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Author
Stach, E.A.

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Enhancement of dislocation velocities by stress assisted kink nucleation at the native oxide / SiGe interface

E. A. Stach[a)]

National Center for Electron Microscopy, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720.

R. Hull

Department of Materials Science and Engineering, University of Virginia, Charlottesville, Virginia 22903;

Abstract

Experiments have shown that the presence of a thin native oxide layer on the surface of a strained SiGe epilayer causes an order of magnitude increase in dislocation velocities during annealing over those observed in atomically clean samples and during crystal growth. This behavior is explained herein by stress-assisted dislocation kink nucleation at the oxide / epilayer interface. Finite element models are used to estimate the magnitude of stress local to steps at this interface due to both intrinsic and thermal expansion stresses, and dislocation theory is used to determine the resulting increase in single kink nucleation.

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[a] Electronic mail: EAStach@LBL.gov

The rate of strain relaxation in lattice mismatched heterostructures is determined by the kinetics of dislocation nucleation, propagation and interaction. Over the past decade the dislocation propagation process in these systems has been studied extensively.[1] The majority of these studies have focused on the rate of dislocation motion during annealing of structures following the completion of epilayer growth. Recently, it has been shown in the SiGe / Si (001) system that significant differences exist between the rate of dislocation motion during epilayer growth and during annealing.[2] In particular, it was found that the presence of a thin native oxide layer on the epilayer surface causes an order of magnitude increase in dislocation velocities over those observed during crystal growth and during annealing of oxide-free samples. In this Letter, it will be shown that this increase may be explained by considering how intrinsic and thermal expansion stresses present at atomic height steps along the oxide / epilayer interface alter the rate of single kink nucleation along the dislocation line.

Dislocation propagation in strained heterostructures is driven by the net excess stress in the epitaxial layer. This stress results from the strain caused by the inherent lattice mismatch between the epitaxial layer and the substrate minus the stress associated with the self-energy of the dislocation.[3] In addition to the driving stress, the periodicity of a crystalline lattice also has a direct influence on the glide motion of dislocations, causing a variation in the self-energy of a dislocation as a function of its position within the lattice. This variation in self-energy results in a periodic force on the dislocation, known as the Peierls force or the Peierls-Nabarro force.[4] Because of the strong covalent bonding present in silicon, germanium and silicon-germanium alloys, the magnitude of the Peierls forces are relatively large and dislocation propagation is substantially more difficult than in metallic materials (with activation energies on the order of 1.0 to 2.5 eV compared to ª 0.1 eV for

metals). These high Peierls barriers cause dislocations to lie within the potential energy troughs. As a result, dislocation glide in semiconductors must occur via the nucleation and propagation of thermally activated kinks along the dislocation line.[5] These kinks are atomic scale disturbances along the dislocation that occur when a small portion of the line is able to surmount the Peierls barrier through thermal activation and advance one lattice spacing. In bulk materials, kink nucleation must necessarily occur in pairs in order to maintain the continuity of the dislocation line. In the case of strained epilayers, however, dislocation kinks may nucleate singly at the epilayer / free surface interface.[6] These kinks, once nucleated, are driven along the length of the dislocation by the applied stress and thus act to advance the entire dislocation forward by one atomic spacing. The presence of very high stresses within a material may assist in the likelihood of kink formation by increasing the probability that a kink or kink pair, once nucleated via thermal activation, will be driven along the dislocation line.[5-7]

In previous experiments, we have systematically measured the rate of dislocation propagation in SiGe / Si (001) heterostructures during epilayer growth,[2] during annealing in ultrahigh vacuum (UHV)[2] and during annealing when the epilayer has a native oxide on its surface.[2,8] The results of these experiments are reproduced as Figure 1. In this graph we plot the measured rate of dislocation motion normalized with respect to both the epilayer excess stress and a composition dependent activation energy according to the equation below:

$$v^* = \frac{v_m}{\sigma_{ex}} \exp\left[\frac{E_v^*}{kT}\right] \tag{2}$$

Here, v_m is the measured velocity and E_v* is the normalized activation energy, which accounts for the 0.6 eV glide activation energy difference between Si and Ge [i.e. E_v*(x) =

(2.2 - 0.6x) eV].[8] From this data we see that there is no significant difference observed between the velocity of dislocations during the growth of the epitaxial layer and during annealing in ultrahigh vacuum (UHV) of the layers following the completion of growth. It is found, however, that the rate of dislocation propagation is significantly enhanced in the samples that have a thin native oxide layer on the surface, and that the magnitude of this enhancement increase scales with increasing germanium content.

As mentioned above, the velocity of dislocations in semiconductors is directly controlled by the nucleation and migration of kinks along the dislocation line. A possible explanation for the observed order of magnitude increase in dislocation velocity following the growth of a thin native oxide layer is that there is an enhanced nucleation of kinks at the oxide – epilayer interface. Using a simple finite element analysis and dislocation theory concepts we will show that the presence of local stresses at steps along the interface may cause enhanced kink nucleation rates consistent with our observations.

In order to determine the magnitude of stress present at steps in the native oxide – epilayer interface, certain assumptions must be made about the level of stress present in the oxide layer during annealing at 600 °C (the temperature at which the dislocation velocity measurements were made). In the case of the experiments of Reference 6, the native oxide was formed on the sample during a room temperature exposure to ambient air. Prior ellipsometry measurements have found that there is a residual compressive stress on the order of 450 MPa present in a native oxide grown on silicon at room temperature.[9] Superimposed on this stress in the experiments of Figure 1 is a tensile thermal expansion stress of 200 MPa caused by raising the temperature of the sample from room temperature to

600 °C.[10] This yields a net compressive stress in the oxide layer of the order of 250 MPa at 600 °C.

The finite element modeling was performed with a commercially available software package.[11] Both monolayer and double atomic layer steps were modeled – as these are typically observed at the native oxide / silicon interface[12] – and the level of compressive stress was varied from 150 MPa to 350 MPa. Similar analyses which compare continuum solutions and atomistic simulations of dislocation cores in semiconductor materials have shown that the continuum solutions are generally accurate to within one to two Burgers vectors.[13,14] This provides justification for the use of a continuum model in the present analysis. Figure 2 shows the results of the finite element calculations for a single monolayer height step, with a residual compressive stress in the oxide of 250 MPa in the region near the step. (The entire model is not shown – it is observed that the level of stress falls off rapidly from the step, consistent with analytical elasticity theory models that predict that the stress due to an applied moment of this type should decrease as $1/r^2$.[15]) Compressive stresses as high as 750 MPa are seen to develop at the step singularity; stresses of the order 500 MPa a short distance away. The stresses quoted are stresses within the growth plane (σ_x), and thus are additive with respect to the compressive excess stress in the film. A number of similar simulations were performed where the magnitude of the residual stress in the oxide was varied, and where double height steps were modeled. The resulting stresses associated with the presence of steps at the oxide / epilayer interface were not found to be strongly sensitive to the residual stress value in the oxide or to the step height. This is consistent with the analytically predicted $1/r^2$ dependence; the amount of residual stress and the step height used in the simulations simply act to shift the distance away from the step at which the stress

falls to zero, but do not substantially alter the maximum step-related stresses. Thus, the finite element models suggest that 500 MPa is a reasonable approximation of the compressive stress local to steps along the oxide – epilayer interface.

Dislocation velocities in semiconductors are determined by both the magnitude of the applied stress and the kinetics of kink formation. The effect of the additional stress caused by the steps at the oxide – epilayer interface is to locally reduce the activation energy associated with kink formation and thus increase dislocation velocities. This additional stress can be accounted for using the Seeger - Schiller correction.[5,7] It would seem most plausible, physically, to consider the formation of single kinks at the epilayer – oxide interface, although the model that follows can be formulated in terms of double-kink nucleation as well (we have done so, and it yields similar conclusions). Considering in detail the process of single kink nucleation, it is apparent that one must think of the nucleation of a single kink in conjunction with an imaginary 'image kink' existing in the vacuum[16] - this will be done in the analysis that follows.

When high stresses are present, the free energy of formation of a kink pair is a function of the separation between the real kink and the image kink. There exists a critical separation (s^*) at which kink-kink attraction due to elastic energy effects is balanced by those external forces which act to tear the kinks apart. These external forces are of the form σbq , with q being the distance between Peierls valleys in the direction of dislocation motion. When the free energy is at a maximum those kinks with separation greater than s^* spread apart and move the entire dislocation line forward while those closer than s^* mutually annihilate. Including the additional effect of step related stress on the free energy of kink formation as a function of s, the kink separation, yields:[5-7]

$$F(s) = F_k - \frac{\mu(1+\upsilon)b^2q^2}{16\pi s(1-\upsilon)} - \frac{1}{2}\sigma_{applied}bqs - \frac{1}{2}\sigma_{step}bqs \tag{3}$$

where F_k is the stress-free activation energy for single kink nucleation (ª 0.7 eV) [17] and $\sigma_{applied}$ is the lattice mismatch stress in the film. The second term describes the elastic interaction between kinks,[5] and the final two terms account for the effect of stresses in the material on kink separation. The function $F(s_o)$ can be minimized to find the critical single-kink separation from the epilayer surface at which the kink energy is maximum, and this critical value back-substituted into the above equation to find the kink formation energy:

$$F_k^* = F_k - \sqrt{\frac{G(1+\upsilon)b^3q^3\left[\sigma_{applied} + \sigma_{step}\right]}{8\pi(1-\upsilon)}} \tag{4}$$

The resulting kink nucleation rate has been shown to be:[5-7]

$$J = \frac{\nu_D bq\left[\sigma_{excess}\right]}{kT}\exp\left[\frac{-\left(E_m + 2F_k^*\right)}{kT}\right] \tag{5}$$

with ν_D is the attempt frequency, approximated here as the Debye frequency ($\nu_D = 1.3 \times 10^{13}$ s^{-1}) and E_m is the kink migration energy (E_m ª 1.25 eV) [17]. Simple geometrical considerations predict that the velocity of dislocations moving via the single kink mechanism is given by:[6]

$$v_{sk} = \frac{Js^*q}{4} \tag{6}$$

Substituting appropriate values of σ_{step} into the above formulations reduces the activation energy for single kink formation by approximately 0.2 to 0.25 eV. Due to the statistical uncertainty in the experimental measurements, the experimental and theoretical activation energies cannot be directly compared to this level of resolution. In Figure 3, we plot the effect of this change in activation energy on the theoretical predication of dislocation velocity for dislocation motion in a 100 nm $Si_{85}Ge_{15}$ layer on Si (100). The curve labeled

"without correction" is predicted using Equations 5 and 6, with σ_{step} = 0. To demonstrate that the model is not particularly sensitive to the exact magnitude of the stress associated with the steps, a lower bound solution with σ_{step} = 250 MPa and an upper bound solution with σ_{step} = 750 MPa are shown. The presence of this stress predicts an order of magnitude increase in dislocation velocities over those determined without the additional step-associated stress. These results show that stress - induced lowering of the kink formation energy at steps at the oxide - epilayer interface provides one viable explanation for the observed increase in dislocation velocities in samples with a native oxide on the epilayer surface shown in Figure 1.

In conclusion, we have used finite element modeling and dislocation theory to explain the experimentally observed order of magnitude increase in dislocation velocities in strained SiGe epilayers which have a native oxide layer. The presence of intrinsic and thermal stresses in the oxide cause highly localized stresses to develop near steps at the oxide – epilayer interface. These stresses may lower the energy barrier associated with single kink formation along the moving dislocation line, thereby increasing the net dislocation velocity. These results indicate that the modification of the surface of epitaxial layers can have dramatic effects on dislocation propagation as well as the overall rate of strain relaxation.

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Figure Captions

1. Experimentally determined dislocation velocities (normalized) as a function of surface condition and temperature. Note in particular that dislocation velocities are an order of magnitude greater when the surface is covered with a native oxide. Reproduced from Reference 2, with permission.
2. Results of the finite element model for a single monolayer step and a 250 MPa compressive stress. The color scale varies from 1 GPa tensile (dark blue) to 1 GPa (red).
3. Theoretical predictions of enhanced dislocation velocity resulting from the stress-assisted single kink nucleation model.

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