# Nanostressors and the Nanomechanical Response of a Thin Silicon Film on an Insulator

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Pseudomorphic three-dimensional Ge nanocrystals (quantum dots) grown on thin silicon-on-insulator substrates can induce significant bending of the silicon template layer that is local on the nanometer scale. We use molecular dynamics simulations and analytical models to confirm the local bending of the Si template and to show that its magnitude approaches the maximum value for a freestanding membrane. The requisite greatly enhanced viscous flow of $SiO_2$ underneath the Si layer is consistent with the dependence of the viscosity of $SiO_2$ on shear stress.

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Silicon-on-insulator (SOI), a composite in which a thin layer of Si is separated from a bulk wafer by an oxide, are becoming widely used in semiconductor device fabrication. It can directly replace bulk Si as a substrate for metal-oxide-semiconductor transistors [1]. Significant advantages arise from the reduction of the effective substrate thickness and from the introduction of the buried oxide layer, including better current control and lower power dissipation, making SOI substrates preferred for low-power-circuit applications, e.g., in portable computers. An alternative use of SOI, as a compliant substrate for heteroepitaxial growth [2], would have a potentially even larger impact on microelectronics.

Our knowledge of SOI is very limited, especially of its mechanical and electrical properties at the nanometer scale. Very recently, we observed [3] a surprising large local bending of the Si template layer in SOI(001) induced by the growth of individual, small, coherent Ge "hut" nanocrystals [4], a behavior that is distinctively different from that observed when these huts are grown on bulk Si(001). The physical origin of this unusual nanomechanical behavior of SOI was, however, unclear. In this Letter, we explore, using molecular dynamics (MD) simulations and continuum mechanics calculations, the physical feasibility of such large local bending occurring in the SOI substrate, and the conditions under which it can occur.

We calculate directly the bending of a thin freestanding Si membrane when an epitaxial Ge nanocrystal (hut island) is grown on it. MD simulations show that the local bending can occur only when the substrate is very thin. The membrane thickness must be comparable to the island height and the density of islands must be sufficiently low that they are elastically "decoupled" from each other, i.e., stressing the substrate independently. Also, we derive a generic formula for calculating the average local bending curvature and stress in a substrate induced by growth of coherently strained nanocrystals. We show that the observed bending curvature in the Si template layer of SOI approaches the maximum value allowed for a freestanding layer. Thus, the $SiO_2$ underneath the Si layer must exhibit a substantial amount of viscous flow during the bending process. Using the dependence of the viscosity of $SiO_2$ on shear stress, we demonstrate that the shear stress produced by the bent Si layer is locally sufficiently large to cause this increase in viscous flow.

The role of strain in the fabrication of electronic and optoelectronic devices that involve thin films of different materials is well established. Because the substrate thickness has generally been much greater than that of the film, strain partitioning leaves the substrate with much less strain than that in the film. As the substrate is made thinner, strain partitioning leads to uniform extended substrate bending. Such substrate bending has been used as a unique probe to monitor the evolution of the growing films [5,6].

In SOI, the template layer (the top layer of crystalline Si) can be made thinner than any freestanding substrate (as little as 3 nm [7]). Because of its thinness, the template layer can now be expected to take up a significant portion of the strain, except, of course, that it is chemically bonded to an oxide underneath. There has so far been no evidence that the strain sharing could be elastic, i.e., that the Si template could expand without forming dislocations [8]. The 3D nanocrystal (hut) [4] that begins to form after about 3 ML (monolayers) of Ge are deposited on Si does, however, produce local elastic deformation on thin SOI [3]. The Ge hut, which is pseudomorphic with the underlying Si, acts as a local nanostressor that bends the underlying Si template layer. Figure 1 shows a scanning tunneling microscopy (STM) image of a Ge hut on bulk Si [4] in registry with the substrate, a corresponding transmission electron microscopy (TEM) image of such a crystal grown on bulk Si, and a TEM image of the Ge hut grown on thin SOI(001), showing the local bending of the Si template layer induced by the nanocrystal. We have observed a bending curvature (inverse of the radius of curvature) underneath the nanocrystal as large as $\sim 0.005\ \mathrm{nm}^{-1}$. This behavior [3] is distinctively different from that observed for Ge growth on thick Si substrates [5,9,10].

  

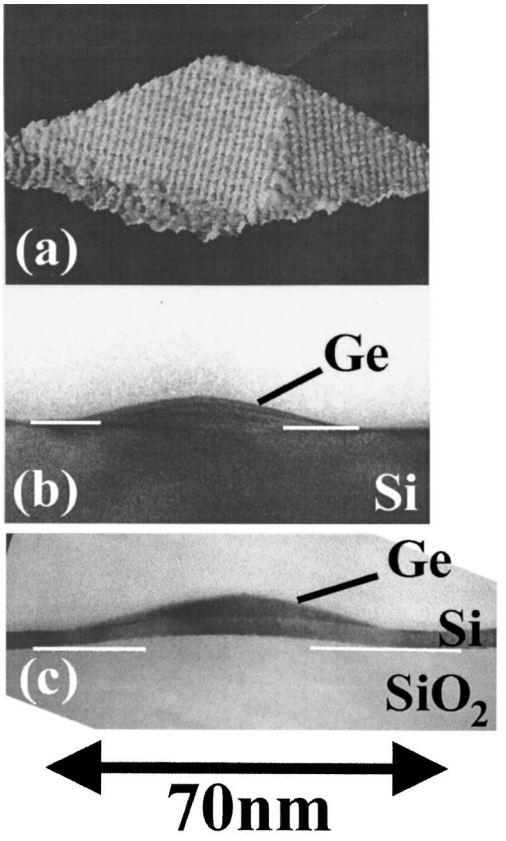


FIG. 1. Ge quantum dot hut crystal on Si(001) and SOI(001). (a) STM image; (b) TEM image on bulk Si; the white lines show the Ge hut-Si substrate interface. (c) TEM image on SOI; about 1.5 nm of pure Ge was deposited by molecular beam epitaxy at a deposition rate of 0.1 Å/s and a substrate temperature of ~700 °C. The white lines show the original Si-oxide interface. The upward bending of the Si template is clearly evident.

We have performed MD simulations to investigate the feasibility of a local bending and the existence of a transition from *extended* to *local* bending with decreasing island density and substrate thickness. Although experimentally a ~10 nm Si membrane is very thin, computationally it is still too large to handle. We use a smaller model system. The key to the new observation of local bending is that the Si substrate thickness is comparable to the equivalent Ge film thickness. We therefore use 4 to 18 atomic layers of Si as a substrate and a Ge nanocrystal consisting of 9 atomic layers with (105) facets, amounting to ~300 to ~2000 atoms. We use an empirical potential for Si and Ge [11] gives a good description of elastic properties of Si and Ge [12].

We construct a simulation cell containing a Ge island sitting on a freestanding Si layer as described above. Initially the Si layer is flat. The system is then relaxed, until the force on all atoms goes to zero, to reach the final "bent" equilibrium configuration. We have repeated the simulations for different system sizes, representing both different substrate thicknesses at constant island density and different island densities at constant substrate thickness. Figures 2(a) and 2(b) demonstrate the effect of substrate thickness. On a very thin substrate and at low island density [Fig. 2(a)], each island induces a large local bending with curvature largest under the island apex and decaying to zero at the island edge. As the substrate thickness increases, the bending becomes more extended (the tendency toward local bending is suppressed [9]). The reduction in local bending is illustrated in Fig. 2(b): clearly, the variation of local curvature underneath the island decreases with increasing substrate thickness. A very thick substrate (18 Si layers) exhibits essentially no local bending [dashed line in Fig. 2(b)]. Figure 2(c) shows schematically the bending of a four-layer substrate produced by densely packed islands: an extended bending with local bending variations. Figure 2(d) compares the local and extended bending as the island density

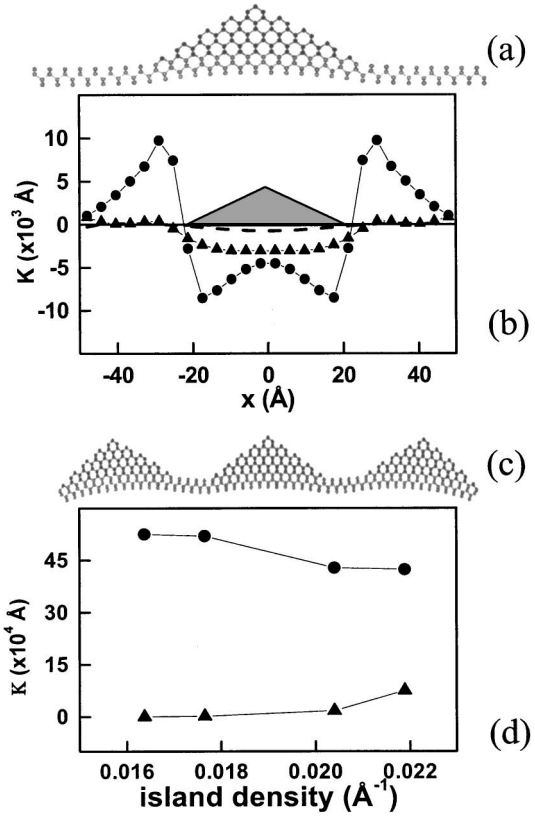


FIG. 2. MD calculation of the bending of a Si membrane induced by coherent 3D Ge islands. (a) Large local bending induced by a single 3D island on a thin Si substrate. (b) Variation across the substrate of the local curvature induced by one 3D island, calculated at the bottom of a substrate of different thicknesses: 4 layers (circles), 12 layers (triangles), and 18 layers (dashed line). (c) Bending of a thin Si substrate induced by a higher density of 3D islands. (d) The dependence on island density of the "average" extended curvature (triangles) and maximum local curvature (circles) under the island apex. The neighboring-island bases are in contact for the highest density shown.

increases: the local bending decreases while the extended bending increases.

We now demonstrate that the observed bending curvature [Fig. 1(c)] approaches the limit for a freestanding Si layer. We derive a formula for estimating the average curvature induced in a freestanding membrane by the growth of a coherently strained nanocrystal. We consider a nanocrystal with a pyramidal shape with base dimensions of $l \times l$ and height $t_i$ (Fig. 3 inset). The equivalent thickness of the corresponding uniform film is then $t_f = (1/3)t_i$. In accordance with experiment [Fig. 1(c)], we assume the bending induced by each island is local and independent of that of other islands (the low-island-density limit). For simplicity, we further assume that the bending is completely localized underneath the island, within the island base, and with a uniform curvature, which we relate to the average curvature in the measurement.

The 3D island always relaxes misfit strain within itself to some extent. The island-induced bending therefore depends on the degree of strain relaxation within the island. To illustrate such an effect of strain relaxation within the island on island-induced bending, we first consider the limit of a 3D pyramidal island (a hut) that has not relaxed any strain internally. Letting $K$ be the average bending curvature and $z_0$ the position of the neutral plane, the strain in the substrate and in the island after bending will be, respectively, $\varepsilon_s = K(z - z_0)$ and $\varepsilon_i = K(z - z_0) + \varepsilon_m$. The strain energy per area of the combined island and substrate is then

$$U = (C_s/2)\int \varepsilon_s^2 dz + (C_f/2)\int \varepsilon_i^2 (1 - z/t_i)^2 dz, \quad (1)$$

where $C_s$, $C_f$ are elastic constants. Minimization of strain energy with respect to $K$ and $z_0$ gives

$$K = -\frac{6(C_f \varepsilon_m)t_f}{C_s t_s^2}\gamma, \quad (2)$$

$$\gamma = [1 + (3/2)\beta]/[1 + 4\alpha\beta + 9\alpha\beta^2 + (54/5)\alpha\beta^3 + (80/21)\alpha^2\beta^4], \quad (3)$$

where $\alpha = C_f/C_s$ and $\beta = t_f/t_s = t_i/3t_s$. $\gamma$ is a weighting function of $\beta$, depending mainly on island shape and island strain.

We consider two different forms of strain relaxation within the Ge island. In general, we can assume that the island is completely coherent (at approximately the Si lattice constant) at the interface and completely relaxed (at the Ge lattice constant) at its top. If the original misfit strain in the island decreases quadratically from $\varepsilon_m$ at $z = 0$ to 0 at $z = t_i$ [13], i.e., $\varepsilon_i = K(z - z_0) + \varepsilon_m(1 - z^2/t_i^2)$, then the effect of the relaxation is to change the numerator of $\gamma$ in Eq. (3) to $9/10 + (6/5)\beta - (3/20)\alpha\beta^2$. If the original strain decreases linearly with height $z$, i.e., $\varepsilon_i = K(z - z_0) + \varepsilon_m(1 - z/t_i)$, then the numerator of $\gamma$ in Eq. (3) becomes $3/4 + (9/10)\beta - (9/40)\alpha\beta^2$.

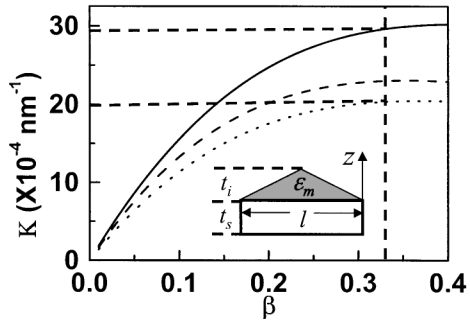


FIG. 3. The dependence of the calculated bending curvature, $K$, on $\beta = t_f/t_s$, the ratio of equivalent film thickness and template thickness. Solid line: 3D island without strain relaxation; dashed line: strain relaxes quadratically with height in the island; dotted line: linear relaxation. Srain relaxation within the island reduces the island-induced bending by 10% to 25%. The vertical line at $\beta = 0.33$ corresponds to the observed island height in Fig. 1(c). The horizontal lines mark the range of calculated curvatures at this island height for various island relaxation assumptions. The average local bending curvature observed in the bent Si layer underneath the coherent Ge islands is in good agreement with these values. The inset shows the parameters used in the calculation: $t_i$ is the thickness of the Ge nanocrystal, $t_s$ is the thickness of the Si membrane, $l$ is the base dimension of the nanocrystal, $\varepsilon_m$ is the misfit strain in the nanocrystal, and $Z$ is the normal to the membrane.

Figure 3 shows the calculated bending curvature for the different forms of strain relaxation in the island as a function of $\beta$, the ratio of equivalent deposited-material thickness to substrate thickness. To compare directly to experiment, we use a Si template thickness of 10 nm and the elastic constants of Si and Ge [14]. For all three strain conditions (fully strained, linearly relaxed, and quadratically relaxed), the calculated curvature, $K$, increases almost linearly with increasing island thickness when $\beta \leq 0.1$ but slows down for film thicknesses beyond $\beta \sim 0.1$. Using the observed island height of $t_i \sim 10$ nm ($t_f \sim 3.33$ nm), we calculate bending curvatures of $K \sim (2\text{–}3) \times 10^{-3}$ nm$^{-1}$ for the range of models for the strain relaxation in the island. This calculated curvature agrees well with the average of the observed curvatures, which range from a maximum of $K \sim 5 \times 10^{-3}$ nm$^{-1}$ right underneath the nanocrystal to a minimum of $K \sim 5 \times 10^{-4}$ nm$^{-1}$ in the region near the island edge.

The above analysis reflects the behavior of a freestanding membrane. The local bending mode (qualitatively) and the large bending magnitude (quantitatively) indicate that the Si template in SOI behaves like a freestanding layer during the growth of Ge nanostressor islands. This result can be achieved in only two ways: either $SiO_2$ exhibits substantial viscous flow or the Si template layer delaminates from the underlying $SiO_2$. For a delamination to exist, a vacuum blister must form in the bent region underneath the island. TEM images (Fig. 1) show

no evidence of a vacuum blister or a void. Delamination appears physically unlikely because it leaves many dangling bonds at the separated $Si/SiO_2$ interface. We therefore address whether a substantial viscous flow of the $SiO_2$ is possible.

The relaxation time of a viscous material can be estimated as $t_{\text{relax}} = \eta/E$, where $\eta$ denotes viscosity and $E$ denotes the Young modulus. For solid $SiO_2$, $\eta \approx 9 \times 10^{17}$ Pa · s [15] and $E = 8 \times 10^{10}$ Pa [16], which gives a relaxation time of $t_{\text{relax}} \sim 10^7$ s. This is much too long, considering the deposition time of Ge on SOI in the experiment is only ~150 s. However, the viscosity of $SiO_2$ decreases almost exponentially with increasing applied shear stress as [15,17]

$$\eta = \eta_0 \frac{\tau_{\max} V_c/2kT}{\sinh(\tau_{\max} V_c/2kT)}, \tag{4}$$

where $\eta_0$ is the low-stress viscosity, $\tau_{\max}$ is the maximum shear stress, $V_c$ is a characteristic volume, $k$ is the Boltzmann constant, and $T$ is the temperature. We suggest that the bending of the Si template layer and the viscous flow of $SiO_2$ proceed in a dynamically correlated fashion: The Ge nanostressor attempts to bend the Si template. This bending induces a shear stress that the Si template layer exerts on the oxide at the Si-oxide interface. This shear stress reduces the oxide viscosity. Any resulting flow allows the Si template to bend more, increasing the shear stress, which in turn reduces the viscosity further, allowing more flow. The bending is thus in the nature of an instability. Using the above value of $\eta_0$, a value of $V_c = 3 \times 10^{-28}$ m$^{-3}$ [15], and the maximum shear stress, $\tau_{\max}$, at the $Si/SiO_2$ interface [15], we estimate, at our growth temperature of $T \approx 1000$ K, that the viscosity of $SiO_2$ can be decreased by 3 to 5 orders of magnitude in the regions underneath the bent Si layer below the Ge islands. The oxide relaxation time (the time for the oxide to deform its shape) is then also shortened by a few orders of magnitude, from a few thousand hours to a few hundred seconds, reasonably within the range of deposition times. Thus, the extremely large bending stress produced by a coherent Ge nanocrystal on the thin Si template layer has the consequence of inducing shear stress on the oxide sufficiently large to produce an unprecedented increase of viscous flow of $SiO_2$. As the oxide flows, it allows the Si template to bend, reaching effectively the conditions corresponding to a freestanding Si membrane.

To conclude, 3D Ge nanocrystals grown pseudomorphically on thin SOI substrates act as nanostressors that produce a novel local bending mode in the thin Si template. MD simulations show that such local bending is most pronounced when strained islands are elastically decoupled from each other, stressing the thin substrate independently. We derive an analytical formula for estimating the bending curvature induced by coherently strained or partially strain relaxed pyramidal islands in a freestanding membrane. The magnitude of local bending in the Si template approaches the maximum value allowed for a freestanding layer of the same thickness, suggesting that the bending of the Si layer is assisted by substantial viscous flow of $SiO_2$ underneath the Si. The reduced viscosity required for this flow is made possible by the very high local shear stress and the strong dependence of viscosity on shear stress. As semiconductor device fabrication incorporates ever thinner layers and smaller laterally defined structures, the concepts elucidated here will become increasingly important. We believe they have general validity in describing the nanomechanical response of thin-film composites.

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