Multimillion-atom molecular dynamics simulation of atomic level stresses in Si(111)/Si_3N_4(0001) nanopixels

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Ten million atom multiresolution molecular-dynamics simulations are performed on parallel computers to determine atomic-level stress distributions in a 54 nm nanopixel on a 0.1 μm silicon substrate. Effects of surfaces, edges, and lattice mismatch at the Si(111)/Si_3N_4(0001) interface on the stress distributions are investigated. Stresses are found to be highly inhomogeneous in the nanopixel. The top surface of silicon nitride has a compressive stress of +3 GPa and the stress is tensile, −1 GPa, in silicon below the interface. © *1998 American Institute of Physics.* [S0003-6951(98)00116-8]

Sub-100 nm pixel sizes pose special challenges in Si electronics. In this regime, the significance of spatial inhomogeneities in the dopant distribution to the device characteristics is being increasingly appreciated.[1] Spatially nonuniform stresses induced by such nanoscale pixellation may have profound impact[2]—rapidly varying stresses at and near edges may lead to defect formation or even initiate a crack. Understanding the stress distribution is therefore essential in the design of nanoscale devices.

On larger (>1 μm) length scales, edge stresses in Si/SiO_2 and Si/Si_3N_4 have been examined utilizing the framework of linear elasticity and finite-element (FE) simulations.[3,4] In nanoscale devices, however, the surface-to-volume ratio is so large that the influence of surfaces, edges, and corners on elastic properties become significant. In addition, chemical bonding at the Si/Si_3N_4 interface introduces types of stresses not present in silicon or silicon nitride materials. These effects have to be included in constitutive relations to achieve realistic description of nanoscale devices in the FE approach. An alternative approach is to use molecular-dynamics (MD) simulations where surface and interface bonding effects are explicitly included at the atomistic level. With recent progress in parallel computer architectures, it has now become possible to carry out direct atomistic simulations for submicron structures with realistic descriptions of the materials involved. In particular, large-scale MD simulations have proven to be useful in the study of dynamic fracture.[5] MD simulations provide spatially resolved stress distributions on the length scales not accessible to experimental techniques, such as MicroRaman spectroscopy.[6] Such numerical experiments can be used to establish the validity of constitutive relations used in FE simulations, in particular the treatment of surface/interface/edge effects.

In this letter, the results of a ten million atom molecular-dynamics study of atomic stress distribution in a $Si/Si/Si_3N_4$ nanopixel are reported. The simulations were performed on 128 processors of the 256-processor HP Exemplar at Caltech requiring a total of 180 h of computational time. We have considered a crystalline Si_3N_4 film forming a coherent Si(111)/Si_3N_4(0001) interface[7] with the Si mesa. An interatomic potential model for the Si/Si_3N_4 interface has been developed using the charge transfer values computed from a self-consistent linear combination of atomic orbitals (LCAO) electronic structure calculation.[8,9] The calculated stress distributions illustrate the role of various surface effects and the 1.1% lattice mismatch between Si(111) and Si_3N_4(0001) surfaces.

A variety of empirical interatomic potentials for atomistic modeling of silicon have been developed over the years.[10–14] For our purposes, we have chosen the well-known Stillinger–Weber potential,[12] which provides a satisfactory description of bulk crystalline silicon. Bulk Si_3N_4 is modeled using a combination of two- and three-body interactions which include charge transfer, electronic polarizability, and covalent bonding effects.[15] This potential provides a good description of the structural and mechanical properties and dynamical behavior[16] (static structure factor, bulk and Young's moduli, and phonon density of states) and fracture behavior of crystalline and amorphous Si_3N_4.[17] To describe the bonding across the Si/Si_3N_4 interface, the interface atoms are treated differently from those in the bulk. LCAO elec-

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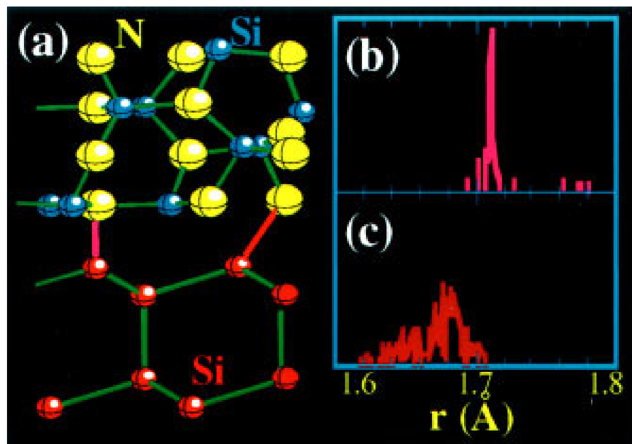

FIG. 1. (a) Si(111)/Si_3N_4(0001) interface. (b) and (c) Si–N bond length distribution for two different bonds marked in magenta and red in (a).

tronic structure calculations[8] provide a guide in determining the charge transfer across the interface.

The Si(111)/Si_3N_4(0001) interface structure is characterized by calculating bond-length and bond-angle distributions. Figure 1(a) shows a schematic view of the interface. Si atoms on the Si(111) surface form bonds with N atoms in Si_3N_4. There are two different types of such bonds (shown in magenta and red, respectively). The bond-length distributions for the two types of bonds across the interface and in bulk Si_3N_4 are shown in Figs. 1(b) and 1(c). The Si–N bond length across the interface is close to that in bulk Si_3N_4 (1.73 Å).

The main issue we address in these simulations is the local stress distribution in Si(111)/Si_3N_4(0001) nanopixels. An efficient algorithm for parallel architectures has been developed to handle multimillion-atom molecular dynamics simulations for the Si/Si_3N_4 system. Additional computational speedup is achieved by using a multiple-time step approach[18] to exploit the separation of time scales and Langevin dynamics approach to reduce the length of equilibration runs for inhomogeneous systems.

The simulated system consists of a 540 Å × 327 Å × 133 Å Si mesa on top of a 1077 Å × 653 Å × 230 Å Si(111) substrate. Periodic boundary conditions are used in the plane of the substrate. The top surface of the mesa is covered with a 83-Å-thick α-crystalline Si_3N_4(0001) film. The lattice Si(111)/Si_3N_4(0001) interface involves a 1.1% lattice mismatch (2 × 2 unit cell of Si is slightly smaller than one unit cell of Si_3N_4). We have also considered a scenario where the parameters of the Si potential are modified so that the lattice constants of Si and Si_3N_4 match exactly. This procedure allows us to isolate the effect of the lattice mismatch on the interfacial stress distribution.

Preparation of the nanopixel is done as follows. First, the Si system and a Si_3N_4 film are separately relaxed to a zero-force configuration using the steepest-descent approach and placed at a distance of 6 Å from each other. The separation distance is then reduced to 1.5 Å in steps of 0.5 Å. At each step, the system is quenched to zero temperature. Subsequently, the system is heated and thermalized at 300 K using the Langevin dynamics.

Atomistic-level stresses are calculated for the two cases of mesas without and with lattice mismatch. The stresses in

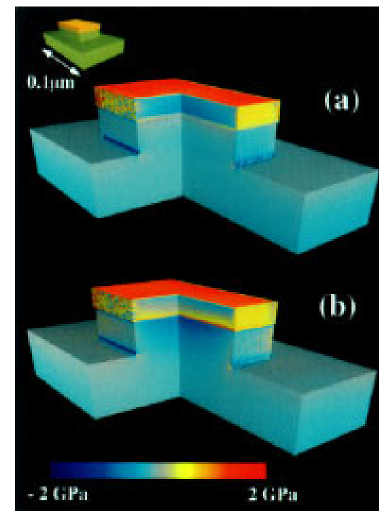

FIG. 2. Stress distribution in a Si/Si/Si_3N_4 nanopixel, (a) without lattice mismatch and (b) in the presence of the 1.1% lattice mismatch. To show the stresses inside the nanopixel one quarter of the system is removed and the value of the hydrostatic stress is color coded.

Si and Si_3N_4 are averaged over the appropriate unit cells, which is necessary to obtain meaningful stress distributions in the case of binary systems such as Si_3N_4 which have atoms of widely different sizes.

Figure 2(a) shows the spatially resolved stress in the absence of the lattice mismatch. Here the stresses are primarily due to the surface effects. In addition, the stress distribution contains stress singularities near the edges of the mesa/substrate boundary. The 1.1% Si/Si_3N_4 lattice mismatch introduces additional contributions to the stress at the interface: compressive stress in Si_3N_4 facing tensile stress in Si [see Fig. 2(b)]. The mismatch-induced stress penetrates deep into the Si mesa to form a tensile stress well.

The hydrostatic $[(\sigma_{xx}+\sigma_{yy}+\sigma_{zz})/3]$ and in-plane $[(\sigma_{xx}+\sigma_{yy})/2]$ stresses along the z axis through the center of the nanopixel are plotted in Fig. 3. The background color corresponds to the color map used in Fig. 2. The stress in the absence of the lattice mismatch is shown in Fig. 3(a). The top surface of the Si_3N_4 film is subject to a strong compres-

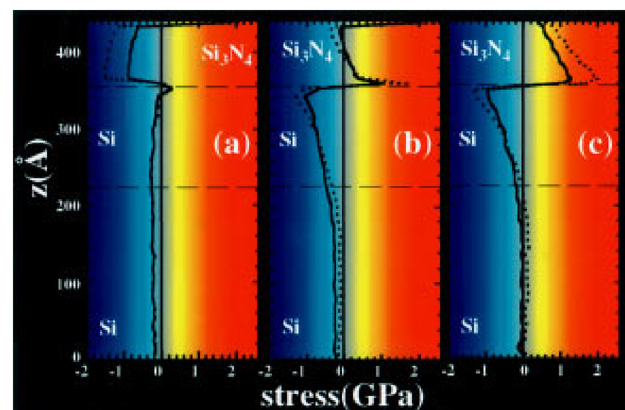

FIG. 3. Hydrostatic $[(\sigma_{xx}+\sigma_{yy}+\sigma_{zz})/3]$ (solid curve) and in-plane $[(\sigma_{xx}+\sigma_{yy})/2]$ (dashed curve) stresses along the z axis through the center of the nanopixel. The background color corresponds to the color map used to show stresses in Fig. 2. (a) lattice matched Si(111)/Si_3N_4(0001) interface, (b) lattice mismatched Si(111)/Si_3N_4(0001) interface, and (c) difference of lattice matched and mismatched interfaces.

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sive stress due to repulsive forces between the N atoms on the surface. Additional stress contributions arise due to intrinsic stress at the interface. As a result, the interior of the Si_3N_4 film experiences tensile stress. The lattice mismatch results in an additional compressive stress in Si_3N_4 above the interface and tensile stress in Si [see Fig. 3(b)]. To isolate the effect of the lattice mismatch, we subtract the stress in the lattice matched system [Fig. 3(a)] from the lattice mismatched data of Fig. 3(b). The resulting stress contribution entirely due to the lattice mismatch is shown in Fig. 3(c). The magnitude and spatial variation of this mismatch-induced stress is consistent with linear elasticity estimates and finite element calculations.[4]

In conclusion, ten million atom molecular dynamics simulations using the space-time multiresolution algorithms have been performed on parallel computers to investigate the stress distribution in a Si(111)/Si_3N_4(0001) mesa on Si(111) substrate. Stress concentration is observed near the interface and at the mesa/substrate edges. A lattice mismatch of 1.1% at the Si(111)/Si_3N_4(0001) interface manifests as a stress well in the center of the mesa. Additional simulations are currently under way to study different geometries of the nanopixel and the effect of amorphous Si_3N_4 in place of crystalline silicon nitride.

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