Strain partition of Si/SiGe and SiO$_2$/SiGe on compliant substrates

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Strain partitioning of crystalline Si and amorphous SiO$_2$ deposited on crystalline SiGe on a compliant viscous borophosphorosilicate (BPSG) glass has been observed. Pseudomorphic epitaxial Si was deposited on SiGe films, which were fabricated on BPSG by wafer bonding and the Smart-cut® process. The strains in SiGe and Si films were found to change identically during a high-temperature anneal which softened the BPSG film, indicating a coherent interface between SiGe and Si films and precluding slippage or the formation of misfit dislocations along the interface. The stress balance between the layers dictated the final state, which confirmed that BPSG was a perfectly compliant substrate and did not exert any force on the layers above it. Similar results were found for amorphous SiO$_2$ deposited on SiGe on BPSG and then annealed. This shows that the viscous BPSG is an effective compliant substrate for the strain engineering of elastic films without the introduction of dislocations. © 2003 American Institute of Physics. DOI: 10.1063/1.1578168

The integration of lattice-mismatched materials has motivated the development of compliant substrates. The ideal compliant substrate structure allows a crystalline thin film above to expand or shrink, thus reducing the strain energy in the system, without the formation of defects such as dislocations. This provides a template for subsequent epitaxy with an in-plane lattice constant different than that of the original substrate. A variety of methods have been utilized to realize compliant substrates, with most of them trying to form a thin template layer that decouples the thick substrates from top epitaxial layers grown later.\textsuperscript{2–10} In practice, pseudomorphic strained layers are often grown on top of these templates, and the whole structure is then annealed to further adjust the lattice constant. Ideally, this relaxation step is accomplished without dislocations (e.g., at the interface between the template and the top layer) so that all layers remain coherent, as has been commonly assumed in many compliant substrate studies.\textsuperscript{1,11–14} However, in the case where such a structure has been examined in detail, coherency was not observed,\textsuperscript{15} leading to uncertainty about the nature of the compliance mechanism. In this letter, we clearly show a coherent relation of bilayers on a compliant substrate of a thin borophosphorosilicate (BPSG) film. This work shows that dislocations are not inherently included in the relaxation of layers on these compliant BPSG films.

Consider two layers on top of a compliant substrate (Fig. 1). When the strain energy is minimized by the coherent displacement of the top two layers and the compliant sub-

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elastic ones in this study. These films are patterned into square islands of various sizes by reactive ion etching to allow for lateral macroscopic expansion. Micro-Raman spectroscopy was used to locally measure the strain in Si$_{0.7}$Ge$_{0.3}$ and Si films.\textsuperscript{19}

In this letter, the coherent relaxation of different samples of four structure types on BPSG is observed. In the first experiment, a compressively strained Si$_{0.7}$Ge$_{0.3}$ (30 nm, strain $\varepsilon_0 = -1.2\%$) on relaxed Si (25 nm) was first transferred to BPSG and patterned into 30 $\mu$m islands (Fig. 2 inset). Upon annealing at 800 °C in nitrogen to reduce the viscosity of BPSG and thus remove the mechanical constraint from the substrate, the compressively strained SiGe layer expands to lessen the strain and the Si layer is stretched to become tensile (Fig. 2). The fact that the same increase in strain ($\sim 0.6\%$) is seen in both layers clearly implies an absence of slippage or misfit dislocations between the Si and SiGe layers. Further, one can predict the final strains of the annealed samples by the stress balance between the layers:

$$\sigma_{\text{SiGe}} h_{\text{SiGe}} + \sigma_{\text{Si}} h_{\text{Si}} = 0,$$

where $\sigma$ represents film stress under equal biaxial stresses ($\sigma_{11} = \sigma_{22} = \sigma$) and $h$ refers to the thickness of the film. Along with the assumption of a coherent interface between the Si and SiGe layers, Eq. (1) predicts:

$$\varepsilon_{\text{SiGe}} = \frac{(1 - \nu_{\text{SiGe}}) E_{\text{SiGe}} h_{\text{SiGe}} + (1 - \nu_{\text{SiGe}}) E_{\text{Si}} h_{\text{Si}}}{E_{\text{SiGe}} h_{\text{SiGe}}},$$

$$\varepsilon_{\text{Si}} = -\varepsilon_0 \frac{(1 - \nu_{\text{SiGe}}) E_{\text{SiGe}} h_{\text{SiGe}} + (1 - \nu_{\text{SiGe}}) E_{\text{Si}} h_{\text{Si}}}{E_{\text{SiGe}} h_{\text{SiGe}}},$$

$E$ and $\nu$ refer to the Young’s Modulus and Possion’s ratio of the film, respectively, whose values are listed in Table I. The good agreement of the observed final strains with the predictions by stress balance is further evidence of the relaxation by compliant BPSG without dislocations.

A second experiment was performed to verify that the stress balance between the layers governs the mechanical equilibrium. Epitaxial unstrained Si of various thicknesses was grown at 700 °C by rapid thermal chemical vapor deposition (RT-CVD) on a compressively strained 30 nm Si$_{0.7}$Ge$_{0.3}$ layer on BPSG before relaxation (Fig. 3 inset). This structure was patterned to 30 $\mu$m square islands and then annealed in nitrogen at 800 °C long enough to reach mechanical equilibrium (1 to 3 h). Figure 3 shows the final equilibrium strains in the two layers as a function of the top Si thickness, both experimentally measured and also predicted by stress balance [Eqs. (2) and (3)]. Again, excellent agreement was observed.

Up to this point, the strain partition has been examined only during the lateral expansion of elastic layers. To demonstrate the full capability of strain engineering using the viscous BPSG film, the lateral shrinkage of elastic layers during the stress balance process was also examined. In a third experiment, 30 $\mu$m square islands of 30 nm Si$_{0.7}$Ge$_{0.3}$ on BPSG were first almost fully relaxed at 800 °C. A 30 nm Si layer was commensurately and selectively deposited on the relaxed Si$_{0.7}$Ge$_{0.3}$ islands by RT-CVD (Fig. 4 inset). The measured tensile strain in the Si layer was about 1.1%, as expected for pseudomorphic epitaxial Si on relaxed Si$_{0.7}$Ge$_{0.3}$. This structure was annealed for 1 h at 800 °C in nitrogen to reach equilibrium (Fig. 4). Again, the stress balance accurately predicts the final strains.

Note that in all three cases described so far, the Si$_{0.7}$Ge$_{0.3}$ thicknesses were above the critical thickness not only for a single thin film on a bulk Si substrate ($\sim 8$ nm), but also for that predicted in a free-standing Si/Si$_{0.7}$Ge$_{0.3}$ bilayer (maximum critical thickness $\sim 16$ nm for Si thickness $>16$ nm in Ref. 12). Thus, dislocations might have been expected by thermodynamic considerations. The fact that the two layers relaxed together in all cases emphasizes the compliant nature of the substrate and that the strain in layers relaxes more

![FIG. 2. Coherent strain evolution of Si and Si$_{0.7}$Ge$_{0.3}$ films as they reach stress equilibrium during an anneal at 800 °C. The strains are measured at the center of a 30 $\mu$m×30 $\mu$m island. The final equilibrium state agrees with the predicted stress balance between Si and Si$_{0.7}$Ge$_{0.3}$ films, depicted by the dotted lines.](image)

**TABLE I. Mechanical properties\textsuperscript{a} of Si and Si$_{0.7}$Ge$_{0.3}$ (linearly interpolated between Si and Ge).**

<table>
<thead>
<tr>
<th>Property</th>
<th>$E$(Si$<em>{0.7}$Ge$</em>{0.3}$) (10$^{11}$ N/m$^2$)</th>
<th>$E$(Si) (10$^{11}$ N/m$^2$)</th>
<th>$\nu$(Si$<em>{0.7}$Ge$</em>{0.3}$)</th>
<th>$\nu$(Si)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>12.2</td>
<td>13.0</td>
<td>0.28</td>
<td>0.28</td>
</tr>
</tbody>
</table>

\textsuperscript{a}See Ref. 21.
quickly through lateral expansion or contraction enabled by the viscous flow of the compliant substrate than through dislocation formation.

Finally, we show the stress balance with a deposited amorphous oxide layer, instead of epitaxial, crystalline layers. A SiO$_2$ layer was deposited on a compressively strained 30 nm Si$_{0.7}$Ge$_{0.3}$ layer on BPSG by plasma-enhanced chemical vapor deposition (PECVD) at 250 °C. The SiO$_2$/SiGe stack was patterned to 30 µm square islands and was then annealed at 800 °C for 2 h to reach an equilibrium state. Open symbols are experimental data. Lines are calculation of stress balance based on the elastic parameters in Table I.

In summary, we have confirmed coherent interfaces and strain partitioning in Si/SiGe and SiO$_2$/SiGe on viscous films. Governed by the stress balance, the layers can either shrink or expand on the viscous BPSG to minimize the strain energy. The formation of dislocations is unnecessary in this process. Thus, the viscous films, such as a BPSG film, are a promising compliant substrate for defect-free strain engineering of lattice-mismatched films.

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![FIG. 3. Biaxial strains of 30 nm Si$_{0.7}$Ge$_{0.3}$ and Si at the center of a 30 µm x 30 µm island as a function of Si thickness after anneals at 800 °C to reach equilibrium. Open symbols are experimental data. Lines are calculation of stress balance based on the elastic parameters in Table I.](Image)

![FIG. 4. Biaxial strain of Si$_{0.7}$Ge$_{0.3}$ and Si at the center of an initially relaxed 30 µm x 30 µm Si$_{0.7}$Ge$_{0.3}$ island before and after an anneal. Open symbols are experimental data and dotted lines are calculation of stress balance.](Image)

![FIG. 5. Biaxial strain of the initially compressively strained 30 nm Si$_{0.7}$Ge$_{0.3}$ at the center of a 30 µm x 30 µm island, after deposition of PECVD SiO$_2$ and an anneal, as a function of PECVD-SiO$_2$ thickness. Open symbols are experimental data and the dashed line is a fitting based on stress balance.](Image)

References: