Multiwavelength micro-Raman analysis of strain in nanopatterned ultrathin strained silicon-on-insulator

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We developed a heterostructure to assess accurately the strain evolution upon nanopatterning of 15 nm thick tensile strained silicon-on-insulator (SSOI). Here the long-standing concern of substrate background in micro-Raman analysis was circumvented by the introduction of an oxide layer underneath the buried oxide. Unprecedented insights into the strain behavior in SSOI nanostructures were obtained by combining deep UV and visible micro-Raman probes. We found that the formation of edges results in a strong relaxation near the surface parallel to an increase in the strain at the Si/oxide interface. This disparity in the strain evolution between surface and interface leads to the coexistence of compressive and tensile strained regions within the same structure at a lateral dimension of 50 nm. This heterogeneous distribution of strain should be taken into account in the design and fabrication of SSOI-based nanodevices. © 2010 American Institute of Physics.

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Ultrathin strained silicon-on-insulator (SSOI) is an emerging material that combines the benefits of strained silicon1 and SOI (Ref. 2) technologies enabling higher performance MOSFETs.3 The potential use of SSOI in near-term generations of CMOS technologies has brought up concerns about the strain stability during device processing.4,5 It was reported that heat treatments up to 1000 °C have no consequences on the strain,4,5 whereas nanoscale patterning affects greatly the amount and distribution of the strain.6–10 Understanding this phenomenon of edge-induced strain relaxation is vital for precise control of SSOI technology. Recent studies have shown that the residual strain in the patterned nanostructures is sensitive to thickness,9 size,6–10 and geometry.9

The examination of the strain behavior in SSOI nanostructures and other strained Si devices necessitates accurate, sensitive and noninvasive probes. Transmission electron microscopy (TEM) methods can map the strain in semiconductor devices on the nanoscale.11–13 Nevertheless, these methods are destructive as they involve the thinning of the material to be probed. Here the relaxation of the strain during the specimen preparation remains a question of concern. Next-generation x-ray nanoprobe14 and Fourier transform holography15 can potentially circumvent these difficulties but their use in routine analyses is rather restricted as they require synchrotron x-ray beams. In spite of its relatively limited spatial resolution, micro-Raman spectroscopy was proven to be an effective and ergonomic instrument for the evaluation of the strain in Si devices.16 Probing SSOI-based nanostructures using micro-Raman faces, however, some complications due to the fact that the oxide is transparent to the laser light leading to a strong background from the underlying Si substrate. This severely limits the sensitivity of the technique and projects large uncertainties on the obtained strain values.

In this paper, we present a heterostructure that permits the precise analysis of the strain in nanopatterned ultrathin SSOI. This heterostructure consists of a 15 nm thick strained Si layer transferred onto SiO2/Ge/Si multilayer as shown in Fig. 1(a). The strained layer was fabricated by the epitaxial growth of Si on a ~500 nm thick Si0.84Ge0.16 buffer layer grown on Si(001) by chemical vapor deposition. The layer transfer was achieved through the ion-cut process16 using a handle substrate made of Si(001) wafer capped with ~120 nm thick Ge layer deposited by molecu-

FIG. 1. (Color online) (a) Cross-sectional TEM image of the strained-Si/SiO2/Ge/Si heterostructure used in this study. The strained Si layer was transferred onto Ge/Si substrate using the ion-cut process. The arrow indicates the bonding interface. Inset: high resolution TEM image and electron diffraction pattern of the strained Si layer. The lines in the high resolution TEM denote the penetration depth of each laser lines used in micro-Raman analysis. (b) Raman spectrum of the heterostructure shown in (a). The signal was recorded using a 488 nm laser. The vertical dashed line denotes the Si–Si peak position in bulk Si.
lular beam epitaxy. Owing to the high absorption coefficient of Ge, the introduction of the Ge layer prevents the laser from reaching the Si handle substrate thereby suppressing the background in Raman signal of the obtained heterostructure [Fig. 1(b)]. Note that the detected Si–Si peak is centered at \( \sim 515.9 \text{ cm}^{-1} \) corresponding to a biaxial tensile strain of \( \sim 0.6\% \) (stress of \( \sim 1.1 \text{ GPa} \)) as expected from the Ge content in the \( \text{Si}_{0.84}\text{Ge}_{0.16} \) buffer layer.

Ordered arrays of SSOI nanostructures were fabricated using electron beam lithography and reactive ion etching as described in Ref. 6. Three sets of patterned square-shaped nanostructures were prepared with a lateral dimension \( L \) of 50, 100, or 500 nm. The postpatterning strain was investigated using a LabRam HR800 UV spectrometer equipped with a deep UV frequency-doubled 244 nm laser, a UV He–Cd 325 nm laser, and an Ar+ 488 nm laser having a penetration depth in Si of \( \sim 6 \text{ nm}, \sim 10 \text{ nm}, \) and \( \sim 570 \text{ nm} \), respectively. This setup enables the determination of Raman shifts with an accuracy of 0.1 cm\(^{-1}\). The components of the in-plane strain \( e_{xx} \) and \( e_{yy} \) are obtained from the measured Raman shifts of the Si–Si LO phonon as described in Ref. 16. In principle, strain values as small as 0.01\% (i.e., a stress of \( \sim 25 \text{ MPa} \)) can be probed.

A first insight into the strain behavior upon nanoscale patterning can be obtained from continuum numerical calculations. Assuming that Si layer is dislocation-free with orthotropic mechanical behavior and that both Si and SiO\(_2\) are linearly elastic, we calculated the three-dimensional maps of the postpatterning strain for the three sets of SSOI nanostructures using finite element method (data not shown). It emerges from these calculations that the formation of free-surfaces upon patterning is associated with a complex redistribution of the strain, which depends on \( L \). As a general trend, a pronounced relaxation is observed in regions close to the surface, whereas the Si/SiO\(_2\) interface exhibits an important increase in the strain. Obviously, these calculations still need experimental validation. It is important to mention that the reports published so far have only demonstrated that the average strain over the entire SSOI nanostructure decreases with the lateral dimension.\(^6\)–\(^9\) In the following we provide clear evidence of the predicted disparity in the strain evolution between surface and interface regions leading to a heterogeneous distribution of strain in SSOI nanostructures.

Typical Raman spectra of the investigated SSOI nanostructures are shown in Figs. 2 and 3 (squares). For the sake of comparison, the Si–Si peak of the initial SSOI material is also shown (circles) and the position of the Si–Si peak in bulk Si is indicated by the vertical broken line. As mentioned above, the measured spectra are background-free and contain only the intrinsic Si–Si modes of the probed SSOI nanostructures. Note that the spectra recorded using the 244 and 325 nm lasers were found to be identical indicating that, within the sensitivity of our setup, the average strain does not change between the top 6 nm and the top 10 nm in the investigated nanostructures. Figures 2 and 3 show the data obtained using the 325 nm and 488 nm lasers, respectively.

At \( L=500 \text{ nm} \), the UV Raman spectrum shows that the Si–Si peak position is shifted up by \( \sim 1 \text{ cm}^{-1} \) with respect to the peak of the unpatterned SSOI (Fig. 2), whereas no clear shift is detected when Raman analysis is performed using the 488 nm laser (Fig. 3). This conflict between the two measurements is very instructive. Indeed, it can be concluded that the average in-plane strain in the whole structure is the same as in the unpatterned SSOI substrate (i.e., \( e_{xx}=e_{yy}=\sim 0.6\% \)). The upshift observed in the UV spectrum indicates, however,
that the strain is partially relaxed in the top 10 nm and drops to $\sim 0.47\%$. It can also be inferred that the strain close to the oxide interface has increased upon nanopatterning to $\sim 0.86\%$ in the bottom 5 nm thick region, which is larger than the initial strain in the SSOI substrate. Note that this is an average value and does not imply a sharp transition between the top 10 nm and the bottom 5 nm thick regions. This increase in the strain near the Si/SiO$_2$ interface agrees well with three-dimensional finite element simulations.\textsuperscript{6,8,9} Additionally, it is worth pointing out that the Si–Si mode becomes broader after the patterning. This can be attributed to the inhomogeneous distribution of the strain resulting from the patterning process.

The difference between the UV and visible laser Raman measurements is also observed for the smallest nanostructures. At $L=100$ nm, the top 10 nm appears to be fully relaxed as the measured Si–Si Raman shift peaks at $\sim 0.7$ cm$^{-1}$ (Fig. 2). Interestingly, the Si–Si mode measured for the total thickness was found to be centered at 518.8 cm$^{-1}$ (Fig. 3), which translates to an average tensile strain of $\sim 0.27\%$ corresponding to a relaxation of $\sim 55\%$ relative to the initial film. Curiously, the average strain at the bottom 5 nm is $\sim 0.81\%$, which is close to the estimated value at $L=500$ nm. At $L=50$ nm, the recorded UV spectrum shows that the Si–Si is shifted up by $\sim 0.7$ cm$^{-1}$ relative to the position in bulk Si (Fig. 2). This indicates that the top 10 nm thick layer becomes under a compressive strain of $\sim 0.1\%$ after patterning of the tensile strained layer. Despite this observed strong contraction near the surface, the average strain measured over the whole thickness remains tensile (Fig. 3) but drops significantly to $\sim 0.11\%$ due to the strong relaxation expected from the higher surface-to-volume ratio at this dimension. Here the estimated average strain in the bottom 5 nm thick region is $\sim 0.53\%$.

Table I summarizes the strain and the corresponding stress measured for SSOI nanostructures at different depths. The obtained result shows that relying on UV-Raman alone to probe the strain can lead to inaccurate conclusions regarding the strain in nanostructures thicker than the penetration depth of the UV laser in Si ($\sim 10$ nm). In fact, the extrapolation of the UV-Raman data to the whole thickness exaggerates the phenomenon of the patterning-induced relaxation of the strain in SSOI nanostructures. Moreover, it emerges from the comparison of the spectra in Figs. 2 and 3 that the region close to the interface Si/SiO$_2$ becomes under a high tensile strain, whereas the top 10 nm relaxes significantly by reducing $L$ (Table I). The ensemble of these observations provides the experimental demonstration of calculation-based mechanisms of the edge-induced strain relaxation in nanopatterned SSOL.\textsuperscript{6,8,9} Interestingly, at $L=50$ nm, both compressive and tensile strained regions coexist within the same nanostructure. This phenomenon can provide an additional degree of freedom in the design and fabrication of strained Si nanodevices.

In summary, we have developed a unique heterostructure to elucidate accurately the strain evolution upon nanoscale patterning of ultrathin SSOI substrates. The introduction of a Ge layer between the handle substrate and the buried oxide suppresses effectively the background and enhances the sensitivity of Raman scattering. By combining UV and visible Raman microprobes unprecedented insights into the phenomenon of edge-induced relaxation in SSOI nanostructures were obtained. We found that the strain in the top 10 nm relaxes significantly, whereas the region near the Si/SiO$_2$ interface becomes highly strained upon nanopatterning. This disparity in the strain evolution between surface and interface is in a qualitative agreement with numerical calculations based on continuum mechanical approach of nanopatterning-induced relaxation.

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Table I. Experimental values of in-plane strain (stress) components in % (MPa) estimated from deep UV and visible micro-Raman probes.

<table>
<thead>
<tr>
<th>$e_{xx}=e_{yy}$ ($\sigma_{xx}=\sigma_{yy}$)</th>
<th>Top 6 to 10 nm</th>
<th>Entire 15 nm thick nanostructure</th>
<th>Bottom 5 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 nm</td>
<td>$\sim 0.10$ ($\sim 180$) compressive</td>
<td>$\sim 0.00$ (0)</td>
<td>$\sim 0.47$ ($\sim 830$)</td>
</tr>
<tr>
<td>100 nm</td>
<td>$\sim 0.11$ ($\sim 195$)</td>
<td>$\sim 0.27$ ($\sim 480$)</td>
<td>$\sim 0.60$ ($\sim 1065$)</td>
</tr>
<tr>
<td>500 nm</td>
<td>$\sim 0.53$ ($\sim 940$)</td>
<td>$\sim 0.81$ ($\sim 1440$)</td>
<td>$\sim 0.86$ ($\sim 1530$)</td>
</tr>
</tbody>
</table>