Models of core reconstruction for the 90° partial dislocation in semiconductors

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Abstract

We compare the models that have been proposed in the literature for the atomic structure of the 90° partial dislocation in the homopolar semiconductors, silicon, diamond, and germanium. In particular, we examine the traditional single-period and our recently proposed double-period core structures. *Ab initio* and tight-binding results on the core energies are discussed, and the geometries are compared in light of the available experimental information about dislocations in these systems. The double-period geometry is found to be the ground-state structure in all three materials. We address boundary-conditions issues that have been recently raised about these results. The structures of point excitations (kinks, solitons, and kink-soliton complexes) in the two geometries are also reviewed.

I. INTRODUCTION

Dislocations are fundamental defects associated with the mechanisms of plastic deformation in solids, playing also a critical role as traps and recombination centers for carriers in semiconductors. In group IV and III-V semicondutors, under usual regimes of plastic deformation, 60° and screw dislocations lying on [110] directions in {111} slip planes are formed. Experimental evidence suggests these to be dissociated into partials both at rest and in motion [1–3]. The screw dissociates into two 30° partials and the 60° dislocation into a 30° partial and a 90° partial. A central issue regards bond reconstruction at the dislocation cores, with most, if not all, of experimental and theoretical works to date indicating that reconstruction does take place. Knowledge of the atomic structure of the core, and of the point-like core excitations (kinks and solitons) which determine the modes of dislocation motion, is crucial to understanding the mechanisms of plastic deformation at a microscopic level.

Here, we review recent theoretical results leading to the proposal of a new core structure for the 90° partial dislocation in homopolar semiconductors [4–6]. This structure has been called the double-period (DP) reconstruction because it involves a doubling of the period along the dislocation direction. In the following, we discuss this and the other models of core reconstruction that had been previously considered for the 90° partial. The traditionally accepted single-period (SP) reconstructed core [7–11] is compared with the DP geometry [4–6]. We also give a brief overview on the types of point excitations occurring in the two geometries.

II. "QUASI-FIVEFOLD" AND SINGLE-PERIOD CORE MODELS

Theoretical works on the atomic-structure of dislocations in semiconductors have heavily concentrated on the 90° partial dislocation [7–11]. From the displacement field predicted for this dislocation by continuous elasticity theory, one obtains an unreconstructed configuration, with the dislocation core displaying 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 along the dislocation direction are present is this configuration, as shown in figure 1(a). By allowing relaxation of this core structure, while keeping the mirror symmetry planes, one obtains a "quasi-fivefold" (QF) structure in which the distance between the two zigzag chains is reduced. The quasi-fivefold denomination is justified since this lead to atomic distances which do not characterize full bond reconstruction [10].

The way for this system to undergo full reconstruction appears straightforward: by breaking the mirror symmetry of the unreconstructed core, reconstructed bonds are formed in the manner shown in figure 1(b). Note that the lattice periodicity along the line is preserved in this geometry, hence we shall refer to this as the single-period structure. All dangling bonds have been eliminated, and all the atoms are fourfold coordinated. *Ab initio* and tight-binding calculations have predicted this structure to be substantially lower in energy (by about 0.2 eV/Å) than the quasi-fivefold core [10,11], being thus the one expected to occur in nature.

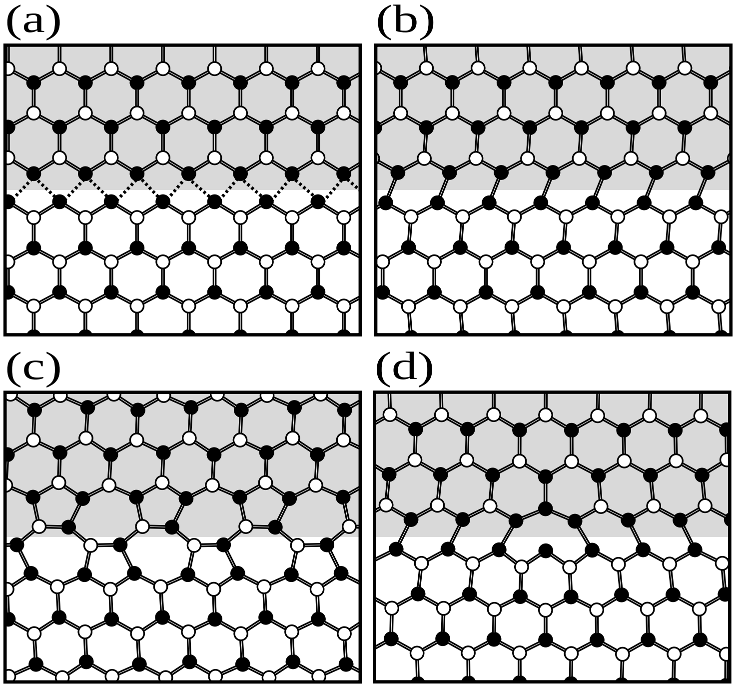

FIG. 1. Models of core reconstruction of the 90° partial dislocation. (a) Symmetric QF reconstruction. (b) Symmetry-breaking SP structure. (c) Ground state symmetry-breaking DP structure. (d) Soliton in the SP core.

III. THE DOUBLE-PERIOD STRUCTURE

Most theoretical works on the 90° partial have addressed the SP geometry. Kinks are fully reconstructed in this structure, with low formation energies, as shown by available theoretical calculations with values ranging from 0.1 to 0.5 eV [9,11–13]. Kinks are thus seen to introduce little strain on the core of the SP geometry. Since a kink and an antikink exert an attractive elastic interaction on each other, and given the already low formation energies above, results indicating a negligible energy for a kink-antikink pair of minimum separation (with the kink and antikink occurring in adjacent sites along the core) should not have been very surprising. Öberg *et al.* reported an energy of only 0.004 eV for this defect, while Nunes [14] computed a value of 0.01 eV. Keating potential calculations on 96-atom supercells of the type employed in our previous works [4,11] give *negative* values (~ -0.3 eV) for the formation energy of the defect.

The full implications of these latter results went unnoticed, however, until it was realized that continuing the process of inserting kink-antikink pairs in the SP core would lead to a new core structure with lower energy than the SP core itself [4]. In addition to the symmetry breaking already present in the SP core, this new structure involves a doubling of the periodicity along the dislocation line, and for that reason it was called the double-period (DP) reconstruction. The atomic geometry is shown in figure 1(c). In the original work, the DP core was introduced for silicon, being later extended to diamond and germanium [5]. In this latter work, the DP core was found to be the ground-state in all three materials, as shown by the *ab initio* and tight-binding total energy (TBTE) results in table I [5]. Recently,

TABLE I. Calculated energy difference in meV/Å, between the SP- and DP-core reconstructions of the 90° partial in diamond (C), silicon, and germanium. 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[a]	−121	160		
Si				
LDA	−69	48		
TETB	−75	39	−57	3
Keating[a]	−40	67		
Ge				
LDA	−58	27		
Keating[a]	−12	36		

[a]Evaluated at LDA-relaxed structure.

Blase *et al.* [15] have shown that the DP core is more stable in diamond over a broad range of stress states, by means of *ab initio* calculations.

Examination of bond lengths and bond angles of the SP and DP structures suggest that the DP core is able to "pack" the atoms more efficiently, as indicated by the smaller average bond-length deviations, at the expense of larger bond-angle deviations. The balance between bond-bending and bond-stretching forces leads to the preference of the three materials for the DP core. The difference is rather subtle, though, as seen by the small differences in maximum bond-length and bond-angle deviations in the two cores, as given in table II [5].

IV. EXPERIMENTAL EVIDENCE

So far, no clear experimental evidence can decide between the two structures. Both geometries are fully reconstructed, hence neither gives rise to deep-gap states which would show an EPR signal. It seems to be safely established by measurements that a rather small density of dangling bonds is to be expected in the core of 90°-partial dislocation [1–3]. 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 [16]. Recent experimental work by Batson [17] indicates a DP-derived structure (called the "Extended DP structure" by this author) to be more consistent with STEM and EELS experiments.

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 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%

V. THE ISSUE OF BOUNDARY CONDITIONS

Lehto and Öberg (LO) have recently investigated the influence of the choice of supercell periodic boundary conditions in the relative stability of the SP and the DP structures [18]. Performing supercell calculations that employed the Keating potential for Si, they concluded that the relative stability of the SP and DP geometries depends on the choice of boundary conditions, with the SP and DP cores being favored for "dipole" and "quadrupole" configurations (these are related to different possible choices of supercell boundary conditions), respectively. Their work raises interesting possibilities, such as the influence of neighboring extended defects, and of the dislocation stress state (as studied in Blase *et al.* [15]) on dislocation core structure, when two competing core structures are very nearly degenerate in energy.

In order to answer the question of which of the two structures is more stable, in the bulk of Si at vanishing stress, we have performed cell-size converged TBTE calculations which clearly show the DP structure to be more stable regardless of the choice of boundary conditions [6]. The results are given in table III. Note that the numbers in this table show a bias of about ~50 meV/Å in the Keating potential, in favor of the SP structure.

VI. KINKS AND SOLITONS

Symmetry breaking in the SP core gives rise to a soliton-type (S) defect at the boundary between two stretches of the dislocation, in which the direction of the bonds is switched, as shown in figure 1(d). Note the presence of a dangling bond in the core of the defect, which explains its formation energy of 1.45 eV. Heggie and Jones [9], suggested a mechanism by which solitons in the SP core may act as nucleating centers for kink-antikink pairs.

TABLE III. Energy of the DP relative to the SP core, in meV/Å per dislocation, for the 90° partial in Si. Three different approximations [TBTE and two different Keating parameterizations (see Nunes and Vanderbilt [6])] are used to compare quadrupole and dipole boundary conditions. Cell size refers to number of atoms in the DP case.

Cell size (atoms)	192	1440	1920
TETB			
quadrupole	−74	−56	−55
dipole	−62	−52	−55
Keating, Ref. [3]			
quadrupole	−27	−1	1
dipole	−14	3	5
Keating, Ref. [4]			
quadrupole	−22	−6	−5
dipole	−13	−4	−3

As discussed by Bulatov *al.* [19], related to the twofold degeneracy of its reconstruction, the SP core supports two kinks and two types of kink-soliton complexes. Referring to figure 2(a), the reconstruction will be said to tilt to the 'left' and to the 'right' on the left and right sides of the kink, respectively. Hence, we call this a left-right (LR) kink, the notation following accordingly for the other kinks. In our terminology, we call kinks

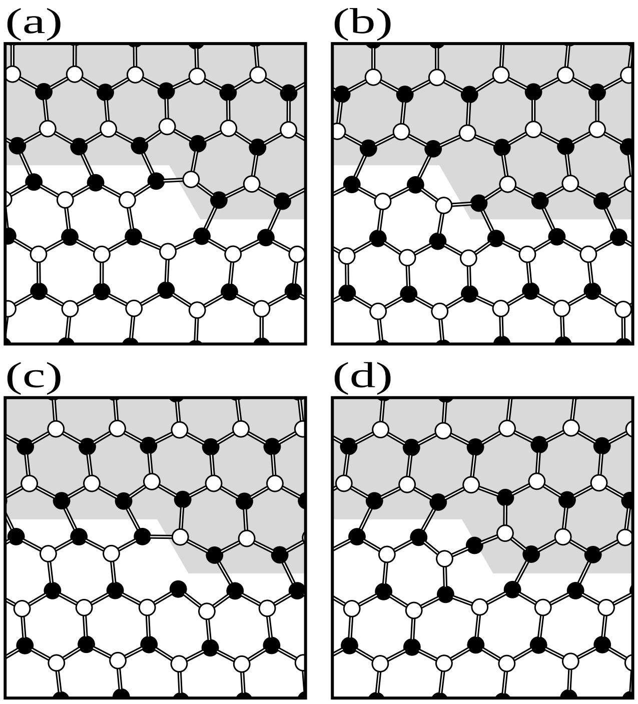

FIG. 2. Core structure of kinks and soliton-kink complexes in the SP core. See text for notation. (a) LR kink. (b) RL kink. (c) LL complex = LR + soliton. (d) RR complex = RL + soliton.

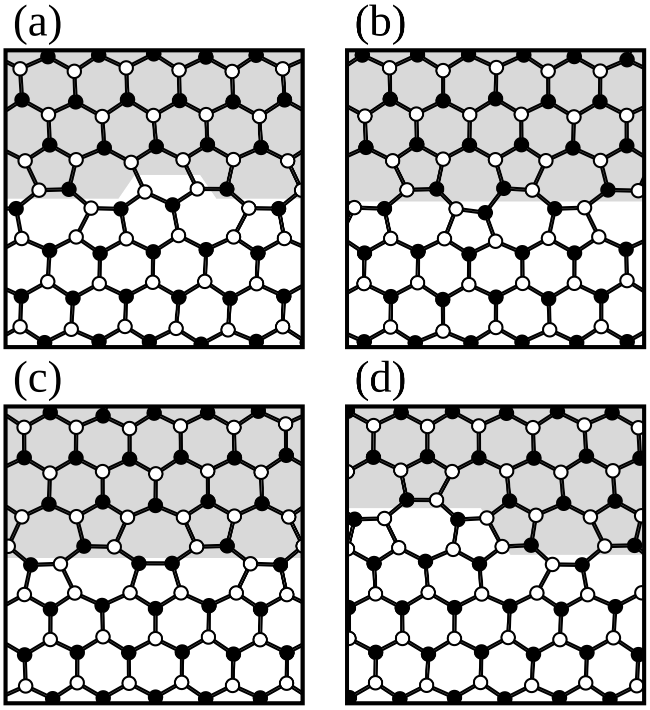

FIG. 3. Examples of several types of core defects in the DP structure. Viewpoint is the same as for figure 1. (a) Phase-switching defect (PSD). (b)-(c) Direction-switching defects (DSD). (d) Kink.

the stable, fully reconstructed excitations shown in figures 2(a) and (b), while kink-soliton complexes are those containing a three-fold coordinated atom in their center, as shown in figures 2(c) and 2(d). Being fully reconstructed, the former have low formation energies (we obtained a value of $\sim$0.12 eV in [12]), while the latter are unstable against the emission of a soliton, in reactions of the type $RR \rightarrow S + LR$, as we have previoulsy discussed [11]. A detailed study of the structure and energetics of these excitations is given in our previous works [11,12].

The period doubling of the DP geometry, combined with the mirror symmetry breaking common to the two structures, gives rise to an even richer structure of core excitations for the DP core. Four equivalent ground states are present(“dnqu”, “qudn”, “pnbu”, “bupn” in the notation of Bennetto *et al.* [4]) related to each other by (110) mirrors and by single-cell translations. An antiphase defect occurs at a translational domain boundary between core segments; being referred to as a “phase-switching defect” (PSD) [figure 3(a)]. As can be seen in figure 3(a), a PSD can be regarded as a short segment of the SP structure inserted into the DP one. Being free of dangling bonds, the PSD is expected to be a low-energy structural excitation. A second class of defects results from a reversal of the mirror symmetry-breaking. These are termed “direction-switching defects” (DSDs); they can be classified by the direction of switching, among other factors. Two examples are shown in figures 3(b) and 3(c), respectively. A DSD will necessarily contain a dangling bond or an over-coordinated atom, so the DSDs are expected to have higher energies than the PSDs.

(The malcoordinated atoms do not appear in figure 3 as they are located just above or below the plane of the figure.)

Finally, turning to the kink structures, because there are four degenerate core structures to choose between on each side of the kink, there should be at least 16 distinct kinks. However, each of these is paired with another into which it can be converted by displacing the center of the kink by one lattice constant along the dislocation [4,19]. Altogether, 8 topologically distinct families of kinks are found in this structure. Furthermore, most of these families may be classified as “kink-defect complexes” incorporating either a DSD, or PSD, or both, which may or may not be energetically bound to the kink. Those including a DSD will retain a malcoordinated atom, and will have no reversal of the mirror symmetry-breaking across the kink; those not including a DSD will be fully reconstructed and will show a reversal of the mirror symmetry-breaking. An example of the latter kind is shown in figure 3(d).

Much work remains to be done to characterize the point excitations of the DP core. Some initial results on kink formation energies were given in Bennetto *et al.* [4], but soliton and kink migration barriers, as well as stability of soliton-kink complexes in this geometry, are crucial aspects determining the mechanisms of dislocation motion, which remain to be addressed. The role of solitonic defects in the nucleation of kink-antikink is also an interesting possibility, to be explored in future studies.

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REFERENCES

[1] P. B. Hirsch, Mater. Sci. Tech. **1**, 666 (1985).

[2] M. S. Duesbery and G. Y. Richardson, Crit. Rev. Solid State Mater. Sci. **17**, 1 (1991).

[3] H. Alexander and H. Teichler, in *Materials Science and Technology*, edited by R. W. Cahn, P. Hassen, and E. J. Kramer (VCH Weiheim, Cambridge, 1993), Vol. 4, p. 249.

[4] J. Bennetto, R. W. Nunes, and D. Vanderbilt, Phys. Rev. Lett. **79**, 245 (1997).

[5] R. W. Nunes, J. Bennetto, and D. Vanderbilt, Phys. Rev. B **58**, 12563 (1998).

[6] R. W. Nunes and D. Vanderbilt, Phys. Rev. Lett., *in press.*

[7] S. Marklund, Phys. Status Solidi B **92**, 83 (1979); J. Phys. (Paris), Colloq. **44**, C4-25 (1983); J. R. Chelikowsky, J. C. H. Spence, Phys. Rev. B **30**, 694 (1984); K. W. Lodge *et al.*, Philos. Mag. A **60**, 643 (1989); L. B. Hansen *et al.*, Phys. Rev. Lett. **75**, 4444 (1995).

[8] R. Jones, J. Phys. (Paris), Colloq. **40**, C6-33 (1979); Philos. Mag. B **42**, 213 (1980); R. Jones et al, Phys. Status Solidi **138**, 369 (1993).

[9] M. I. Heggie and R. Jones, Philos. Mag. B **48**, 365 (1983); **48** 379 (1983); Inst. Phys. Conf. Ser. **87**, 367 (1987) ; M. I. Heggie, R. Jones, and A. Umerski, Phys. Stat. Sol **138**, 383 (1993).

[10] J. R. K. Bigger *et al.*, Phys. Rev. Lett. **69**, 2224 (1992).

[11] R. W. Nunes, J. Bennetto, and D. Vanderbilt, Phys. Rev. Lett. **77**, 15417 (1996).

[12] R. W. Nunes, J. Bennetto, and D. Vanderbilt, Phys. Rev. B **57**, 10388 (1998).

[13] S. Öberg, P. K. Sitch, R. Jones, and M. I. Heggie, Phys. Rev. B **51**, 13138 (1995).

[14] R. W. Nunes, PhD. Thesis, 1996.

[15] X. Blase, K. Lin, A. Canning, S. G. Louie, and D. C. Chrzan, Phys. Rev. Lett. **84**, 5780 (2000).

[16] H. R. Kolar, J. C. H. Spence, and H. Alexander, Phys. Rev. Lett. **77**, 4031 (1996).

[17] P. Batson, Phys. Rev. Lett. **83**, 4409 (1999).

[18] N. Lehto and S. Öberg, Phys. Rev. Lett. **80**, 5568 (1998).

[19] V. V. Bulatov, J. F. Justo, W. Cai, and S. Yip, Phys. Rev. Lett. **79**, 5042 (1997).