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Theoretical study of pressure effect on the dislocation core properties in semiconductors

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The effect of an applied pressure on the core of screw dislocations in semiconductors such as Si, β-SiC, and diamond has been investigated by carrying out tight-binding and first-principles calculations of the variations in dislocation core energies and in energy barriers for dislocation translation. Pressure is found to have a sizable effect and can lead to either decreases or increases in the latter quantities. It is also shown that it is advisable to take into account all pressure-dependent parameters for accurately determining this effect. Nevertheless, we found that for the investigated materials, the effect of pressure was not strong enough to induce structural transformations of the dislocation core. The mobility of the cores was also found to be dependent on pressure, which tends to increase or decrease the energy barriers according to the direction of the dislocation displacement.

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I. INTRODUCTION

Investigations of materials plasticity are usually done without considering the possible effect of an applied pressure. Obviously, in normal conditions, the only experienced pressure is atmospheric and it is too small to have any impact. However, a large pressure is present in specific cases that may considerably modify the mechanical properties of materials. An example is given by the plasticity properties of materials present in the earth mantle, into which a huge lithostatic pressure has to be considered. Other cases concern several mechanical properties experiments such as indentation and scratch tests. Very high stress can be present locally in the tested materials, giving rise to stress tensors with large components. Finally, another relevant situation is the deformation of materials in low-temperature/high-stress conditions.[1–3] For instance, it is possible to use high-pressure confinement apparatus to plastically deform semiconductors in this regime. In fact, pressure helps to prevent the failure of samples that should normally occur since temperatures in those experiments correspond to a brittle behavior. Nevertheless, until now, all theoretical investigations of dislocations in the low-temperature regime have been done without considering the effect of pressure.[4–8] For a model semiconductor such as silicon, typical applied pressures in experiments are in the order of one to several gigapascals,[3] which is large enough to play a non-negligible role. Therefore, in all these different situations, one may wonder what is the effect of pressure on the plastic behavior and, in particular, on the stability and mobility of core dislocations.

Pressure may have several possible kinds of effects on dislocations. An applied pressure will alter the elastic response of the material. The effect of this is a change in elastic constants. Pressure tends to make materials stiffer, and the strain field associated with dislocations is then expected to be different from a zero-pressure case. Pressure may also have a direct effect on the nonelastic part of the dislocation, i.e., the core. First, dislocation core stability may change, with transformation from one configuration to another. Second, dislocations displacements could be made easier (for instance, by lowering the Peierls stress) or harder depending on the pressure. Considered together, these factors could have a definite impact on dislocation cores and therefore on the plastic properties of material. Nevertheless, to our knowledge very little is known, although there have been attempts to investigate the effect of pressure on dislocation cores in several classes of materials. For instance, Durinck *et al.*[9] computed the Peierls stress of dislocations in olivine, an important compound in geology since it dominates in the upper earth mantle. In this material, the complexity of the dislocation cores prevents a full atomistic description; therefore, the authors determined the Peierls stress by combining generalized stacking faults calculations and the Peierls-Nabarro model.[10,11] They showed that, in the presence of a pressure of 10 GPa, some slip systems would harden whereas others would become softer, a result which cannot be fully explained with elastic effects. Pressure effects have also been considered in the case of bcc metals such as tantalum.[12] It has been shown that the structure of a screw dislocation core could be significantly modified upon the application of 10 MPa pressure. However, they found no particular pressure dependence of the Peierls stress compared to the shear modulus variation. Regarding semiconductors, Umeno and Černý[13] recently computed the theoretical shear stress as a function of an applied pressure in diamond, silicon, germanium, and two different silicon carbide polytypes using first-principles calculations. They showed that in diamond, the ideal shear strength is being increased by compression. This finding is coherent with a hard-sphere model, for which compression results in a squeezing of the spheres and a larger resistance against shear, a picture well suited for fcc metals. However, they found an inverse behavior for silicon or germanium, while the silicon carbide shear stress decreases in both compression and dilation. Finally, it has been early shown that iron-based materials and aluminum exhibited a nonideal Schmid behavior, and Bulatov *et al.*[14] proposed that the observed pressure dependence is due to the interaction of a transient activation dilatancy of the moving dislocations with external pressure. These different studies suggest that pressure is an important parameter to account for and call for further investigations.

In this paper, we describe the results of first-principles and tight-binding calculations carried out in order to better un-

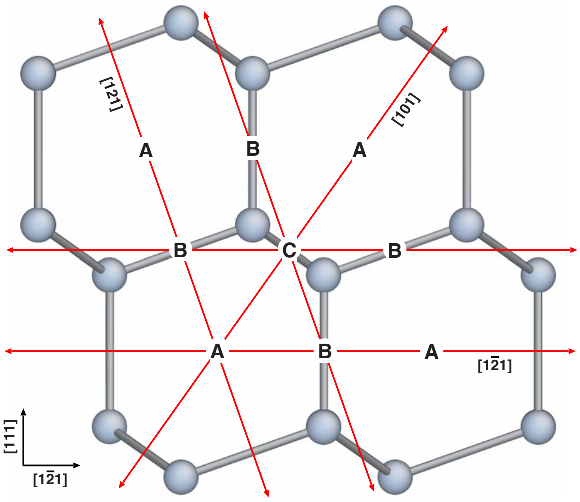

FIG. 1. (Color online) Ball-stick representation of the cubic diamond structure projected along the $[10\bar{1}]$ direction. The positions for the different core configurations discussed in the text are shown (C being C_1 or C_2). Directions for dislocation migration are represented as thin red (gray) lines.

derstand how pressure would affect the mobility properties of semiconductor dislocation cores. We have considered three different materials, i.e., silicon, diamond, and cubic silicon carbide, which are especially interesting for both fundamental research and applications. Also, for silicon and silicon carbide, low-temperature deformation experiments with confinement pressure have already been done, opening the way to comparison between experiments and numerical simulations. After a brief description of the methods and of the computational systems, the effect of pressure on the stability of dislocation cores is detailed. Then, we show how pressure could modify the dislocation mobility using two different approaches. Our results are then discussed in relation with available experiments.

II. MODELS

Experimental investigations of dislocations operating in the low-temperature/high-stress regime have been essentially made in silicon and in III-V compounds.[1–3] The results indicate that these dislocations have a Burgers vector (BV) of $a/2\langle 110\rangle$ and are not dissociated. The glide planes are assumed to be the "shuffle" {111} set planes (widely separated and marked as ABA in Fig. 1), in agreement with the common idea that dislocations in the "glide" {111} set planes (narrowly spaced and marked as BCB in Fig. 1) are necessarily dissociated, as observed in the high-temperature/low-stress regime.[19] In silicon dislocations with characters screw, 60°, 30°, and 41°, have been observed.[3,20,21] Among all these possible orientations, the screw dislocation has received a special attention since it usually governs the plasticity. Also the screw dislocation can cross slip, i.e., move along different directions without diffusion, which is especially interesting for investigating the effect of pressure on dislocation motion. Theoretical investigations showed that three different screw core structures are stable (Fig. 1). One, labeled A in this work, is located in shuffle planes.[5,22–24] The two other possible cores are located in glide planes, one having a structure with a single period along the dislocation line (named C_1),[5,22,24] whereas the other (C_2) is reconstructed along the dislocation line with a double period.[25] For silicon, Wang *et al.*[25] showed that C_2 is the most stable configuration. In this work, we have considered these three possible core structures in the case of three different cubic materials, silicon, silicon carbide in the β phase (cubic), and diamond. Note that another high-symmetry core configuration has been proposed (named B in the following) on the basis of atomistic potential calculations,[23,26] but that is found to be unstable within first-principles accuracy.

The study of the dislocation core stability as a function of pressure has been done by performing self-consistent charges density-functional-based tight-binding (DFTB) calculations[27] using the DFTB+ code and the associated Slater-Koster parameters.[28] The computed lattice parameter, elastic constants, and first derivatives with respect to pressure are reported in Table I. First-principles calculations using the VASP code[29] have also been performed, either to check the results of the DFTB calculations, or for calculating minimum-energy paths (MEPs) for dislocation core mobility. We have used ultrasoft peudopotentials with plane-wave energy cutoffs of 140 eV (Si), 240 eV (SiC), and 280 eV (C), respectively, and the PW91 generalized gradient approximation (GGA) for exchange-correlation.[30] Within these conditions, lattice parameters and bulk modulus of 5.476 Å and 100 GPa (Si), 4.395 Å and 200 GPa (SiC), and 3.571 Å and 419 GPa (diamond) have been calculated, respectively, in very good agreement with experiments. The Brillouin-zone integration has been performed with two special k points along $\hat{Z}$, i.e., the dislocation line orientation, for both methods. MEPs have been computed, thanks to the nudged elastic band (NEB) method, using three relaxed images in the band.[31] The recently proposed technique for combining NEB

TABLE I. Lattice parameter, elastic constants, and related pressure derivatives for Si, β-SiC, and diamond computed using the DFTB+ code. Reference data are given in parentheses. [Pressure derivatives are taken from Refs. 15 and 16 (Si), Ref. 17 (SiC), and Ref. 18 (C).]

	a_0 (Å)	C_{11} (GPa)	C'_{11}	C_{12} (GPa)	C'_{12}	C_{44} (GPa)	C'_{44}
Si	5.460 (5.43)	160 (167)	4.0 (4.19)	69 (65)	3.0 (4.02)	76 (81)	1.1 (0.80)
β-SiC	4.382 (4.36)	479 (390)	4.5 (3.49)	203 (142)	3.5 (4.06)	235 (256)	1.1 (1.58)
C (dia)	3.563 (3.57)	1178 (1079)	5.9 (6.98)	241 (124)	3.0 (2.06)	633 (578)	3.2 (3.98)

TABLE II. Bulk moduli (in GPa), pressure derivatives, and estimated pressures (in GPa) for 1% and 2% compressions computed using the DFTB+ code and the Birch-Murnaghan equation of state for Si, β-SiC, and diamond.

	B	B'	P (ϵ=1%)	P (ϵ=2%)
Si	98	3.42	3.1	6.6
β-SiC	287	5.1	9.3	20.3
C (dia)	530	5.1	17.3	37.5

and dislocations in periodic boundary conditions has been employed.[32]

Cells used in this work were oriented along $\hat{X}$=[112], $\hat{Y}$=[111], and $\hat{Z}$=[110] directions. A specific cell geometry was used, yielding an infinite quadrupolar arrangement of dislocations with periodic boundary conditions and including only two dislocations in the cell.[5,33] Dimensions of systems are $12\times 12\times 2$ for tight-binding calculations and $12\times 12\times 1$ for first-principles calculations. Additional tight-binding calculations performed in bigger cells have shown that such system sizes are large enough to obtain accurate values and trends. Initial dislocation core configurations have been generated using elasticity theory and elastic constants reported in Table I. The effect of a hydrostatic pressure is obtained by applying a strain along all cell directions. In this work, we have considered strains not larger than 2% in order to remain in the validity range of linear elasticity. Corresponding pressures are given in Table II and have been calculated using a Birch-Murnaghan equation of state fitted on DFTB+ bulk computations.

III. DISLOCATION CORE STABILITY

The results of stability calculations as a function of pressure for all possible core configurations are reported in Table III. Clearly, the double period glide configuration C_2 has the lowest energy, in all cases. The shuffle core configuration A is stable, with a higher energy. For silicon, this is the second best solution, with an energy difference in very close agreement with a previous work.[25] DFTB calculations suggest that the single period glide core C_1 is not stable and relaxes to the A configuration (or possibly C_2 with a 2% compression). We have performed first-principles GGA calculations which confirm this result, in contrast to previous local-density approximation calculations.[5] Considering β-SiC, all core configurations are stable and the stability ordering remains the same than in silicon. Finally, in diamond, the single period core C_1 becomes competitive compared to C_2 although slightly higher in energy. The shuffle core A is stable but with a very high energy. In the considered range, the applied pressure does not change the stability ordering. However, it has a sizable effect on the magnitude of the energy difference. In fact, for silicon and silicon carbide, it appears that pressure increases the stability of the shuffle core compared to both glide cores. Also, for all materials, there is an important increase in the energy of the single period glide C_1 configuration relatively to the double period configuration C_2.

TABLE III. Energy differences (in eV per Burgers vector) between different screw dislocation core configurations for each material computed with DFTB+. The most stable configuration, i.e., C_2 here, is taken as the energy reference.

	0%			1%			2%		
	A	C_1	C_2	A	C_1	C_2	A	C_1	C_2
Si	0.60	→A	0	0.52	→A	0	0.43	→A/C_2	0
β-SiC	0.54	0.61	0	0.41	0.73	0	0.28	0.87	0
C (dia)	1.66	0.23	0	1.64	0.33	0	1.64	0.45	0

Comparing two configurations that are equivalent in terms of system size, geometry and applied strain, it has to be noted that the energy difference directly shows how pressure would favor one configuration over the other. But it remains relative and does not allow us to determine the effect of pressure on a dislocation core configuration independently. Such information can be obtained by calculating the dislocation core energy E_C as a function of the applied strain. The total energy of a relaxed configuration can be written as

$$E = E_{\text{bulk}} + E_{\text{inter}} + 2E_C, \tag{1}$$

where E is the total energy of a system including two dislocations, E_{bulk} is the energy of an equivalent system with no dislocations, and E_{inter} is the interaction energy between dislocations (including the interaction between the two dislocations in the cell and half the interaction energy between the dislocation dipole and images due to periodic boundary conditions). The latter depends on the distance between dislocations, i.e., of the geometry of the system, and is usually calculated in the framework of anisotropic elasticity theory, thus depending on elastic constants.[34] Assuming that the dislocation core radius r_0 is equal to the Burgers vector, E_{inter} can be determined in the framework of anisotropic elasticity theory and Eq. (1) allows us to determine E_C. However, it is important to note that all terms in Eq. (1) will directly or indirectly depend on strain and that corrections have to be made. The first is E_{bulk}, which includes the largest part of the energy increase due to the applied strain. The simplest and most accurate way to proceed is to compute E_{bulk} for an equivalently strained bulk system, thus leading to cancellation of errors associated with total-energy calculations. For the second term E_{inter}, one has to take into account that: (i) the interactions are modified due to the reduction in the distances between all dislocations and (ii) the elastic constants vary as a function of pressure. These variations are easily determined using pressure derivatives (Table I).

We have determined dislocation core energies E_C as a function of the applied strain from DFTB calculations and with all the above-mentioned corrections (Fig. 2). We found that core energies increase or decrease approximately linearly with the applied strain. The amplitude of the energy variation can be rather large, e.g., −10% for the shuffle core A in silicon or +8% for the glide core C_1 in silicon carbide and diamond. It also appears that the energy variation depends on the material. The applied pressure tends to lower

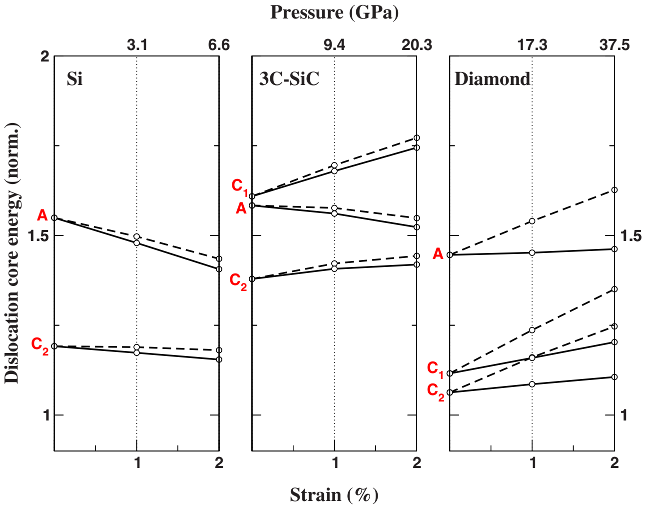

FIG. 2. (Color online) Dislocation core energies as a function of the applied pressure, for each configuration and material (white dots joined by full lines), computed with DFTB+. The energy is normalized by the material-dependent factor $Kb^2/4\pi$ for a better comparison. The core energies calculated without corrections for the E_{inter} contribution are also reported as white dots joined by dashed lines.

the dislocation cores energies in silicon, whereas an opposite behavior is observed for diamond. In the case of silicon carbide, there is no marked tendency on core energies either decreasing (A configuration) or increasing (C_2 and C_1 configurations).

Overall, our results suggest that the variation in the core energy as a function of pressure will depend on both the core configuration and the material. For instance, the energy of the glide core configuration C_1 strongly increases under pressure for both silicon carbide and diamond. The analysis of the structure provides insights for understanding this result. In fact, the C_1 structure is characterized by a central bond linking two atoms which are sp^2 hybridized. This bond is in a compressive state with a length lower than the equilibrium one. Pressure tends to further shorten this bond, leading to a dramatic increase in the core energy. Conversely, the shuffle A configuration energy tends to be lowered (except for diamond, for which it slightly increases), which may be surprising. One possible explanation lies in the specific geometry of the core, which is characterized by four largely stretched and distorted bonds (linking atoms on both sides of shuffle planes; marked by "B" in Fig. 1). Applying a pressure would bring atoms closer, thus lowering the amplitude of bonds stretching and distortion. Finally, we found that the C_2 core is only weakly sensitive to the applied pressure, with small variations in the core energy. This configuration shows a reconstructed core and is thus more complicated, preventing a simple analysis. It is also interesting to analyze the trends going from the "softer" silicon to the "harder" diamond. Overall, we found that, in silicon, an applied pressure would decrease the core energy, while for harder materials an opposite behavior is observed. This suggests that dislocation cores in silicon are in a tensile state, whereas they are in a compressive state in diamond. Silicon carbide shows an intermediate behavior.

IV. DISLOCATION CORE MOBILITY

The various possible paths for the migration of a dislocation in the cubic diamond lattice are represented in Fig. 1. Along ⟨112⟩ orientations, screw dislocations move in {111} planes, with paths ABA for shuffle planes or CBC for glide planes. Another possible displacement direction is ⟨110⟩, with a ACA path encompassed in a {001} plane. Considering that, in two of these paths, C could be either C_1 or C_2, we should investigate five different possible core displacements. However, in this work, we have limited our investigations to paths involving C_1 for many reasons. First, although the C_2 core is found to be the most stable configuration, it is characterized by a Peierls stress which is 50% higher than the shuffle configuration A.[25] It is then not clear whether this configuration plays an important role in the low-temperature/high-stress regime. A second issue is that very little is known about the atomistic mechanisms allowing the reconstructed C_2 core to migrate unlike the other core configurations. Such an investigation is out of the scope of the present study. Finally, there is likely an additional energy barrier due to core reconstruction for the C_2 configuration, and the quick determination of the Peierls energy by simple energy differences that is described in the following would lead to inaccurate quantities.

Two different methods have been employed for investigating the mobility of dislocation cores. Quick estimates of the Peierls energy barriers have been determined by computing the tight-binding-energy differences between stable and high-symmetry saddle configurations along migration paths. These saddle configurations are for instance the B configuration in all materials (see Fig. 1) or the C_1 core in silicon. The total energy of these unstable configurations has been determined by using as few as possible constraints on two atoms in the core during relaxation. In the case where the two considered configurations along the path are stable, this method still allows us to estimate the energy barrier provided that one of the computed configurations is very close to the highest-energy configuration along the MEP; i.e., it is weakly stable. Our investigations of the stability of the different configurations suggest that this is the case here. In the second step, results for silicon have been refined by performing first-principles NEB calculations.

We first describe the results obtained from DFTB calculations represented in Fig. 3. In the case of silicon, the lowest-energy barrier corresponds to the ABA path, i.e., to a screw dislocation displacement in the shuffle plane. With no pressure, the calculated value is about 0.5 eV per Burgers vector, in very good agreement with a previous first-principles result.[32] Applying pressure leads to a slight decrease in the energy barrier. It has been shown in Sec. III that the core energy of the configuration A was decreasing as a function of pressure, which implies that the core energy of the configuration B is decreasing at a larger rate. A possible explanation is related to the structure of the screw dislocation at position B, which is characterized by two opposite rows of three-coordinated atoms, all showing a single dangling bond. Homogeneously straining the lattice brings these two rows closer, thus minimizing the energy penalty due to dangling bonds. Other displacement directions such as ACA and BCB

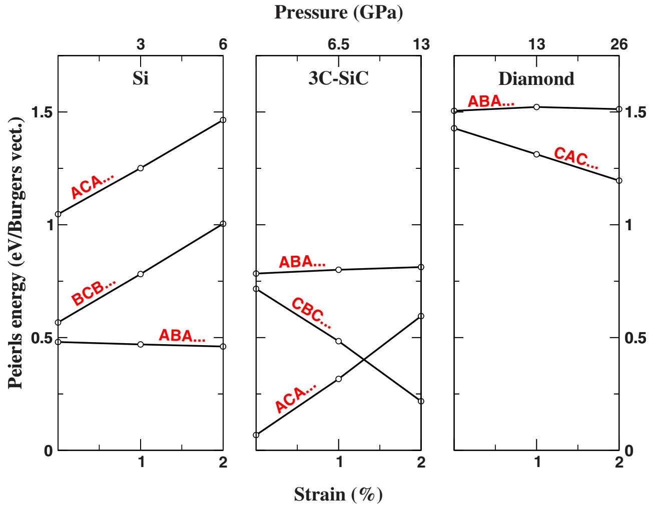

FIG. 3. (Color online) Energies required for translating the dislocation cores (Peierls energies) as a function of the applied pressure, for different paths and materials (white dots joined by full lines). For carbon, the CBC direction is not represented since it is associated with a very-high-energy barrier (>2.7 eV).

lead to larger Peierls energies increasing with pressure. In order to confirm these results that have been obtained with energy differences calculated in the tight-binding approximation we have performed first-principles NEB simulations for the ABA and ACA paths. The computed MEPs, represented in Fig. 4, confirm DFTB calculations. In fact, the energy barrier along ABA (ACA) decreases (increases) as a function of the applied pressure. Also, for the ACA path, the energy variations in Figs. 3 and 4 are similar. The only minor difference comes from the energy decrease for the ABA path, which is much larger in first-principles results with values of 0.41 eV per BV at zero strain and 0.31 eV per BV at 2%. These results then suggest that pressure could significantly enhance the screw dislocation mobility in the shuffle set for silicon.

Analysis of data for silicon carbide reveals a different behavior since the lowest-energy MEP at zero pressure corresponds to an ACA path. In this case, the screw dislocation would move in a {001} plane, alternatively visiting shuffle A and glide C_1 configurations. This result has to be considered with caution because A and C_1 are two stable configurations for β-SiC, and a simple energy difference could be a very rough approximation in that case. In the case of an applied pressure, it is interesting to note that there might be a transition between two glide modes at about 1.3%, with a displacement direction in glide set planes being favored at higher pressure. Finally, for carbon, we found that the ACA path is always favored and that the energy barrier, much higher than in silicon and silicon carbide, is decreasing with pressure.

V. DISCUSSION

In all cases, we found that an applied pressure has a noticeable effect on both stability and mobility properties such as core energies and energy barriers for dislocation translation (Peierls energy) and increases or decreases these energies depending on dislocation core configuration or displacement directions. This is a further confirmation of a previous work on olivine which suggested that slip systems in this material could become softer or harder depending on the applied pressure.[9] Although covalent materials considered in our work have a simpler structure than a silicate such as olivine, similar conclusions are drawn here. In a general situation, taking into account the effect of an applied pressure is therefore necessary.

The most important point is that surely it is extremely difficult to predict how dislocation properties will be affected by pressure. For few cases, it seems that simple arguments based on electronic and atomic structure analysis could explain the computed variations. But in many others, such an approach fails. Because it is not possible to draw simple and general rules, atomistic calculations have to be performed.

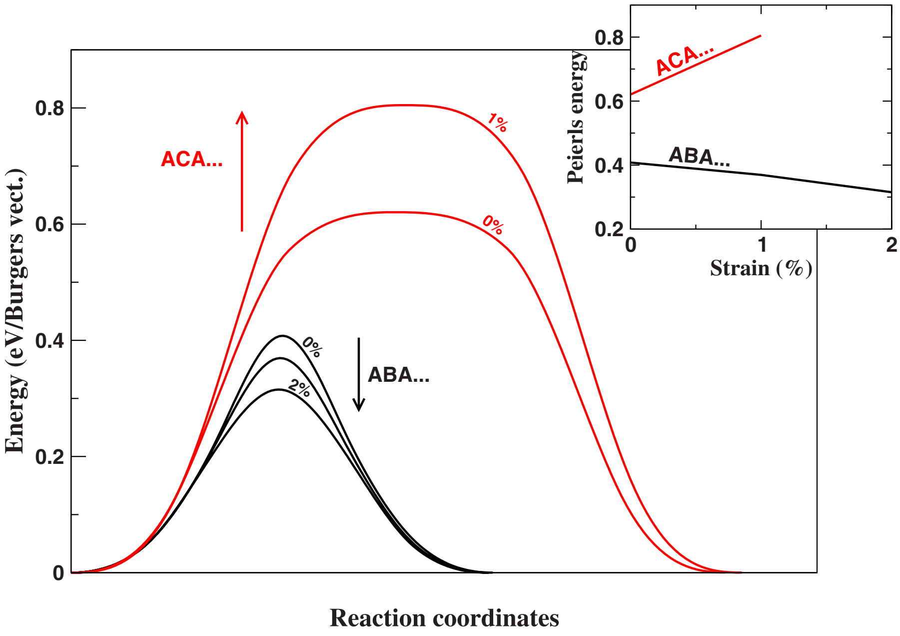

FIG. 4. (Color online) Minimum-energy paths associated with the displacement of a screw dislocation along the ABA (black lines) and ACA [red (gray) lines] directions, as a function of an applied homogeneous strain, in silicon. Peierls energies (in eV per Burgers vector), determined as the maximum energy along MEP, are reported in the inset graph.

This issue may also be more critical for covalent materials than for metals for instance.

Another point concerns the determination of core energy using periodic boundary conditions, a widely used technique in first-principles calculations of dislocations. As explained above, in the determination of interactions between dislocations, it is advised to take into account the variations in both the structural parameters and the elastic constants as functions of pressure. To emphasize this point, we have drawn as dashed lines in Fig. 2 the calculated core energies using both lattice and elastic constants of nonstrained materials. Without corrections, core energy variations show qualitatively similar variation, albeit large differences in amplitude could occur. For instance, taking into account corrections in the case of diamond leads to strong reduction in the pressure effect. Therefore, in the relevant situations, not only pressure has to be taken into account in calculations, but it also has to be very carefully dealt with.

In this work, a pressure has been applied by homogeneously straining the materials, with strains up to 2%. The pressure corresponding to the strain is easily obtained from the bulk modulus. For instance, a strain of 2% corresponds to an applied pressure of about 6.6 GPa for silicon, i.e., in the range of values considered in confinement pressure experiments.[3] For silicon, the semiconductor with the largest amount of experimental data on plasticity, our calculations show that there is no transition in stability between the C_2 glide core and the A shuffle core in this pressure range. In fact, assuming that the core energy variations represented in Fig. 2 are linear and can be extrapolated to large strains, such a transition would occur for a strain of about 6.7%, i.e., an applied pressure of about 29 GPa, which is much higher than the pressure for phase transition from the cubic diamond to the β-Sn structures in silicon. Nevertheless, our results show that due to the applied pressure, the stability of the A core is increased relatively to C_2 and that the screw dislocation mobility in a shuffle plane is made easier. These calculated trends are then in agreement with experiments exhibiting mobile nondissociated shuffle dislocations during high-pressure confinement experiments in the low-temperature/high-stress regime.

Finally, it is instructive to compare our investigations on pressure dependence on dislocation cores properties in the case of semiconductors with what is known for fcc metals. Bulatov *et al.*[14] suggested that there is an additional dilation for moving dislocations compared to dislocations at rest and that this is the coupling of this dilation with an external pressure which is responsible for the observed pressure dependence at the macroscopic scale. Here, we have determined the variation in the core width for dislocations at rest and in the transition state, a quantity which is accessible from NEB calculations.[32] For both ABA and ACA paths, we found a dislocation core which is 20% wider in the transition state. Therefore, in a semiconductor such as silicon, a wider core for a dislocation in motion does not necessarily imply an increase in the Peierls energy with a growing pressure. However, we noticed that the width difference between dislocations in motion and at rest follows the same variation as a function of pressure than the computed Peierls energy, i.e., decreases for the ABA path, and increases for the ACA path. This result indicates that properties of dislocation cores in covalent materials are drastically different than in metals. In covalent materials, it is necessary to take into account the structure and chemistry of the dislocation core at the atomistic level since this fully determines the properties of dislocations.

VI. CONCLUSION

We have performed tight-binding and first-principles calculations of the effect of an applied pressure on the core of screw dislocations in semiconductors such as Si, β-SiC, and diamond. More specifically, the variations in dislocation core energies and in energy barriers for dislocation translation as a function of pressure have been computed and discussed. Overall, we found that the pressure has a noticeable effect, either increasing or decreasing both quantities, suggesting that pressure should be carefully taken into account in the treatment and analysis of the results. This is especially important for investigations where a large applied pressure is present. Nevertheless, this effect is not strong enough to change the stability ordering in any of the investigated materials. Decrease or increase in the energy barrier for dislocation core mobility, depending on the investigated direction, has also been shown, in agreement with available experiments in the case of silicon. These results suggest that electronic structure calculations are required for investigating dislocation core properties in semiconductors.

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