrinsic Si-Si peak position moves closer to the bulk frequency indicating a more pronounced relaxation. The smallest structures $80 \text{ nm} \times 200 \text{ nm}$ and $80 \text{ nm} \times 80 \text{ nm}$ seem to be fully relaxed. The origin of the observed relaxation resides in the formation of free surfaces during the patterning process. In general, this edge effect leads to the relaxation of the tensile strain following different mechanisms: 1- The edges of the strained nanostructure move inwards and drag the underlying substrate along with them;¹¹ 2- The edges move inwards without any distortion of the substrate;^{12,13} and 3- The edges bend up and the central region bends down, making it concave.⁹ For nanoscale-sized structures surface stress due to atomic rearrangement at the patterning-induced free surfaces can also affect the strain state. However, the contribution of the surface reconstruction can only be significant for dimensions in the order of a few nanometers.¹⁴ Therefore, it is reasonable to ignore the surface effects in the structures investigated in this work.

By considering the mechanism 1 alone, a two-dimensional model relates the relaxation to the lateral size and predicts that the strain at the center of a patterned structure decreases exponentially with a time constant t_E given by:¹⁵

$$t_E = \frac{\eta l^2}{c_{11} h_f h_s} \quad (2)$$

where η is the viscosity of the substrate, l the lateral dimension, c_{11} the elastic stiffness coefficient, h_f the thickness of the patterned structure, and h_s the thickness of the substrate. This model was employed to describe the relaxation during thermal annealing of

patterned compressively strained $\text{Si}_{0.7}\text{Ge}_{0.3}$ islands on borophosphorosilicate.^{16,17} In spite of its approximate nature, the formula given in (2) predicts nicely the influence of the size on the edge-induced relaxation. In particular, it can be inferred that faster and easier relaxation would take place when the lateral dimension becomes smaller in a qualitative agreement with our Raman data (Fig. 2). Indeed, for $200 \text{ nm} \times 200 \text{ nm}$ structures, Si-Si phonons peak is centered around 519.5 cm^{-1} . The post-patterning strain in this case remains isotropic, that is, the strain is biaxial and $\varepsilon_{xx} = \varepsilon_{yy} = 0.16\%$ corresponding to a relaxation of $\sim 73\%$ of the initial strain. However, at the lateral dimension of 80 nm a complete relief of the strain is observed.

Due to their asymmetry, the residual strain in rectangular nanostructures is no more isotropic (the strains in the two in-plane directions, ε_{xx} and ε_{yy} , are different). Unfortunately, in backscattering geometry, Raman selection rules forbid the detection of the TO phonons. Therefore, the individual stress tensor elements can not be resolved. In order to gain more insights into the complexity of the relaxation phenomenon, we performed detailed three dimensional (3D) finite-element (FE) simulations using the program Ansys 11.0. Selected data of the 3D distribution of the simulated equivalent strain are shown in Fig. 3. We note that the edges and the surface undertake a strong contraction and the residual equivalent strain drops to values below 0.1% . Expectedly, for the square nanostructures (Fig. 3 (a) and (b)) the relaxation process is symmetric along the two in-plane directions. A pronounced contraction is observed for the smallest structure $80 \text{ nm} \times 80 \text{ nm}$ (Fig. 3 (b)) in agreement with the experimental data (Fig. 2). It is worth pointing out that the strain becomes anisotropic in rectangular nanostructures (Fig. 3(c-d)). Independently of the size and shape, the lateral relaxation induces a vertical

distortion of the lattice (initially $\varepsilon_{zz} = 0$). Additionally, the simulations show that the relaxation induces a very strained region at the interface Si/SiO₂ (the gray zones in Fig. 3). Close examination of the cross section of the simulated 3D maps (not shown) indicates that the edge of the interface Si/SiO₂ becomes highly strained upon nanopatterning. This indicates that the relaxation induces a distortion of the SiO₂ layer as it is expected from the mechanisms 1 and 3 described above.

To discuss the anisotropic relaxation in rectangular nanostructure, we compare in figure 4 the simulated profiles of the in-plane longitudinal strain (dashed lines) and in-plan transverse strain (solid lines) for 120 nm \times 200 nm, 80 nm \times 200 nm, and 120 nm \times 400 nm nanostructures. The corresponding width to length ratio (w/L) is indicated. Since the strain is not homogeneous as a function of depth, figure 4 gives the profiles simulated at the surface (black lines) and at a depth of 30 nm (red lines). At the surface, the relaxation is slightly larger along the short dimension for $w/L = 0.6$ and 0.4 . At $w/L = 0.3$ the strain is highly anisotropic and the relaxation becomes important along the long dimension. This is also the general trend for all the structures in the region below the surface. Note that the transverse in-plane strain remains invariable for all structures. Interestingly, for 120 nm \times 400 nm structure the strain along the short dimension remains very close to the profile calculated at the surface. This indicates a relatively high uniformity of the transverse strain as a function of depth in this structure. Also, the strain along the short dimension is relatively high in this structure. The observed anisotropy in the relaxation is related to Poisson effect by which the contraction along the long dimension can induce an additional tensile strain along the short dimension.¹⁸ Hashemi et al. have exploited this anisotropic relaxation to fabricate uniaxial tensile strained Si

nanowires ($w \ll L$) by patterning a biaxial tensile strain film.¹⁹ We anticipate that further manipulation of the strain in nanopatterned SSOI can be achieved by adjusting their thickness. For instance, based on (2) it can be deduced that the relaxation can be significantly reduced in thinner nanostructures. Finally, the modification of the mechanical properties of the underlying oxide by tuning its stoichiometry²⁰ can also be employed to control the relaxation.

In conclusion, we studied the influence of the size on the strain evolution upon nanoscale patterning of 60 nm-thick SSOI substrates. UV micro-Raman analysis demonstrated that the strain in patterned structures relaxes due to the formation of free surfaces. Under our experimental conditions, the biaxial strain is completely relieved in the patterned structures with a lateral dimension of 80 nm. The evolution of the strain was also studied by 3D FE simulations. The simulated 3D maps demonstrate that the relaxation is pronounced at the edges and at the surface. Independently of the size, the simulations indicate that the Si/SiO₂ interface becomes highly strained and the patterned structures exhibit a out-of-plane distortion. The anisotropic relaxation in rectangular nanostructures was also discussed.

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Figure captions

FIG. 1 SEM images of the ordered arrays of some of nanoSSOI structures investigated in this work: (a) $200\text{ nm} \times 200\text{ nm}$ and (b) $80\text{ nm} \times 200\text{ nm}$. The scale bar is $1\text{ }\mu\text{m}$.

FIG. 2 nanoSSOI Si-Si intrinsic modes extracted for different dimensions. The corresponding sum of longitudinal and transverse in-plane strain is indicated. The open symbols present the experimental data and the solid lines the *Voigt* function fits. Dashed lines show the Si-Si peak positions for both the initial SSOI substrate and the bulk Si.

FIG. 3 3D FE simulations of the equivalent strain distribution within nanoSSOI with different dimensions: (a) $200\text{ nm} \times 200\text{ nm}$; (b) $80\text{ nm} \times 80\text{ nm}$; (c) $80\text{ nm} \times 200\text{ nm}$; and (d) $120\text{ nm} \times 400\text{ nm}$. The highly strained regions at the interface of nanoSSOI and SiO_2 are off scale ($\sim 1.4\%$).

FIG. 4 Simulated profiles at the surface (black lines) and at a depth of 30 nm (red lines) of the in-plane longitudinal principal strain (dashed lines) and in-plan transverse strain (solid lines) for $120\text{ nm} \times 200\text{ nm}$ (top), $80\text{ nm} \times 200\text{ nm}$ (middle), and $120\text{ nm} \times 400\text{ nm}$ (bottom) nanostructures. The horizontal axis is normalized to the width or length of the patterned nanostructures.