Core reconstruction of the 90° partial dislocation in non-polar semiconductors

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(June 23, 1998)

We investigate the energetics of the single-period and double-period core reconstructions of the 90° partial dislocation in the homopolar semiconductors C, Si, and Ge. The double-period geometry is found to be lower in energy in all three materials, and the energy difference between the two geometries is shown to follow the same trends as the energy gap and the stiffness. Both structures are fully reconstructed, consisting entirely of fourfold coordinated atoms. They differ primarily in the detail of the local strains introduced by the the two reconstructions in the core region. The double-period structure is shown to introduce smaller average bond-length deviations, at the expense of slightly larger average bond-angle bending distortions, with respect to the single-period core. The balance between these two strain components leads to the lower energy of the double-period reconstruction.

61.72.Lk, 61.72.Bb, 61.82.Fk

A fundamental understanding of plasticity in solids clearly requires a knowledge of the atomistic structure at the cores of dislocations. In particular, the microscopic mechanisms of dislocation motion are intimately related to the defects (e.g., kinks) that can occur within the dislocation, which in turn are connected with the underlying lattice symmetries and the nature of the reconstruction in the core.[1] Recently, advances in computer power and computational methodology have led to an active area of research focused on the theoretical study of the atomistic structure of these dislocation cores and their defects.[2–21] However, in at least one important case, even the structure of the dislocation core itself remains fundamentally in doubt.

In tetrahedrally bonded semiconductors, the two most frequently occurring dislocations are the 30° and the 90° partial dislocations, lying on {111} planes along [110] directions.[22–24] These materials are of obvious technological importance, and the detailed understanding of the atomic structure at the dislocation cores is of great interest, since dislocations influence both the electronic and the mechanical properties of semiconductor devices. Indeed, a great deal of theoretical effort has been devoted to study the properties of dislocations in these materials.[2–21] In the particular case of silicon, the theoretical study of the dislocation cores at the atomistic scale has revealed a rich structure of point excitations (kinks and reconstruction defects) in the core of the 30° and 90° partials.[2–5,16–20]

Most of these works have concentrated on understanding the structure of the 90° partial dislocation. Until recently, a consensus had emerged at the theoretical level, about the nature of the reconstruction at the core of the defect. In its unreconstructed configuration, the core of the 90° partial displays a zigzag chain of threefold-coordinated atoms running along the dislocation direction, with broken bonds lying nearly parallel to the slip plane. Mirror symmetry planes are present is this configuration, as can be seen in Fig. 1(a). A variant of this structure is one in which the dashed lines in Fig. 1(a) are considered to be covalent bonds, resulting in a "quasifivefold" reconstruction that also retains the mirror symmetry.[6] On the other hand, a reconstruction that breaks the mirror symmetry of the unreconstructed core, while preserving the lattice periodicity along the line, is shown in Fig. 1(b). In this case all dangling bonds have been eliminated, and all the atoms are fourfold coordinated. Such a reconstruction was predicted to be substantially lower in energy than both the unreconstructed and the quasifivefold-reconstructed cores,[2,6,11–13,15] and thus to be the one expected to occur in nature. We will refer to this symmetry-breaking reconstruction as the single-period (SP) reconstruction.

However, our recent theoretical work on the core reconstruction of this dislocation in Si produced a surprise. In Ref. 3, we proposed an alternative core structure for the 90° partial in which, in addition to symmetry breaking of the SP core, the periodicity along the dislocation line is doubled. This double-period (DP) reconstruction, which is shown in Fig. 1(c), can be derived from the SP one by introducing alternating kinks at every lattice site along the core. This geometry is consistent with all available experimental information about the 90° partial. Like the SP core, the DP structure is fully reconstructed, and thus neither one gives rise to deep-gap states which would show an EPR signal. EPR experiments in Si indicate a very small density of dangling bonds in the core of dislocation.[22–24] Moreover, both cores consist entirely of fivefold, sixfold, and sevenfold rings, both being consistent with images produced by transmission electron microscopy, at the current level of resolution of this technique.[25] The results we obtained in

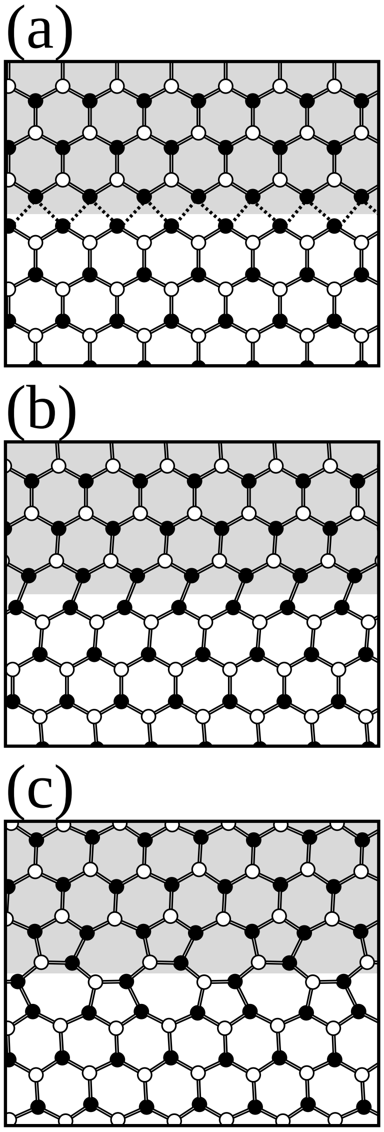

FIG. 1. (a) Symmetric reconstruction of the 90° partial dislocation in homopolar semiconductors. Shaded area indicates stacking fault. (b) The single-period (SP) symmetry-breaking reconstruction. (c) The double-period (DP) symmetry-breaking reconstruction.

Ref. 3 show the DP structure to be lower in energy than the SP one, by means of Keating-potential, total-energy tight-binding (TETB), and *ab initio* local-density (LDA) calculations.

In the present work, we investigate the issue of DP versus SP reconstruction in the homopolar diamond-structure semiconductors C, Si, and Ge. As in our previous work on Si, we present LDA, TETB, and Keating-potential results for the energies of the two core reconstructions. The trend in the energy difference between the DP and SP cores is seen to correlate with the stiffness of each material, with the DP core being more (less) strongly favored in C (Ge), as revealed by our *ab-initio*

TABLE I. Calculated energy difference in meV/Å, between the SP- and DP-core reconstructions of the 90° partial in C, Si, and Ge. Cell size refers to the double-period cell. $E_{\rm DP}$ is the energy of the double-period reconstruction. For the single-period case, $\overline{E}_{\rm SP}$ and $\Delta E_{\rm SP}$ are respectively the average and difference of the energies for the two different relative arrangements of mirror symmetry-breaking.

	192-atom supercell		588-atom supercell	
	$E_{\rm DP}-\overline{E}_{\rm SP}$	$\Delta E_{\rm SP}$	$E_{\rm DP}-\overline{E}_{\rm SP}$	$\Delta E_{\rm SP}$
C				
LDA	-235	126		
TETB	-100	74	-76	14
Keating	-21	123	34	24
Keating[a]	-121	160		
Si				
LDA	-69	48		
TETB	-75	39	-57	3
Keating	-27	40	-7	8
Keating[a]	-40	67		
Ge				
LDA	-58	27		
Keating	-21	32	-5	6
Keating[a]	-12	36		

[a]Evaluated at LDA-relaxed structure.

and TETB calculations. This is in contrast with the Keating-potential calculations which, despite predicting the correct ground-state and trend between Si and Ge, favor the SP structure over the DP core in the case of C.

As in Ref. 3, we employed supercells of 96 and 192 atoms for the SP and DP cores respectively, containing a dislocation dipole in the quadrupole arrangement suggested in Ref. 6. These were fully relaxed (with average forces no larger than 0.01 eV/Å in each case) using an LDA approach, with core states represented by Troullier-Martins pseudopotentials, as implemented in the fhi96md package.[26] All the energy differences were converged to within $\sim$5% with respect to plane-wave cutoff. For Si and C, these cells were also relaxed with a TETB model, using an $\mathcal{O}$(N) density-matrix technique[27] to solve for the electronic structure. (The corresponding TETB results for Ge would be expected to resemble those for Si.) The tight-binding Hamiltonian of Kwon *et al.*[28] was used for Si, while the model proposed by Xu *et al.* was applied to C.[29] The convergence of the TETB results with respect to cell size was checked by relaxing larger cells, with 576 (288) atoms for the DP (SP) structure. Keating-potential results were used in order to investigate qualitatively the strains associated with the two structures. For these, we use the original set of parameters introduced by Keating[30] for the three materials. Further details about the supercells and the technical aspects of our TB calculations can be found in Refs. 2–4.

We discuss first the LDA results for the 192-atom supercell as shown in Table I. The calculated energy of the SP core depends on whether the breaking of mirror symmetry occurs with the same sense, or with opposite sense, for the two dislocations in the supercell. (There is a corresponding energy splitting in the DP core, but this is of a much smaller magnitude and was not taken into consideration.) As in Ref. 3, the average energy of these two possibilities is denoted by $\overline{E}_{\rm SP}$, while the difference is denoted by $\Delta E_{\rm SP}$; the latter is expected to vanish in the limit that the supercell gets large. Focusing for the moment on the $\overline{E}_{\rm SP}$ values, it can be seen that the DP structure is preferred by a substantial margin for all three, and that this preference follows the same trends as the stiffness and the size of the band gap of the material. That is, C shows the strongest tendency toward stabilization of the DP core, followed by Si and then Ge.

Since we cannot easily afford to repeat the LDA calculation for a larger supercell, we have carried out parallel calculations on 192-atom and 588-atom supercells of C and Si using the TETB method. Table I shows first of all that the TETB results are in qualitative agreement with the LDA ones for both materials, although in the case of C the corresponding values are underestimated by a factor of about two. Secondly, the TETB results give us a good estimate of the importance of the finite supercell-size effects. That is, by inspecting the TETB results for the two supercells, it appears that one can say that $\overline{E}_{\rm SP}$ gives the energy of the true isolated SP structure to within an error bar of approximately $\pm\Delta E_{\rm SP}/2$. Applying this heuristic to the LDA results, we see that the supercell-size error is almost certainly insufficient to reverse the sign of the predicted $E_{\rm DP} - E_{\rm SP}$. Returning now to the discrepancy between the TETB and LDA results for C, this could be attributed at first sight to the fact that the model of Xu *et al.* that we use for C results in elastic constants which are too soft [$(C_{11} - C_{12})$ and C_{44} are smaller by 35% and 17% with respect to experimental values, respectively]. On the other hand, the TETB results for Si that we obtained using the model of Ref. 31, which also underestimates the elastic constants, are practically identical to those shown in Table I for the Kwon model.

In order to gain some further insight on the difference between the SP and DP structures, we look at the maximum deviations of bond lengths and bond angles for the LDA geometries, as shown in Table II. The main trend as a function of the material considered is the smaller variation of bond angles, and greater variation of bond lengths, in C relative to Si and Ge. This is consistent with the fact that the ratio of bond-angle bending to bond-stretching forces is bigger in C, compared to Si and Ge. However, we are mainly interested in the trends in going from the SP to the DP structure. For all three materials, we find that the pattern of deviations looks surprisingly similar for the two structures. In particular, the maximum and minimum bond-length and bond-angle variations are *not* systematically smaller in the DP structure, in spite of its lower energy. However, a trend becomes more visible when inspecting the root-mean-square deviations: we see that the rms bond-length variations are systematically slightly larger in the SP core. While it also appears that the bond-angle variations go the other way, being slightly smaller for the SP core, this seems to be a weaker effect. These results suggest that advantage of the DP structure is that it allows a better packing of the atoms, as measured by bond-length variations, at the expense of a slightly greater bond-bending strain.

TABLE II. Minimum, maximum, and root-mean-square variations of bond lengths and bond angles for the LDA-relaxed SP and DP structures, relative to the corresponding bulk diamond values.

	bond length		bond angle	
	SP	DP	SP	DP
C				
min	−5.3%	−4.4%	−11%	−14%
max	+5.4%	+6.2%	+20%	+22%
rms	3.1%	2.8%	3.4%	3.6%
Si				
min	−2.2%	−2.1%	−11%	−15%
max	+3.0%	+3.5%	+22%	+23%
rms	2.6%	2.3%	4.0%	4.1%
Ge				
min	−2.2%	−2.1%	−11%	−15%
max	+3.1%	+3.5%	+22%	+22%
rms	2.8%	2.5%	4.0%	4.1%

In view of the fact that the variations in bond lengths and bond angles between the SP and DP structures are so subtle, it is not at all clear whether a Keating model could be expected to reproduce the correct trends in $E_{\rm SP}$ vs. $E_{\rm DP}$ for the three materials. In order to test this, we also present in Table I the energies for the two core structures as computed using the Keating potential. This was done both by consistently relaxing and evaluating the energy using the Keating model, and by simply evaluating the Keating energy of the LDA-relaxed supercells. Note that in the case of C, the DP-SP energy difference for the Keating-relaxed geometry is substantially smaller than the corresponding LDA result. Also, this set of numbers predicts an incorrect trend for this quantity among the three materials, as compared to the LDA results. For the larger supercell this quantity is even in qualitative disagreement with the TETB result, in the case of C. (We evaluated the Keating energy for the TETB geometries in these larger cells, and found the correct qualitative behavior, with $E_{\rm DP} - \overline{E}_{\rm SP} = -85$ meV/Å for C.) On the other hand, for the LDA geometries, the Keating results follow the same trends as those obtained with the other methods. From these results, we conclude that the Keating potential cannot be trusted to capture the energy difference between the SP and DP structures on a quantitative (or perhaps even qualitative) level.

To summarize, we investigated the energetics of the SP and DP core reconstructions of the 90° partial dislocation in the homopolar semiconductors, C, Si, and Ge. We find the DP core to be favored in all three materials, and observe that the energy difference between the two geometries follows the same trends as the energy gap and the stiffness in these materials. The nature of this difference is primarily associated with the local strains introduced by the the two reconstructions. The DP structure is shown to introduce smaller average bond-length deviations, at the expansion of slightly larger average bond-angle bending distortions, with respect to the SP one, with the delicate balance between these two strain components favoring the DP reconstruction.

ACKNOWLEDGMENTS

Partial support was provided by the DoD Software Initiative. J.B. and D.V. acknowledge support from NSF Grant DMR-96-13648.

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