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Mechanical stability of ultrathin Ge/Si film on SiO_2: The effect of Si/SiO_2 interface

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We perform two-dimensional linear elastic finite element analysis to investigate the mechanical stability of ultrathin Ge/Si film grown on or bonded to SiO_2, using *imperfect interface elements* between Si and SiO_2 to model Si/SiO_2 interfacial slippage. We demonstrate that the overall composite film is stable when only the tangential slippage is allowed, however, it becomes unstable when normal slippage is allowed: the coherently strained Ge island induces a large local bending of Si layer, and separates the Si layer from the underlying SiO_2 forming a void at the Si/SiO_2 interface. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1926421]

Current semiconductor technology is approaching fundamental and practical limitations to scaling. Different methods have been proposed to enhance device performance other than shrinking the gate oxide thickness and channel length. Two emerging approaches are based on the use of silicon-on-insulator (SOI) substrate and use of strained silicon layer to eliminate substrate current leakage and to improve carrier mobility in the channel. SOI, a composite material used to separate a thin layer of Si from a bulk wafer by an oxide, is becoming prevalent in semiconductor device fabrication. For example, metal-oxide-semiconductor (MOS) transistors[1] (switches used in microprocessors) are built on top of a thin Si layer of SOI. The SOI reduces the capacitance of the switch, achieving faster operation and lowering power consumption. Strained Si technology is based on engineering the strain in silicon, altering its band structure. For example, a tensile-strained Si layer can be grown on a relaxed SiGe buffer layer. Recent results[2,3] on the application of these concepts to 90-nm silicon MOS field-effect transistors indicated significant performance enhancements in carrier mobility. Furthermore, International Business Machines[4] (IBM) has combined these two methods together to bond strained Si layer with SOI, as an attempt to fabricate higher-clocked switches by lowering their power demands.

Despite the promises made by the strained Si (Ge) layer on SOI, one major technical issue is the mechanical stability of such a strained layer structure, particularly when its thickness is reduced down to the nanometer scale. For instance, it is well known that when Ge is grown on Si, misfit strain induces surface instability and leads to a three-dimensional (3D) island formation.[5] Recently, we have demonstrated that a thin Si layer on SOI (down to ~10 nm) becomes unstable against Ge deposition. The strained Ge 3D islands induce an anomalously large local bending of Si layer underneath the Ge islands.[6] Our theory further showed that the magnitude of the observed local bending approaches the linear elastic limit for a freestanding Si layer, and such bending instability may occur generally for a very thin freestanding Si layer when the Ge island density is low.[7]

Because experimentally no vacuum blister (void) was observed at the Si/SiO_2 interface, it is suggested that the local bending of Si is achieved by a local nonlinear viscous flow of SiO_2 which makes Si layer behave like a freestanding film.[6,7] In this letter, using finite element analysis (FEA), we examine the mechanical stability of ultrathin Ge/Si/SiO_2 composite film within the linear elastic regime, without viscous flow of SiO_2. We focus our study on the effect of Si/SiO_2 interface by employing *imperfect interface elements* between Si and SiO_2 to simulate different bonding and relaxation mechanisms at the Si/SiO_2 interface.

The quality of Si/SiO_2 interface affects strongly the mechanical stability of the overall Ge/Si/SiO_2 composite film. It depends on the fabrication techniques and formation processes. The Si/SiO_2 interface formed by thermal oxidation or chemical vapor deposition is expected to be different from which is formed by bonding Si with SiO_2. To account for an imperfect interface, we include normal or tangential displacement discontinuities at the interface to allow interfacial slippages. Our analyses show that the overall composite film is stable without localized bending when only the tangential slippage is allowed; whereas it becomes unstable when the normal slippage is allowed: the strained Ge island induces a large local bending underneath the island and debonds the Si layer from the underlying SiO_2 forming a void.

We perform FEA using the JANFEA software[8] and employ imperfect interface elements[9,10] to model the Si/SiO_2 interface. JANFEA supports linear elastic imperfect interface elements that are created by defining two separate paths along a line within a material. The element will develop normal and tangential displacement discontinuities related to the stress in the corresponding direction according to the linear law:

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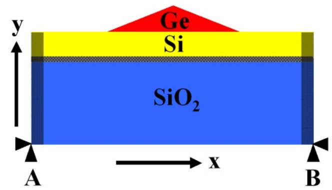

FIG. 1. (Color online) Schematics of our 2D FEA model.

$$[\mu_n] = \frac{\sigma_n}{D_n}, \quad [\nu_t] = \frac{\tau_t}{D_t}, \tag{1}$$

where σ_n is the interfacial normal stress and τ_t is the interfacial tangential stress. D_n and D_t are interface parameters that define the stiffness of the interface for the development of normal or tangential displacement discontinuities at the interface, as denoted by the square brackets $[\mu_n]$ and $[\nu_t]$, respectively. If both D_n and D_t are infinite, displacement discontinuities will be zero and the interfacial slippage is eliminated; if both D_n and D_t are zero, interfacial stresses will be zero and the interfacial slippage is most pronounced. Choosing finite values of D_n and D_t independently allows us to model the different degrees of slippage in the normal and tangential directions.

Figure 1 shows the two-dimensional (2D) FEA model, consisting of a Ge hut island[5] (10-nm height) grown on SOI substrate with a very thin Si layer (10 nm). The SiO_2 layer is 100 nm thick and ~1000 nm long. The Si/SiO_2 interfacial elements are schematically shown as hatched grids. We note that the interface elements describing a line or an element without volume should be considered more like the boundary conditions rather than an element of the material. The interfacial stresses in the interface elements are therefore not used to calculate the average nodal stresses. The boundary condition applied in our model is to fix the displacements along both x and y axes at two endpoints (A and B), as shown in Fig. 1. Also, we use large values of D_n and D_t at both end zones (~50 nm) to prevent interpenetration between Si and SiO_2 and sliding along their interface. The generic misfit strain (~4.2%) at Ge/Si interface is introduced by the relative thermal expansion. The FEA uses eight-noded quadrilaterial elements providing a 2D plane stress analysis. The material properties,[11–13] including the Young's modulus (E), Poisson's ratio (υ), and thermal expansion coefficient (α), of the solid Si(100), Ge(100), and SiO_2 used in our FEA are listed in Table I.

Initially, the whole composite film is flat. The system is then relaxed by the thermal expansion until the nodal displacements and stresses are converged, reaching the final bent equilibrium structure. We first consider the case of large D_n ("infinite") and small D_t ("finite"). This corresponds to the physical condition that only tangential slippage is allowed at the interface as the interface will virtually have $[\mu_n]=0$. We fix D_n at $\sim 10^{20}$ and decrease D_t from 10^{14} to 10^8 to obtain three different equilibrium bent structures as shown in Figs. 2(a)–2(c).

TABLE I. The material properties used in FEA.

Material	E (GPa)	ν	α(1/K) at 293 K
Si(100)	130.0	0.280	2.60
Ge(100)	103.2	0.278	6.10
SiO_2	80.0	0.170	0.55

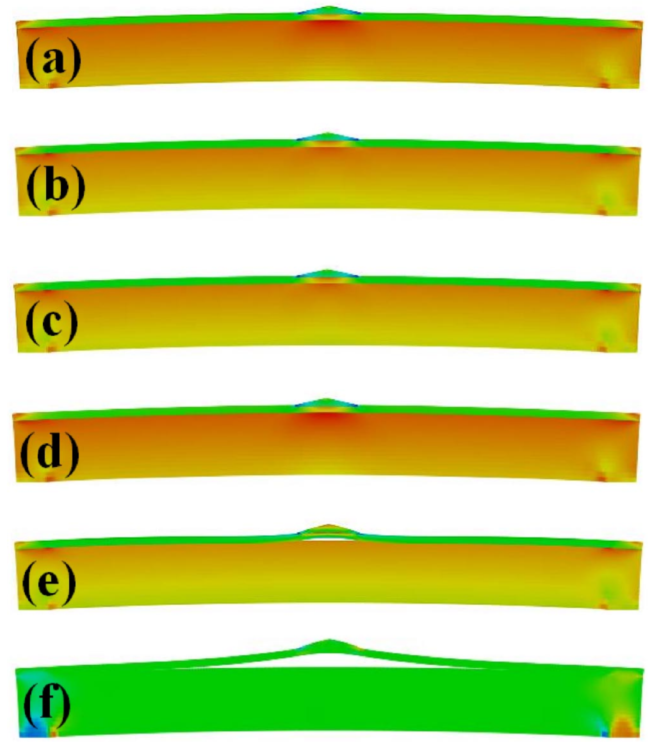

FIG. 2. (Color online) The distributions of the average tangential nodal stress (σ_{xx}) obtained by FEA at six different values of D_n and D_t. The color ranging from blue to red represents the smallest to largest tangential stress. The left panel is for fixed $D_n=10^{20}$ at three different D_t values: (a) $D_t=10^{14}$, (b) $D_t=10^{11}$, and (c) $D_t=10^8$. The right panel is for decreasing both D_n and D_t: (d) $D_n=D_t=10^{14}$, (e) $D_n=D_t=10^{10}$, and (f) $D_n=D_t=10^8$.

The strained Ge island tends to bend the thin Si film and induces an extended bending across the whole composite film. The bending magnitude increases slightly with decreasing D_t from Figs. 2(a)–2(c). In addition to the equilibrium bent structure, Fig. 2 also shows the distributions of the average tangential nodal stress (σ_{xx}) in the composite thin film. Because the Ge island is ~4.2% compressively strained, it induces a large tensile stress (large σ_{xx}) in the Si layer right underneath the Ge island, and a large compressive stress in the SiO_2 below. The tensile stress in the Si layer is maximum under the middle of the island base and decreases towards the island edges. It then becomes compressive in the vicinity of the island edges, similar to the case of the Ge island on a bulk Si substrate.[14] One interesting point is that a larger tangential interface slippage at smaller D_t further decreases the overall stress in Si and SiO_2. Overall, we conclude the composite film to be mechanically stable under the condition with no normal slippage, because no local bending of Si template layer is observed underneath the Ge island.

We next consider the situation when both normal and tangential slippages are allowed at the interface by using small values of both D_n and D_t simultaneously. Figures 2(d)–2(f) show the three equilibrium bent structures by decreasing D_n and D_t from 10^{14} to 10^8. Most noticeably, the

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composite film now becomes unstable; with decreasing D_n and D_t, the Ge island gradually induces a large local bending of the Si layer, which is accompanied by the debonding of the Si template layer from the underlying SiO_2. Once the Si layer separates from the underneath SiO_2 [Figs. 2(e) and 2(f)], the stress in the Si layer becomes more localized and much larger, while the stress in the underlying SiO_2 diminishes. Figure 2(f) shows that the magnitude of the local bending of Si approaches the limit for a freestanding Si film.

Our analyses show that within the linear elastic regime, the local bending of the Si layer induced by the Ge island may only occur and approach the limit for a freestanding Si film if the Si layer separates from the SiO_2 forming a big void at the Si/SiO_2 interface [Fig. 2(f)]. Therefore, it provides an indirect support to the suggestion that the experimentally observed large local bending[6,7] is assisted by the local nonlinear viscous flow of SiO_2, because no void was observed in the experiment.[6,7] A direct proof, however, requires simulation of the nonlinear viscoelastic property of SiO_2. Currently, we are developing a nonlinear viscoelastic material point method[8] for such simulations.

In conclusion, we have performed FEA to investigate the mechanical stability of an ultrathin Ge/Si film on SiO_2 within the linear elastic regime, focusing on the effect of Si/SiO_2 interface. We demonstrate the mechanical response of the overall composite film to the interface slippage by employing *imperfect interface elements*. We illustrate that the overall composite film is stable when only the tangential slippage is allowed. However, it becomes unstable when normal slippage is allowed: the coherent strained Ge island induces a large local bending of Si layer, which is separated from the underlying SiO_2 forming a void at the Si/SiO_2 interface. Thus, the quality of Si/SiO_2 interface is expected to play an important role in controlling the stability of those device structures employing the strained Si/SiO_2 film. Because the techniques involving strained Ge/Si on SOI have been proposed to make next-generation semiconductor devices, the concept we elucidate here will become increasingly important, especially as the dimension of the devices continue to shrink towards the nanometer scale.

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