Effect of Ge on dislocation nucleation from surface imperfections in Si-Ge

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Nucleation of dislocation loops from sharp corners playing the role of stress concentrators located on the surface of $Si_{1-x}Ge_x$ strained layers is studied. The surface is of {100} type and the concentrator is oriented such as to increase the applied resolved shear stress in one of the {111} glide planes. The mean stress in the structure is controlled through the boundary conditions, independent of the Ge concentration. Shuffle dislocations are considered throughout, as appropriate for low temperature-high stress conditions. The effect of Ge atoms located in the glide plane, in the vicinity of the glide plane and at larger distances is studied separately. It is observed that Ge located in the glide plane leads to the reduction of the activation energy for dislocation nucleation. The activation volume in presence of Ge is identical to that in pure Si. Ge located in {111} planes three interplanar distances away from the active glide plane has little effect on nucleation parameters. The far-field Ge contributes through the compressive normal stress it produces and leads to a slight reduction of the activation energy for shuffle dislocation nucleation. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4745864]

I. INTRODUCTION

Modern semiconductor devices employ strained layers which are introduced to control the carrier mobility in the channel of field emission transistors. The local strain is produced by $Si_{1-x}Ge_x$ regions placed in the close proximity of the channel. In these regions, a fraction *x* of the Si atoms is replaced, at random, with Ge (*x* is below 0.3). The Ge atom is ~4% larger than Si and hence, at constant pressure, the volume of the alloy is larger than that of Si. When incorporated in the Si wafer, the lateral constraint prevents $Si_{1-x}Ge_x$ from expanding and a compressive stress develops. Typically, two $Si_{1-x}Ge_x$ regions are built on both sides of the channel with the goal of obtaining a large, approximately uniform stress/strain state in a region below the gate with nanometer-scale thickness. Stresses in the GPa range are not uncommon in these devices.

These large stresses add to those produced during processing by implantation and thermal cycling. This increases the probability of dislocation nucleation, which is generally detrimental to the proper function of devices. Since conductive states are created in the highly distorted dislocation core region, these defects produce leaks and shorts. In the current technology, dislocations are trapped at interfaces below the surface layer in which devices are integrated, however, the treading segments of these defects connect to the surface, necessarily crossing the active device layer. In addition, with increased device density and more complex, finer scale patterns at the metal-semiconductor interface, dislocations nucleating from features at the surface may interact with each other and form metastable configurations which cannot be trapped in the sub-surface, therefore, remaining in the electrically active region. Designing the device in ways that prevent dislocation nucleation becomes important for the reliability of the entire circuit.

Evidence of dislocation nucleation from surface imperfections such as steps and ledges is ample. Kammler et al.¹ observed dislocations being emitted from the corners of SiN pads on Si, provided the size of the pads is large enough (i.e., that sufficient strain energy is stored in the initial strain field). They also observed that the resulting dislocation structure does not depend on the geometric details of the nucleation site, but the critical load at which nucleation happens is sensitive to these factors. The dislocation structure below the concentrator could be modeled accurately using dislocation dynamics.² These simulations do not incorporate any information about the nucleation process. Direct, real time observations of dislocation nucleation in epitaxial Ge islands growing on Si have been performed by LeGoues et al.³ and the process was modeled analytically by Johnson and Freund.⁴ Additional indications that stress concentration at surface steps and ledges leads to preferential nucleation from these sites are obtained from nanoindentation. In this test, pop-in events are observed at a smaller applied force in the presence of surface steps than when indenting in a nominally atomically flat surface.⁵ Interestingly, Kiley *et al.*⁶ observed that one does not have to indent on a surface step in order to observe such critical force reduction. Nucleation from the step results even when indentation is performed on a terrace some distance away. This indicates that the ledge plays the role of a stress concentrator.

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Nucleation from surface imperfections in Si has been studied extensively using atomistic models.^{7–10} The general understanding resulting from these works is that nucleation is a thermally activated process which depends on the local stress/strain state, on the geometry of the concentrator and on temperature. Typically, dislocations nucleate as prismatic half-loops from straight ledges and move into the crystal by a kink propagation mechanism. Nucleation takes place without the assistance of thermal fluctuations at a critical resolved shear stress (RSS) or associated strain, γ_{ath} . Under these conditions, the critical nucleus size vanishes. Nucleation at lower strain levels is possible at finite temperatures. The activation energy for nucleation was determined using the nudged elastic band (NEB) method^{7,10} or statistically, by direct molecular dynamics (MD) simulations,¹¹ and was observed to depend strongly on the applied strain. The pure Si case is taken as the reference process for the systems discussed in this article.

Si has a diamond cubic structure with {111} being the preferred glide planes. Dislocations can move in the glide or the shuffle set of {111} planes. A debate was carried out approximately 10 years ago regarding whether one set of planes or the other is favored. At this time, it appears that a consensus has been reached that at low temperatures nucleation and motion in the shuffle set is favored, while at high temperatures dislocation activity takes place predominantly in the glide set. Motion/nucleation at low temperatures requires large stresses, while smaller stresses are necessary at high temperatures. An important result supporting this conclusion was provided by Shima *et al.*⁸ who computed the variation of the activation energy for dislocation nucleation with the applied shear stress for the two systems and showed that the two curves cross; at low stresses (below RSS $= 4.7 \,\mathrm{GPa}$), the activation energy for the glide set is smaller, while at RSS above this threshold the activation energy for the shuffle set is below that for the glide set. Applying a compressive stress normal to the glide plane reduces the activation energy for nucleation in the shuffle plane, while leaving the activation energy for nucleation in the glide set unchanged. Guided by these findings, we study in this work the nucleation of shuffle dislocations.

We investigate the effect of Ge on the nucleation of dislocations from stress concentrators. The nature of dislocations and dislocation mobility in Si_{1-x}Ge_x has received much less attention than the same phenomena in pure Si. Dislocation nucleation in $Si_{1-x}Ge_x$ has not been studied to date, despite the important role played by Si_{1-x}Ge_x in devices. The structure of dislocation cores in presence of Ge has been discussed by Marzegalli et al.¹² who indicate that shuffle dislocations are favored by the presence of high compressive normal strains, a conclusion similar to that discussed above for pure Si. The same group also reports results of atomistic simulations of dislocation motion in a Ge/SiGe epitaxial film.¹³ The problem of Ge clustering at dislocations in Si_{1-x}Ge_x was studied using Monte Carlo simulations by Remediakis *et al.*¹⁴ who reported the core size and energy with clustered and randomly distributed Ge.

The present article is structured around the question of whether nucleation is more likely to take place in the Si or in the $Si_{1-x}Ge_x$ regions of a device. To answer this question, we consider randomly distributed Ge and evaluate the activation energy for nucleation from a surface ledge using an atomistic model. The data for various Ge fractions, *x*, are compared with results for pure Si. The model and the simulation methodology are discussed in Sec. II, while the simulation results are discussed in Sec. III. Conclusions are presented in closure.

II. MODEL AND SIMULATION METHODOLOGY

The model used in this work is shown in Fig. 1 and is similar to that used in Ref. 7 for similar purposes. It is obtained by cutting from a block of dimensions 42×21 $\times 42 a_0^3$ a region (ABCDEF) of dimensions $10 \times 21 \times 10 a_0^3$, where $a_0 = 5.43$ Å is the lattice parameter of Si. The crystal is oriented as indicated in the figure, such that the AB edge of the re-entrant corner is contained in the (111) glide plane. The corner is considered atomically sharp (as in Refs. 7, 8, and 10). This detail is important in nucleation as the stress state next to blunt corners is less concentrated than at sharp corners. The effect of the corner bluntness on the probability of dislocation nucleation was discussed in Ref. 10.

Periodic boundary conditions are applied in all directions and the stress in the simulation cell is controlled by adjusting the position of the periodic boundary planes. Specifically, knowing the stress field which is to be applied in the far field, the corresponding strain field is computed using the anisotropic constitutive law of the crystal. The desired strain is imposed by affinely displacing all atoms. Relaxation is then performed while holding the boundaries of the model in the desired position. In most cases considered here, a pure shear stress in the direction of the Burgers vector is applied in the far field.

The corner AB is a stress concentrator and represents a preferred nucleation site for dislocations. However, the other corners of the rectangular hole, e.g., EF and CD, are also stress concentrators with the same singularity. In simulations in which the athermal strain is applied, i.e., when nucleation is entirely mechanically activated, a very small perturbation is produced in the vicinity of the AB corner in order to favor



FIG. 1. Schematic representation of the model used in this work. The lattice spacing in pure Si, a_0 , is 5.43 Å.

nucleation from this site. The perturbation consists in very small random displacements applied to atoms close to the corner.

Note that the model is large enough such that the periodic boundary conditions in the y-direction do not force the nucleating dislocation to be straight. As discussed below, dislocations nucleate from the corner as half-loops and then become straight (aligned with the y-direction) as they move deeper into the material. The Burgers vector in this {111} plane can be oriented either parallel to or at 60° with AB. Hence, once beyond the half-loop stage, the resulting dislocation is of screw or 60° type. Since the resolved shear stress in the direction of the y-axis is smaller than that in the direction making a 60° angle with AB, the nucleation of 60° dislocations is favored.

The model contains 284,580 atoms. The interatomic interactions between Si-Si, Ge-Ge, and Si-Ge are represented with the Stillinger-Weber three-body potential, which has been used extensively in atomistic simulations of Si mechanics.¹⁵ The parameters for Si-Si are determined in the original publication. For Ge-Ge, the parameters are determined by fitting the energy and size parameters to the cohesive energy and lattice constant. For Si-Ge, a simple arithmetic average of Si-Si and Ge-Ge interactions was considered for the size parameter.¹⁶

The objective of this work is to evaluate the effect of Ge on the activation energy for dislocation nucleation from the stress concentrator. The activation energy is evaluated using the NEB method.¹⁷ The NEB requires a sequence of replicas that interpolate between the initial, defect free state and the final state in which a dislocation has nucleated. Using a set of replicas with configurations close to those of structures along the actual reaction pathway is critical for the proper convergence and accuracy of the method. To obtain these replicas, a molecular dynamics simulation was performed at 1 K and the stress was increased until athermal dislocation nucleation was observed. A dislocation with two 60° and one screw segment and Burgers vector $\frac{1}{2}$ [101] nucleates in the shuffle plane at a resolved shear strain $\gamma_{ath} = 5.45\%$. After nucleation, the dislocation moves quickly into the sample. Sixteen configurations are selected from this sequence and are used as replicas in the NEB method. The initial, defectfree state of the crystal (which corresponds to an energy minimum) is used as the first replica. The last replica of the NEB set is not an equilibrium configuration since under the action of the applied stress the dislocation moves deeply into the crystal. Hence, one of the configurations selected from the MD run is taken as the last replica of the NEB transition path. Both ends of the NEB set are fixed. An alternative would be to use the free-end NEB,¹⁸ however, the last replica is taken far enough from the saddle point and it is assumed that the fact that it is kept fixed does not influence the identification of the transition state. We have tested this conjecture by selecting other configurations as the last replica of the NEB set, configurations which are farther along the reaction pathway from the transition state, and observed that this has no effect on the saddle point configuration.

The NEB is used at stresses much smaller than the athermal threshold, however, the replicas selected from the MD trajectory are all loaded with a resolved shear strain $\gamma_{ath} = 5.45\%$ corresponding to athermal nucleation. Using such high energy replicas directly in NEB would lead to serious convergence problems. Furthermore, such high resolved shear strain situation is very rare in real devices and thus a lower value is more interesting for practical reasons. In order to reduce the total energy of these replicas, an affine strain, which effectively unloads each replica to the desired strain level, is applied before the replicas are used in NEB. This unloading strain is applied only to the atoms located at a distance larger than about 10 Å from the active glide plane in order preserve the atomic configuration in the vicinity of the glide plane. The resulting configurations have energies closer to the actual minimum energy path (MEP) and the NEB convergence is faster.

III. RESULTS AND DISCUSSION

As discussed in previous works, dislocation nucleation takes place preferentially from the corner due to the stress concentration there. For a sharp corner and for the situation in which the ledge height is larger than 3 {111} interplanar distances, continuum mechanics provides an accurate solution for the stress state at the concentrator.^{10,11} This stress state is described by a power function of the distance from the concentrator, r, $\sigma_{ij} \sim r^{-\lambda}$, with two singularities: $\lambda_1 = 0.455$, $\lambda_2 = 0.09$ (values for the isotropic material case). As seen in our previous work,¹⁰ the atomistic model correctly represents the stress concentration up to a distance to the corner of about 0.3 nm. At distances closer to the corner, surface effects dominate. These include surface reconstruction and the relaxation of the outer atomic planes. The critical nucleus size (see below) is larger than the region where these effects are important and hence nucleation is not significantly influenced by them.

Let us consider the case of pure Si first. As mentioned in Sec. II, an undissociated shuffle dislocation half loop nucleates from the corner at a resolved shear strain $\gamma_{ath} = 5.45\%$. This is considered the athermal threshold strain at which nucleation is mechanically activated (no thermal activation). The value compares well with that reported by Izumi and Yip⁷ for pure Si ($\gamma_{ath} = 5.1\%$). The fact that the dislocation nucleates in the shuffle plane and is undissociated is expected based on results from the previous works reviewed in the Introduction.

As the resolved shear strain is reduced below the athermal threshold, an energy barrier to nucleation can be measured. Figure 2 shows the MEP obtained from NEB, corresponding to nucleation in pure Si at a resolved shear strain of $\gamma/\gamma_{ath} = 0.7$. The activation energy is large: 11.7 eV at this applied strain. The barrier height depends strongly on the applied strain.

Figure 3 shows the critical dislocation nucleus corresponding to the transition state for two far field applied strains. The loop has a Burgers vector $1/2[\bar{1}01]a_0$ and segments aligned with $\langle 110 \rangle$ directions. Two segments are of 60° type and one is screw, as indicated in the figure. Similar



FIG. 2. The MEP for nucleating a dislocation loop from the corner AB in Fig. 1, in pure Si, and under an applied strain $\gamma/\gamma_{ath} = 0.7$.

half-hexagonal dislocation loops were observed in MD simulations⁷ and in experiments performed at low temperature.¹⁹

The color coding in Fig. 3 shows the absolute value of the slip vector, which represents the relative displacement of the atoms on the two sides of the glide plane. This relative displacement takes place in the direction of the Burgers vector. As was observed in Ref. 5, slip takes place in the direction of the smallest energetic barrier (the saddle corre-



FIG. 3. Snapshots representing the transition states (critical nuclei) of dislocation nucleation from a sharp corner in pure silicon under resolved shear strains (a) $\gamma/\gamma_{ath} = 0.7$, (b) $\gamma/\gamma_{ath} = 0.55$.

sponding to the unstable stacking fault energy) even when the largest RSS is in a slightly misoriented direction. In the case of $\gamma/\gamma_{ath} = 0.7$ (Fig. 3(a)), the largest magnitude of the slip vector is approximately 80% of the Burgers vector. As the resolved shear strain decreases to $\gamma/\gamma_{ath} = 0.55$ (Fig. 3(b)), the maximum of the slip vector increases, approaching the full Burgers vector of the dislocation. The activation volume and the critical nucleus size increase as the applied strain decreases. A similar result was reported for pure Si by Izumi and Yip⁷ who indicated that the maximum slip vector length in the critical nucleus decreases from 0.95b for $\gamma/\gamma_{ath} = 0.6$ to approximately 0.6b for $\gamma/\gamma_{ath} = 0.95$.

Let us consider now the Si-Ge case. To construct this model, a fraction of Si atoms are replaced with Ge. This leads to a compressive stress, primarily due to the size misfit between Ge and Si. However, the actual stress in the glide plane, both the resolved shear stress (in the direction of the Burgers vector) and the stress normal to the glide plane are controlled through the boundary conditions.

Ge atoms are expected to contribute to nucleation through several mechanisms: Ge located in the glide plane changes the local bonding and hence the γ -surface, while Ge located far from the active glide plane creates a background hydrostatic compressive stress which may influence nucleation. In addition, the spatially varying misfit stress field of Ge located close to the glide plane (this field is not purely hydrostatic), but at distances larger than the cut-off radius of the interatomic potential, may have an effect on nucleation as well. To determine the contribution of each of these mechanisms, we study them separately.

A. Ge located in the glide plane

To determine the effect of Ge atoms in the glide plane, we consider a pure Si model in which a fraction of the Si atoms in two {111} planes ending at corner AB (Fig. 1) are replaced with Ge. This represents a range of 3 Å on both sides of the glide plane, i.e., a layer containing the glide plane and of thickness equal to twice the cut-off radius of the interatomic potential used for Ge. The far field is then adjusted to bring the mean resolved shear stress and the stress normal on the glide plane to zero. Since variability is introduced by the random distribution of Ge, several replicas of the system are considered for each situation. The Ge concentration is kept as a parameter.

The NEB method is then used to determine the MEP. Replicas used as the initial guess for the NEB procedure are obtained, as described in Sec. II, by running a MD simulation at 1 K using the actual atomistic structure of specified Ge concentration. Fig. 4 shows the variation of the nucleation activation energy with the Ge concentration in the glide plane, for a far field resolved shear strain of γ = 3.85%. The activation energy decreases as the Ge concentration increases. For the pure Si case, x = 0, $E_a = 11.7 \text{ eV}$, while for the system with 30% Ge, the activation energy is smaller by approximately 2 eV. Some variability results for each Ge concentration due to the randomness of the Ge atoms distribution in the glide plane. The 3 replicas considered at each Ge concentration are within 0.5 eV from each other in all



FIG. 4. Dependence of the activation energy for dislocation nucleation on the fraction x of Ge (in Si_{1-x}Ge_x) located in the glide plane, and under a resolved shear strain $\gamma = 3.85\%$ ($\gamma/\gamma_{ath} = 0.7$). The multiple points at given x represent results from different replicas of the system. The inset shows the random distribution of Ge substitutional atoms (blue/dark) in the predominantly Si (grey/light) glide plane.

cases. This effect is attributed to the modification of the γ -surface induced by the presence of Ge.

We further investigate the variation of the activation energy with the applied resolved shear strain. Figure 5(a) shows this parameter for systems with 30% Ge in the glide plane. Data for pure Si are also included for reference. The activation energy for the Si-Ge system is lower than that for pure Si at all applied resolved shear strains. The plot has a general decreasing trend and crosses the horizontal axis at the athermal critical strain, γ_{ath} . The athermal threshold strain for Si is $\gamma_{ath} = 5.45\%$, as mentioned previously. The corresponding threshold strains for the Si-Ge system are slightly smaller and decrease with increasing the fraction of Ge. For x = 10% Ge, $\gamma_{ath} = 5.27\%$, for x = 20% Ge, $\gamma_{ath} = 5.15\%$, and for x = 30% Ge, $\gamma_{ath} = 5.1\%$.

The data in Fig. 5(a) are replotted in Fig. 5(b) after the horizontal axis has been normalized by the respective values of γ_{ath} for pure Si and Si_{0.7} Ge_{0.3}. The two curves overlap. This indicates that the activation volume, which is proportional to the slope of this curve, is identical in Si and in Si-Ge at all applied strains. The activation volume decreases as the applied strain increases. Specifically, it is ~100b³ for $\gamma/\gamma_{ath} = 0.48$ (RSS = 2 GPa) and 40b³ for $\gamma/\gamma_{ath} = 0.67$ (RSS = 3.25 GPa). Izumi and Yip⁷ calculated an activation volume of 80b³ for pure Si at $\gamma/\gamma_{ath} = 0.6$ and ~60b³ at $\gamma/\gamma_{ath} = 0.7$. For comparison, the activation volumes for the nucleation of partial dislocations in metals are much smaller, on the order of 10b³, even at relatively low values of γ/γ_{ath} .¹¹

It is also interesting to compare the dislocation nuclei (configurations at the saddle-point) corresponding to $\gamma/\gamma_{ath} = 0.76$ and $\gamma/\gamma_{ath} = 0.58$ for a system with 30% Ge (Fig. 6). As in Fig. 3, the color code in Fig. 6 represents the slip vector magnitude in the direction of the Burgers vector at the location of each atom. The bi-color figures on the right hand side indicate the position of Ge atoms (shown in dark blue) in the respective replica. Comparing Figs. 3 and 6, one may conclude that the presence of Ge does not modify significantly the saddle point configuration of the nucleating dislocation. To make this comparison quantitative, the magnitude



FIG. 5. Variation of the activation energy with (a) the resolved shear strain, and (b) the normalized resolved shear strain, for pure Si (black square) and Si_{0.7}Ge_{0.3} (red triangles). The normalization of the horizontal axis in (b) is made with the critical strain for athermal nucleation, γ_{ath} , for the respective system.

of the slip vector normalized by the length of the Burgers vector, |s|/b, measured across the nucleus and along the line shown in Figs. 6(a) and 6(b), is represented in Fig. 6(c). The coordinate ξ representing the distance from the corner, is reported in Fig. 6(c) normalized with the Burgers vector length, ξ/b . Data are shown for both Si (from Fig. 3) and Si_{0.7} Ge_{0.3} (from Fig. 6). This supports the conclusions stated above: (a) the slip in the critical nucleus is smaller than the Burgers vector when the applied strain/stress is large, and increases as the applied strain decreases, (b) Ge does not have a major effect on the slip vector or the size of the critical nucleus.

Similar observations have been made for pure Si⁷ and for Ni:²⁰ the largest slip in the critical nucleus is smaller than the full Burgers vector at large applied stresses. It is interesting to link this observation with the recent finding of Aubry *et al.*²¹ who evaluated the γ -surface in Cu using the classical procedure, but with the crystal subjected to a resolved shear stress. They concluded that both the unstable stacking fault energy and the stacking fault energy decrease with the applied stress and the slip corresponding to these measures decreases as well. Making use of the standard approach employed to link these measure to dislocation nucleation,^{22,23} one may conclude that under a large applied shear stress a smaller relative displacement of two adjacent glide planes is required in order to nucleate a dislocation.

B. Ge located in the vicinity of the active glide plane

We investigate next the effect of the short range misfit field produced by Ge, while excluding the effect of bonding. 034315-6 Li et al.



FIG. 6. Snapshots representing the critical nuclei (transition state configurations) for dislocation nucleation in Si_{0.7}Ge_{0.3} and under resolved shear strain (a) $\gamma/\gamma_{ath} = 0.76$, and (b) $\gamma/\gamma_{ath} = 0.58$. The colors in the figures on the left represent the magnitude of the slip vector for each atom. The figures on the right indicate which atoms are Si (grey/light) and Ge (blue/dark). The magnitude of the slip vector along the two lines indicated in (a) and (b), *s*, is shown in (c), after normalization with the Burgers vector length. Data are shown for both Si_{0.7}Ge_{0.3} (critical nuclei shown in (a) and (b)) and for pure Si (critical nuclei shown in Fig. 3). The coordinate ξ represents the distance from the corner, and in (c) it is normalized by the Burgers vector length.

To this end, the pure Si model is employed again and a fraction, x, of the Si atoms located in (111) planes at distances between 10 and 13 Å from the active glide plane (which is of shuffle type) and on both sides of it, are replaced with Ge. The region between these two parallel planar regions of Si-Ge, including the active glide plane, contains pure Si. The distance is selected larger than the cut-off radius of the Ge interatomic potential, such that Ge atoms are outside the planar core of the nucleating dislocation. However, the stress produced by these substitutional atoms is still effectively acting on the glide plane. This stress is spatially varying, since the Ge atoms are close enough to the glide plane, it is not purely hydrostatic, but is rather small. For 30% Ge, the mean normal stress on the glide plane is compressive and approximately equal to 0.1 GPa. The resolved shear stress has mean zero (due to the random Ge distribution), but fluctuates with small amplitude. The effect these Ge atoms have on the nucleation process is expected to be weak.

To quantify this contribution, the activation energy for dislocation nucleation is computed using the method described above. The variation of this parameter with the concentration of Ge is shown in Fig. 7 for a resolved far field applied strain of $\gamma = 3.55\%$. The plot also includes the data points corresponding to x = 30% Ge from Fig. 4, i.e., for Ge located in the glide plane. It is observed that Ge located in



FIG. 7. Variation of the activation energy for dislocation nucleation with the fraction of Ge located in the vicinity of the active glide plane (black squares). The effect of Ge located in the glide plane is also shown (red triangles) only for x = 0.3, for reference (Fig. 4). The applied shear strain is $\gamma = 3.55\%$.

the neighborhood of the glide plane has essentially no effect on the activation energy. The variability from sample to sample is on the order of 3%.

C. Far field Ge

The Ge atoms located at distances larger than 4 atomic planes from the active glide plane are expected to influence nucleation only through the mean stress they produce. If the model is constrained, Ge introduces a compressive hydrostatic stress in Si; the pressure is described approximately by p = -11.6x GPa for Ge fractions x < 0.3. This is evaluated using a cubic model in which x% of the Si atoms are replaced by Ge under fixed boundary conditions.

To study the effect of this compressive stress on nucleation, a slightly modified model was used (Fig. 8). This is obtained from that shown in Fig. 1 by shifting the ABEF face into the ABE'F' position. Hence, the active glide plane, i.e., the (111) plane which passes through AB, becomes the



FIG. 8. Schematic representation of the model used to study the effect of compressive stresses acting normal to the glide plane on dislocation nucleation. The step surface ABEF in Fig. 1 is shifted to ABE'F', such that the two surfaces ABCD and ABE'F' are symmetrically located (at an angle $\alpha = 125.27^{\circ}$) relative to the glide plane.

bisector of the angle CAE'. This symmetric configuration allows independent control on the normal and the resolved shear stress in the glide plane, including in the stress concentration region close to the corner. With an asymmetric model such as that shown in Fig. 1, a shear stress concentration appears when one attempts to control the normal stress on the glide plane. For example, when a normal stress of magnitude 3.5 GPa (corresponding to a far field Ge concentration of 30%) is applied, a shear stress with a maximum value of 0.5 GPa is measured close to the corner. This coupling is not present in the configuration shown in Fig. 8. We note that the coupling does not exist even for the geometry in Fig. 1 at locations far from the corner since this effect is due to the structure of the asymptotic field components.

In the simulation, up to 30% of the Ge substitutional atoms are placed in the far-field of the modified model, as shown schematically in the inset of Fig. 9. The main figure shows the variation of the activation energy with the far-field Ge concentration. The activation energy decreases with increasing the compressive stress acting on the glide plane, at constant resolved shear strain (of $\gamma = 3.85\%$).

In metals and alloys, a compressive stress applied on the glide plane generally leads to a modification of the γ -surface which makes dislocation motion and nucleation more difficult. Therefore, from this perspective, the present result is surprising. However, other studies have shown that a compressive stress applied normal to the glide plane reduces the barrier for motion and for the nucleation of shuffle dislocations in Si. Our data can be compared with those of Shima *et al.*⁸ who indicate that the activation energy for dislocation nucleation in the glide set is largely independent of the normal stress acting on the glide plane, while a compressive stress reduces the activation energy for nucleation in the shuffle system. In Ref. 8, the authors report a reduction of the activation energy of 2 eV when 2 GPa compressive normal stress is applied and at 4 GPa resolved shear stress. Our results are in agreement with this estimate; for example we evaluate a 2.1 eV reduction when 2.5 GPa compressive stress acts together with a resolved shear stress of 3.25 GPa.



FIG. 9. Variation of the activation energy for dislocation nucleation with the fraction of Ge located far from the glide plane and under a resolved shear strain $\gamma = 3.85\%$. The inset shows the region in which Ge atoms (blue) are randomly located. The grey area surrounding the glide plane starting from the corner is pure Si.

Further evidence supporting the present result comes from the density functional theory analysis presented in Ref. 24, where it is indicated that the ideal shear strength decreases when a compressive stress is applied on Si, Ge, and SiC. Our finding can also partially explain the fact that gliding in the shuffle planes is more favorable under hydrostatic pressure (5–15 GPa) and low temperature.²⁵

IV. CONCLUSIONS

Dislocation nucleation in Si-Ge is qualitatively similar to nucleation in pure Si, however, the activation energy is reduced due to the presence of Ge. This effect is primarily due to the Ge atoms located in the glide plane. Ge atoms located at a distance from the glide plane larger than the cut-off radius of the interatomic potential influence nucleation only through the strain produced. Specifically, the compressive stress produced by the substitutional Ge atoms reduces the activation energy for nucleation in the shuffle plane. The activation volume and its variation with the resolved stress/strain are identical in Si-Ge and in Si.

Ge atoms diffuse under the action of non-uniform stress fields. In presence of stress concentrators, these point defects form clusters. The results presented here are expected to apply in such cases too, provided that the solute concentration in the region where the critical nucleus develops is approximately constant.

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