Dislocation core studies in empirical silicon models

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Several modern empirical potentials for silicon are used to calculate the configurations and energies of dislocation cores and their mobility-related excitations. The degree of consistency with experiment is found to vary systematically with the magnitude of the defect distortion. The results suggest that the distorted structures encountered with this important class of defects should be incorporated into the construction of the potentials.

Dislocations in semiconducting materials are of topical interest both from a technological and a fundamental point of view. The present consensus is that the experimental evidence,[1-4] supported by electronic-structure calculations,[5] suggests that 2–5% of the atom sites within the dislocation core harbor localized in-gap electron-energy levels, which can destroy the electronic properties of bulk and epilayered solid-state devices by forming intrinsic conductive paths or developing space charges. Provided that the dislocations do not move, the effect need not be catastrophic, because the device logic can be structured to avoid dislocated areas; the consequence is a loss in circuit density. The key question is dislocation mobility, a property that depends critically on the dislocation core.[6]

From a fundamental point of view, the properties of the dislocation core in semiconductors are also highly interesting. While the theory of the dislocation core in metallic materials is reasonably well understood,[7-9] the same cannot be said for semiconductors. The presence of covalent bonding, a lattice basis and an energy gap straddling the Fermi level, introduces core couplings that elude the scope of established theory. For example, there are two distinct classes of (111) glide plane, the *shuffle* and *glide* sets:[10] dislocation motion is associated with production of large quantities of lattice vacancies,[3,11] suggesting a strong mutual binding: electrically active impurities, photon and carrier injection each has a strong effect on dislocation mobility,[12,13] implying that electrically active core sites are associated with dislocation motion.

Fully self-consistent quantum-mechanical calculations are feasible only for computations of small clusters or cells of less than 100 atoms. Dislocation mobility problems, however, can require cells containing thousands of atoms, because of the r^{-1} strain field. Therefore there is a tangible need for work with empirical interatomic potential functions, if only to isolate those configurations which merit more formal treatment. Most attention in semiconductors, both on dislocations and on empirical potentials, has been directed towards Si. The early work on dislocations, reviewed by Marklund,[14] was directed almost exclusively toward core energies, using heuristic methods or empirical potentials[15,16] fitted to limited data to establish the atomic positions in a dislocated environment. The calculated structural energies often required supplementation by uncertain electronic terms.

The more modern empirical potentials,[17-21] fitted to larger data bases and nominally including electronic effects, might be expected to provide a better description. However, the comparative studies necessary to discriminate between the different proposed forms are not available. The work reported here fills this gap by comparing and contrasting the performance of several recently developed empirical potentials for Si in predicting the structures and energies not only of the dislocation core, but also of mobility-related core defects and their interactions with vacancies.

Three different empirical potentials for Si have been considered, each of which contains only pair and interbond angle terms. The potential developed by Stillinger and Weber[17] (SW), providing a reasonable description of the properties of molten Si, is of intermediate range (3.77 Å), extending nearly to the second-neighbor shell. The second potential, suggested by Tersoff,[18] was fitted to density-functional [local-density-approximation (LDA)] calculations of several Si polytypes. It was found necessary to extend the range of this potential in order to use molecular-dynamics (MD) methods; a limit of 3.77 Å, to match the SW range, was chosen. The third potential considered is that due to Kaxiras and Pandey[21] (KP). Fitted to LDA calculations of helical atom interchange, this potential is relatively long ranged, extending to 5.5 Å and including five neighbor shells.

TABLE I. Comparative dislocation energies in eV/b (DE) and dislocation defect energies in eV of the antiphase defect (APD), the kink pair complex (KPC), the trapped vacancy (V), and the APD-trapped vacancy (APD+V) in the perfect lattice (dc) and for 30° and 90° partials, for the Tersoff, SW, and KP potentials (see text). Estimated precision is ±5%.

	DE	APD	KPC	V	APD+V
SW dc				4.54	
SW 30°	1.57	0.84	2.39	1.92	0.35
SW 90°	1.79		1.64	1.54	
Tersoff dc				4.02	
Tersoff 30°	3.12	−0.13	3.67	1.35	1.71
Tersoff 90°	3.96	0.37	1.80	2.33	1.35
KP dc				2.90	
KP 30°	3.10	2.55	3.56	2.32	−1.07
KP 90°	3.93		0.84	1.96	

Dislocations in the diamond cubic lattice have Burgers's vector $b=\frac{1}{2}a(1,1,0)$ and can move on {111} shuffle or glide set planes; however, dissociation involving low-energy intrinsic stacking faults can take place only on the glide set.[10] That both stationary and mobile dislocations are dissociated in Si (Ref. 22) is a strong indication that the active dislocations belong to the glide set; attention will be confined to these.

At low deformations, dislocations in Si are almost exclusively confined to ⟨111⟩ directions, hence either of screw or 60° character. These perfect dislocations are built from just two types of partial dislocation, with 30° and 90° character.[2] Both of these have been considered, modeled as partial dislocation dipoles with a separation of $2a$ (a is the lattice constant); this device permits the use of the fully periodic boundary conditions, thereby avoiding surface effects. The calculations were performed using constant-pressure MD, using the Verlet[23] algorithm with time step 5×10^{-16} s. The model sizes varied from 720 to 3780 atoms, depending on the periodicity of the defect considered. In all cases the configurations were equilibrated at 100 K before quenching to 1 K to extract ground-state energies.

The dislocation energies, shown in the DE column of Table I, contain both core and long-range elastic terms. The latter term, which depends only on the elastic constants, is about 10% smaller for the 30° partial. The energies shown refer to a single partial dislocation. The KP and Tersoff results are in close agreement, roughly double the SW value. This indicates a higher core energy for the KP and Tersoff dislocations, reflecting the larger angular stiffness for these potentials. Since core energies are not measurable experimentally, this energetic distinction does not provide a criterion for choice between the potentials.

The first quantifiable criterion is whether or not the potential support *reconstruction* (indicated from experiment and band-structure calculations cited above) of the partial dislocation cores, i.e., whether the atomic structure within the core can distort sufficiently to permit unpaired electrons to form bonding orbitals with each other. Figure 1(a) shows a ⟨111⟩ projection of the positions of atoms immediately above (closed symbols) and below (open symbols) the slip plane for a 90° partial dislocation with atoms placed at the positions dictated by linear anisotropic elasticity theory. Circular symbols are used for atoms with full fourfold coordination; squares for those with threefold coordination (dangling bonds). The center of the partial dislocation is shown as a dashed line parallel to ⟨110⟩. There are rows of atoms (labeled A and B) parallel to and on either side of the dislocation core, with dangling bonds. With the Tersoff potential, a moderate localized symmetry-breaking deformation of the structure allows the dangling bonds to pair and recover the fourfold coordination for all atoms at the expense of some structural and angular distortion [Fig. 1(b)]. The long cross-core bond in the reconstructed structure has a length of $1.11a_{NN}$ (a_{NN} is the near-neighbor spacing in the perfect lattice), probably not long enough to force local electronic levels far into the gap; the remaining bonds, with lengths of $0.99a_{NN}$, $1.03a_{NN}$, and $1.06a_{NN}$, are not severely stretched. The bond angles range from 95° to 112°. The KP and SW potentials, in contrast, predict a symmetrical dislocation core structure [Fig. 1(c)] in which the A and B atoms each have three neighbors at

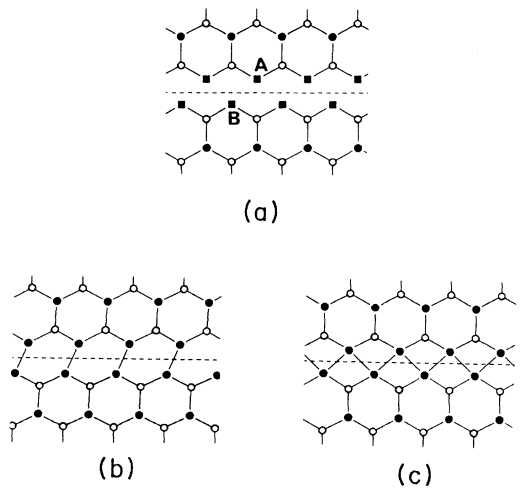

FIG. 1. Spin-plane projection of atom placement within the core of a 90° partial dislocation dipole: (a) unreconstructed, (b) symmetry-breaking reconstruction, and (c) symmetrical reconstruction.

distances close to the ideal (KP, $1.01a_{NN}$, $1.06a_{NN}$, and $1.06a_{NN}$; SW, $0.99a_{NN}$, $0.99a_{NN}$, and $1.00a_{NN}$), plus two at a somewhat larger distance (KP, $1.15a_{NN}$; SW, $1.22a_{NN}$) than nearest neighbor, but much closer than second neighbor ($1.63a_{NNS}$). The bond angle range is larger (KP, 76°–150°; SW, 78°–150°) than for the Tersoff potential. It is not immediately clear what effect the quasifivefold coordination will have on the band structure, but the larger deformation of the cross-core bonds, particularly for the SW potential, is more suggestive of in-gap bands. The Tersoff potential therefore offers a better representation of the 90° partial.

Analogous diagrams for the 30° partial are shown in Figs. 2(a) and 2(b). In this case there are also dangling bonds, at the atoms labeled *A*. Reconstruction (involving a Peierls transition[14]) is possible by the symmetry-breaking deformation shown in Fig. 2(b). All three potentials predict similar fourfold coordinated reconstructed structures, in agreement with experiment and band-structure calculations. The largest bond deformation is $1.10a_{NN}$ for the in-core bond of the Tersoff potential. Bond angles are less distorted than for the 90° partial, ranging from 90° to 122°.

In the broken-symmetry cores, a defect in the reconstruction [termed an antiphase defect[24] (APD) or soliton[25]] becomes possible. The dangling bond associated with this defect, shown in Figs. 3(a) and 3(b) for the 90° partial (for the Tersoff potential) and the 30° partial (for all three potentials), is a plausible source of the observed small electrical activity of the dislocation.[3,4] Calculated APD energies range from −0.13 eV for the Tersoff potential (indicating an instability towards an ordered one-dimensional lattice of alternating APD's and reconstructed core segments, with a 30% concentration of electrically active sites) to a high for the KP potential of 2.55 eV, a value too large to permit any appreciable thermal concentration. The SW value of 0.84 eV would predict a thermal concentration of 10% at 900 K, ostensibly in closest agreement with experiment. The situation may be modified by the position of the APD dangling-bond level with respect to the Fermi level, but the KP APD energy remains too high for it to be a thermal defect.

Dislocation motion takes place by the kink pair creation and migration mechanism.[2,6,10] Experimentally activation energies for kink pair creation and migration lie in the range of 2–3 eV per partial.[2] Calculation of the creation energy of the kink pair complex (KPC in Table I) is complicated by the fact that for the 30° and the asymmetric 90° partials, kink pairs may be fully reconstructed or may be combined with an APD to include a dangling bond.[25,26] The energies listed in Table I pertain to kink pairs containing a single dangling bond, a choice deemed reasonable because the motion of reconstructed kinks requires the intermediate creation of dangling bonds. All three potentials predict KPC energies much larger for the 30° than for the 90° partial. This would imply a lower mobility for screw (containing two 30° partials) than for 60° dislocations (containing one 30° partial and one 90° partial), a feature not observed experimentally. In this respect none of the potentials is completely satisfactory. For the KP and Tersoff potentials, the calculated energies for the 30° partial KPC, each about 3.5 eV, are too large.

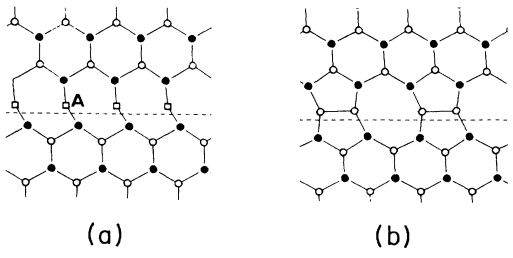

FIG. 2. Slip-plane projection of atom placement within the core of a 30° partial dislocation dipole: (a) unreconstructed, and (b) reconstructed.

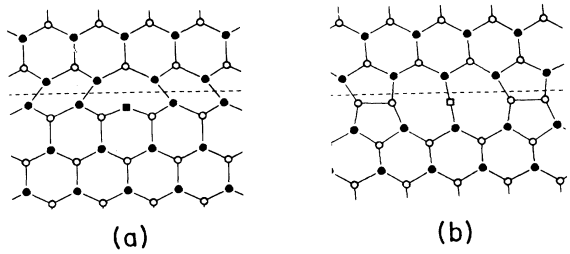

FIG. 3. Slip-plane projection of atom placement within the core of an APD dipole: (a) 90° partial, and (b) 30° partial.

Finally, the interaction between the dislocation core and vacancies will be considered. The vacancy energy itself is somewhat in question. Some LDA calculations[27] suggest values similar to those given by the SW and Tersoff potentials (Table I). On the other hand, Pandey[28] claims a lower value, close to that obtained (2.9 eV) with the KP potential. The energies of a vacancy sited at partial dislocations and at APD's of each kind are shown in Table I. All three potentials suggest that the partial dislocation cores and APD's in particular are preferred sites for vacancies, in agreement with experiment. The negative energy found for the vacancy bound at the KP 30° APD, implying an instability with respect to the shuffle core, is not supported experimentally.

To summarize, the results indicate that the modern procedure of matching empirical potentials for covalent materials to liquid or solid polytype data, while necessary, is not sufficient for simulation of dislocation processes. All three of the potentials considered provide an acceptable picture of the low-strain 30° partial dislocation. The 90° partial dislocation, requiring a greater distortion of the bond angles and lengths, is represented well only by the Tersoff potential. The APD and KPC dislocation core excitations, involving even more highly deformed environments, are not described well by any of the potentials. The trend of decreasing performance with increasingly distorted structures reflects the risk inherent in applying an empirical potential to structures far removed from its implicit database.

The need for an empirical potential that can describe

the structure and mobility of dislocations is unquestionable. A prerequisite, not yet satisfied, is an acceptable description of the fundamental mobility-related dislocation excitations. The moderate success of current potentials for the less distorted defects is encouraging, but the construction of a suitably parametrized functional form that can support both ordered and strained states remains a challenge. Certainly, any such potential must include within its data base the wide range of stable, highly deformed configurations present in the dislocated environment.

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