Dislocation Migration across Coherent Phase Interfaces in SiGe Superlattices

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ABSTRACT

In this work we present a molecular dynamics study of a symmetrically strained SiGe superlatticesubjected to compression. We measure the velocity of a dislocation nucleated at a step in the superlattice on a slip system that cuts across the interfaces, and compare it with that in single crystal Si and Ge for the same geometry. Simulation results of this work show that the phase interfaces in the short-period SiGe superlattice are free of misfit dislocations and that the average dislocation velocity in the SiGe superlatticesample is about two orders of magnitude lower than that in the Si and Ge single crystals for the same geometry and size. The effect of the coherent phase interfaces on the average dislocation velocity is quantified, and the underlying mechanism is identified. This work demonstrates that the coherency stress plays a dominant role on dislocation migration in coherent SiGe superlattices. It shows that a phase interface can impede or assist the migration of a dislocation depending on whether the sign of the stress field along the interface opposes or reinforces that of the dislocation core.

I. INTRODUCTION

The nucleation, multiplication and migration of dislocations in crystalline materials gives rise to plastic deformation [1]. Yield strength and flow stress depend to a large extent on the “dislocation mean free path” [2], which is the distance traveled by a dislocation segment before it is impeded by interactions with other dislocations or obstacles such as grain boundaries, phase boundaries, etc. Phase interfaces between dissimilar materials can act as barriers to the migration of dislocations [3], which may account for the very high hardness and wear resistance seen in nanoscale thickness multilayers or superlattices that have high density of phase interfaces [4-6].

Nanostructured multilayers contain alternating layers of two different materials, with layer thicknesses ranging from several nm to hundreds of nm. Multilayers may be amorphous or polycrystalline, and may have highly coherent or semi-coherent interfaces. In contrast, superlattices are defined by alternating, interpenetrating crystal structures with nanoscale periodicity on the order of a few lattice spacings, and are of single crystalline character [7]. The role of the local interface structure and the misfit dislocations on the mechanical behavior of metallic multilayers have been intensely studied over the past decades [3, 8-15]. Atomistic simulations have demonstrated the effect of the local interface structure on interface-controlled dislocation nucleation behavior [12, 16, 17] as well as the effect of the layer thickness on the flow stress [10, 15, 18].

Different from that in metallic multilayers, semiconductor superlattices grown by molecular beam epitaxy can have interfaces that are atomistically flat and free of misfit dislocations [19, 20]. It has been theoretically predicated [5, 21] and experimentally observed [22, 23] that there is a critical layer thickness below which defect-free phase interfaces in the superlattice can be expected. The resulting superlattice has a single crystal structure and coherent phase interfaces [24-26]. The dynamics of dislocations in such semiconductor superlattices in general and the effect of the atomistically flat phase interfaces on dislocation migration in particular are less investigated.

Experimental study of dislocation–phase interface interaction in superlattices with a high interface density is very difficult due to the extremely fine length and time scales involved in the dynamic process of the interaction between dislocations and interfaces. Quantitative prediction of dislocation mobility from first principles electronic structure calculations currently is still not feasible. Mesoscale dislocation simulation tools, such as the Dislocation Dynamics [27-29], on the other hand, assume dislocation mobility as an a priori input [30]. To provide atomic-level detail of the dynamic process of dislocation-interface interaction, molecular dynamics

(MD) simulations are essentially the only accessible pathway.

The objective of this work is to explore the effect of coherent phase interfaces on the migration of dislocations in silicon germanium (SiGe) semiconductor superlattices. To isolate the effect of coherent interfaces, we focus on short-period SiGe superlattice structure that has been reported to have defect-free, atomistically flat interfaces. The rest of paper is organized as follows. After the introduction, Section II introduces computational model and simulation setup; Section III presents the simulation results for dislocation traversing the superlattice structure. Results for the SiGe superlattice are compared to that for single crystal models of Si and Ge to provide a comparative quantitative understanding of the effect of coherent SiGe interfaces. This paper ends with summary and discussion in Section IV.

II. SIMULATION SETUP

FIG1. The finite SiGe superlattice model where Si layers are in blue and Ge layers are in pink. A constant downward velocity is applied to the atoms in the red box at the top, while atoms in the lower blue box are fixed.

Equal-layer-thickness SiGe superlattices can be grown by molecular beam epitaxy on a buffer layer with a lattice constant on the top surface equal to the average lattice constant of Si and Ge [24]. Superlattices grown in this way have a tensile strain in the Si layer and a compressive strain of equal value in the Ge layer, resulting in symmetrically strained superlattices. For symmetrically strained SiGe superlattices [24], the slip planes and slip directions are continuous across the phase interfaces. There is no mismatch between Si and Ge crystal structures and Burgers vectors. The computer model that mimics the symmetrically strained SiGe superlattice is shown in Fig. 1, in which each Si and Ge layer contains ten unit cells in the cross plane Z direction. A step was created in the top layer of the model to act as a stress

concentrator at which dislocations may nucleate under applied stress. The total approximate model size is 15.0 nm $\times$ 29.8 nm $\times$ 22.2 nm and contains 476,960 atoms in total. Each layer of germanium and silicon atoms is approximately 5.5 nm in thickness.

The open-source molecular dynamics simulation code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is used for the simulations. The Stillinger-Weber potential[31] is employed to describe the interactions between atoms. Non-periodic boundary conditions are applied to the global simulation box. Three groups of atoms are defined in the model shown in Fig. 1 - those in the upper region (red outlined box, comprising atoms in the surface step), those in the lower region (blue outlined box, within two Å of the bottom of the domain), and all other atoms, which are unconstrained. For the purpose of comparison, MD simulation of the same computer model with periodic boundary conditions is also performed to quantify the effects of the free boundary surfaces.

The simulations are first conducted using the NVE ensemble for 1,000,000 steps with a timestep of 1.0 fs to obtain the equilibrium structure of the superlattice in the absence of external force, and then run for another 1,000,000 steps at a low temperature (0.1K) with the NVT ensemble using the Nosé-Hoover thermostat so as to minimize the effect of the thermal fluctuation on dislocation mobility and again to equilibrate the system.

III. RESULTS

A. Model with non-periodic boundary conditions

Figure 2 presents the distribution of the X-direction normal stress component in the superlattice after equilibration. It is seen from Fig. 2 that the Si layers are under tension, while the Ge layers are under compression. The maximum local tensile or compressive stress is 3.283 GPa. It is also seen from Fig. 2 that the relaxed superlattice has a single crystal structure and the interfaces are defect-free and coherent. Note that the stress calculated in LAMMPS is the atomic virial stress, which for homogeneous strain or when the stress is averaged over an area larger than the atomic interaction range is identical to the true stress, i.e., the Cauchy stress[32]. The distribution of other normal stress components of the local virial stress in the superlattice are similar, while the shear stress components are negligible compared with the normal stress components.

After the equilibration, compression is applied to the surface step, as shown in Fig. 1. Velocities of atoms in the upper box are prescribed to achieve an imposed strain rate of 0.0027% ps⁻¹, with the atoms in the lower blue box being fixed. The rest of the atoms are subject to

integration as part of the NVT ensemble at 0.1K. For comparison purposes, computer models of single crystal Si and Ge with the same size as that of the SiGe superlattice are also constructed, and their responses to the same loading conditions are simulated.

FIG2. The finite-size SiGe superlattice model after equilibration, showing the distribution of the X-direction normal component of the virial stress, the single crystal structure of the superlattices, and the coherent interfaces. Note also the influence of free surfaces for the finite model domain, revealing that the stress field is inhomogeneous.

FIG 3. Evolution of the dislocations (blue atoms) nucleated at the step discontinuity and the completely slipped area (red atoms) in (a) Si single crystal, (b) Ge single crystal and (c) SiGe superlattice under compression.

Simulation results are visualized using the visualization software Ovito [33]. Fig. 3 presents 3D snapshots of the time sequences of dislocations in the Si single crystal (Fig. 3a), the Ge single crystal (Fig. 3b), and

the SiGe superlattice (Fig.3c), respectively. The atoms in Fig 3 are colored according to level of volumetric strain; only those atoms associated with dislocations and completely slipped area are displayed. From Fig. 3a we see that the dislocation line in single crystal Si tends to form a hexagonal loop in two slip planes: the (111) and the ($\bar{1}\bar{1}1$), whereas in Fig.3b we observe a hexagonal loop forming at only the (111) slip plane in the Ge sample. Compared with that in single crystal Si and Ge, the dislocation morphology in the SiGe superlattice shown in Fig. 3c is more complex. Before reaching the Si-Ge interface, the dislocation migration in the Si layer is quite similar to that in the Si single crystal. However, due to the existence of the interface, the dislocation line segment on the (111) plane in the first Si layer was hindered at $t = 1.992$ ns, as shown in Fig.3c, and then the other dislocation line segment on the adjacent ($\bar{1}\bar{1}1$) slip plane continued moving forward in the Si layer before the dislocation line segment on the (111) plane transmitted across the interface at $t = 1.994$ ns. After that, more dislocation kinks were formed at $t = 2.655$ ns, as shown in Fig.3c.

To analyze the time evolution of dislocation velocity, an angled plane of atoms is extracted from the 60 degree mixed dislocation, as shown in Fig.4. This is the (110) plane that the intersection point of the two dislocation line segments is moving on. We choose those atoms participating in the plane to trace the dislocation movement. The position and time data are then exported from the time sequence of the trajectories of the dislocated atoms in the selected (110) plane for the analysis. Average positions of atoms in each timestep are used to plot the dislocation position as a function of the simulation time. The dislocation position-time history is then differentiated to yield the instantaneous dislocation velocity.

FIG.4 The (110) plane used to extract data for dislocation velocity. Only those dislocated atoms in this plane were used to characterize the dislocation velocity.

In Fig. 5, we plot the dislocation velocity versus time in the single crystal Si model. It is seen from Fig.5 that the dislocation velocity consists of three stages:

nucleation, acceleration and deceleration. As the dislocation approaches the boundary of the specimen at $t = 2.195$ ns, the velocity starts to drop. There is no steady motion of the dislocation in the single crystal Si sample due to the small sample size.

In Fig. 6, we plot the time history of the dislocation velocity in Ge single crystal. It is seen from Fig. 6 that the dislocation velocity in single crystal Ge is slower than that in single crystal Si. Different from the velocity-time history in Si, the dislocation velocity in single crystal Ge has four stages: nucleation, acceleration, a slow deceleration, and a fast deceleration. The difference in the dislocation velocity profile in Si and Ge is due to their different dislocation velocities and different dislocation morphologies. The velocity of the dislocation in Ge is much lower.

FIG 5. Plot of dislocation velocity versus time in the single crystal Si model. The dislocation nucleated at $t = 2.185$ ns and completely moved out of the crystal at $t = 2.200$ ns. The total time for the dislocation to traverse the crystal is 0.015 ns.

FIG6. Plot of dislocation velocity versus time in the single crystal Ge model. The dislocation nucleated at $t = 2.985$ ns and completely moved out of the crystal at $t = 3.010$ ns. The total time for the dislocation to traverse the crystal is 0.025 ns.

FIG. 7 (a) Plot of dislocation velocity versus time in the SiGe superlattice model. The dislocation nucleated at 1.885 ns and reached the boundary surfaces at $t = 3.500$ ns. The total time for the dislocation to traverse the superlattice is 1.615 ns. (b) Zoomed-in plot of dislocation velocity versus time in the Si layer from $t = 1.985$ ns to $t = 1.995$ ns and (c) in the Ge layer and the second Si layer from $t = 2.640$ ns to $t = 2.660$ ns.

Figure 7 plots the dislocation velocity versus time in the SiGe superlattice model. The dislocation nucleated at 1.885 ns. The plateau in Fig. 7a just after the first peak corresponds to the dislocation reaching the first Si-Ge interface and remaining at the interface. The dislocation transmitted across the first Si-Ge interface at about 2.642 ns with increase of applied displacement. Thereafter, the dislocation quickly passed through the layers of Ge and Si

(2nd major peak) until it reached the 2nd Si-Ge interface. The dislocation remained at the second Si-Ge interface until 3.470 ns when it transmitted across the interface. From Fig. 7 we see that the dislocation motion was impeded by the two Si-Ge interfaces for more than 1.6 ns, while the total time of the dislocation migration in the Si or Ge layers is only about 0.01 ns. Dislocation migration is therefore blocked by the Si-Ge interfaces. Note that the transmission across Ge-Si interfaces occurred very abruptly and the Ge-Si interface appears to have no effect on hindering the dislocation migration.

From the zoomed-in plot of dislocation velocity in Fig. 7b, it is seen that the highest instantaneous dislocation velocity in the first Si layer of the SiGe superlattice is about 1000 m/s, which is much smaller than that in single crystal Si model shown in Fig. 5. Fig. 7c shows that the dislocation velocity in the first Ge layer is also much smaller and decreases slightly as it approaches the Ge-Si interface. However, the dislocation velocity increase rapidly after transmission across Ge-Si interfaces, exceeding 2500 m/s in the second Si layer before the dislocation being impeded by the second Si-Ge interface.

Figure 8 presents snapshots of time sequences of the distribution of the virial stress components. The snapshots are taken at the times corresponding to the dislocation being blocked at the first Si-Ge interface, having transmitted across the first Si-Ge interface, and being blocked at the second Si-Ge interface, respectively. For comparison, we also plot the stress fields in single crystal Si in Fig. 8a. Our simulation results show that the stress fields of dislocations are highly singular, and that the XY-component of the stress field in SiGe is similar to that in Si. From Fig. 8a-d we see that the stress fields associated with the dislocation core are compressive on the top and tensile on the bottom, which opposes the stress field along the Si-Ge interface that is tensile on the top and compressive on the bottom. In addition, before the transmission of the dislocation across the first Si-Ge interface in the superlattice, the applied stress has completely overcome the z-direction component of the coherency stress in the Si layer. In fact, the entire SiGe system is under compression in the loading direction. However, in the in-plane direction, i.e., the X-direction, the Si layers are still under tension while the Ge layers are under compression.

Figure 8 also provides a visualization of the change of the atomic-scale structure of the superlattice under compression after the dislocation transmission. From Fig. 8c we see that steps have been introduced in each of the three interfaces of the superlattice structures. Clearly, the behavior of dislocations crossing the Si-Ge interfaces modifies the initially atomistically flat phase interfaces, but no residual Burgers vector is found at the interfaces.

FIG.8. (a) The XY- shear stress component in the Si single crystal model and (b) in the SiGe superlattice model ; atoms that are colored in red have tensile stress equal or high than 2GPa and those that are colored in blue have compressive stress equal or higher than 2GPa; (c) The X-direction and (d) the Z-direction normal stress component in the SiGe superlattice model during dislocation traversing the superlattice. Atoms that are colored in red have tensile stress equal or higher than 4GPa and those that are colored in blue have compressive stress equal or higher than 4GPa.

B. Model with periodic boundary conditions

To quantify the effect of the free boundary surfaces on dislocation behavior, the same model system under compression is simulated with periodic boundary conditions (PBCs) applied to the in-plane directions of the SiGe superlattice model. Figure 9 shows that the X-direction normal component of the virial stress is nearly uniform, and therefore the effect of the free boundary surfaces on the internal stress in the finite-size superlattice model shown in Fig. 2 is removed. Accordingly, we

observe a homogeneous compressive stress field in the Ge layers and a homogeneous tensile stress field in the Si layers.

FIG 9. The equilibrated SiGe superlattice model with PBCs applied along the X- and Y-directions, showing the distribution of the X-direction normal component of the virial stress, the single crystal structure of the superlattice, and the coherent interfaces.

FIG.10 Snapshots of a time sequence of the dislocation (blue atoms) and the area swept out by slip (red atoms) in the compressed SiGe model with PBCs.

Figure 10 presents 3D snapshots of a time sequence of a dislocation in the SiGe superlattice with PBCs. In the absence of free boundary surfaces, instead of forming a loop, the dislocation nucleated at the step remains straight on the slip plane as the dislocation traverses the specimen.

FIG. 11 (a) Plot of dislocation velocity versus time in the SiGe superlattice for a MD simulation with PBCs. The dislocation nucleated at 2.22ns and transmitted across the 2nd Si/Ge interface at 3.444 ns. (b) Zoomed-in plot of dislocation velocity versus time in the Si layer from $t = 2.226$ ns to $t = 2.230$ ns, and (c) in the first Ge layer and the second Si layer from $t = 3.438$ ns to $t = 3.455$ ns. The total time for the dislocation to traverse the superlattice is about 1.98 ns.

In Fig. 11, we plot the dislocation velocity versus time in the SiGe superlattice model. It can be seen from Fig. 10 or Fig. 11 that the dislocation was impeded by the first Si-Ge interface from about $t = 2.230$ ns to $t = 3.438$ ns; after its transmission across the first Si-Ge interface, the dislocation quickly reached the Ge-Si interface at $t = 3.440$ ns and immediately transmitted across the Ge-Si interface at $t = 3.445$ ns. At $t = 3.450$ ns, the dislocation reached the second Si-Ge interface and was again impeded by the interface.

Note that the effect of the phase interfaces on the motion of the dislocation in the SiGe superlattice subjected to the PBCs corresponds precisely to that of the superlattice with free lateral boundary surfaces presented earlier in this paper. In both cases, the Si-Ge interfaces act

as a strong barrier to the dislocation motion whereas the Ge-Si interface exhibits no such effect on the motion of a dislocation.

VI. SUMMARY AND DISCUSSIONS

The simulation results of this work have demonstrated the effect of the coherent phase interfaces on dislocation migration along slip systems that intersect these interfaces. The time for a dislocation to traverse the nano-sized single crystal Si, Ge, and superlattice SiGe system is 0.015ns, 0.025ns, and 1.615ns, respectively. Although the instantaneous dislocation velocity can be higher in the SiGe superlattice than that in the Si or the Ge single crystals, the average velocity in the finite-size SiGe superlattice sample is about two orders of magnitude lower than that in the Si or Ge single crystal models with the same geometry and size.

The computer models in this work are of sufficiently small size to avoid interface misfit dislocations, with a surface step introduced to facilitate dislocation nucleation. These models are not designed for measuring the strength of the materials but rather for investigating the migration of specific types of dislocations through a series of interfaces. The significant reduction of the average dislocation velocity, however, implies an increased strength of SiGe superlattices relative to the constituent materials, i.e., that of Si or Ge single crystal materials.

The strengthening mechanisms of multilayers or superlattices have been attributed to the modulus, lattice parameter, gamma surface, and slip-plane mismatches between the constituent materials [34]. The mismatch of lattice parameters gives rise to coherency stresses and possible misfit dislocations at the interfaces. Simulation results of this work show that the phase interfaces in the short-period SiGe superlattice investigated in this work are dislocation-free and coherent. For coherent interfaces in the absence of misfit dislocations, it has been believed that the coherency stress is the primary strengthening mechanism and that a stress must be applied to overcome the coherency stress in the superlattices for a dislocation to transmit across the interfaces [9, 34, 35]. In SiGe superlattices, the Si layers are under tension while the Ge layers are under compression. This work reveals that dislocation migration is significantly impeded by the Si-Ge interfaces, whereas overall the Ge-Si interface assists the migration of the dislocation. Note that the stress field associated with the dislocation core opposes the sign of the normal stress field along the Si-Ge interface, but it is consistent with the stress field along the Ge-Si interface. Simulation results of this work thus demonstrate that, although there is a difference between Si and Ge in dislocation velocity, the coherency stress plays the dominant role in impeding dislocation through the system.

of interfaces. Coherent interfaces can impede or assist the migration of a dislocation, depending on whether the sign of the stress field along an interface opposes or reinforces that of the dislocation core.

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