

Electronic and elastic properties of edge dislocations in Si

Feng Liu, Mark Mostoller, V. Milman,* M. F. Chisholm, and Theodore Kaplan
Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831

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Ab initio, tight-binding, and classical calculations have been done for $(a/2)\langle 110 \rangle$ edge dislocation dipoles in Si at separations of 7.5–22.9 Å in unit cells comprising 32–288 atoms. These calculations show states associated with the cores relatively deep in the band gap (~ 0.2 eV) despite the absence of dangling bonds. The shifts in the electronic states depend significantly on separation d and are correlated with a concentration of strain in the cores as the dislocations become more isolated. The strain energies exhibit a logarithmic dependence on d consistent with linear elasticity for all system sizes.

Extended defects like interfaces, grain boundaries, and dislocations are receiving increasing attention, particularly in semiconductors, because of their potential impact on device performance. These defects can degrade device performance by serving as undesirable sinks or sources of carriers.¹ In the growth of multicomponent structures, lattice mismatch between components can result in the formation of misfit dislocations at the interfaces.² At one time, it was believed that the observed electrical properties might arise from intrinsic changes in local bonding, i.e., dangling bonds or overcoordination. However, many studies of the atomic structures of dislocations and tilt boundaries have revealed structures which retain tetrahedral coordination, with bond and angle distortions too small to introduce localized states in the gap.

There have been a few recent *ab initio* studies of dislocations and related structures in Si. These include the work of DiVincenzo *et al.* on the $\Sigma 9$ twin boundary,³ of Bigger *et al.* on the 90° partial dislocation,⁴ and of Arias and Joannopoulos on a $\langle 110 \rangle$ screw dislocation.⁵ In the first two of these, only shallow gap states are reported, and the third is silent as to electronic structure. We present here results of *ab initio*, tight-binding, and classical calculations of $(a/2)\langle 110 \rangle$ edge dislocation dipoles which show states relatively deep in the gap despite the absence of dangling bonds or overcoordination. Calculations were done for dipole separations of 7.5–22.9 Å along the direction of the Burgers vector in the relaxed samples. For the smallest (32-atom) system, the presence of the dislocations pushes the top of the valence band upward by a small amount into the gap for bulk Si. As the separation increases, this shift increases and converges to a value of almost 0.2 eV above the bulk band edge, much deeper in the gap than reported in previous calculations for systems containing dislocations. We also find that the calculated strain energies for all separations from the smallest to the largest can be fit to a single logarithmic curve of the form predicted by linear elasticity theory, as was found by Arias and Joannopoulos for screw dislocations.⁵ A value for the core energy E_c is extracted subject to some ambiguity in determining the core radius r_c .

In the calculations, unit cells containing a dislocation dipole with a separation of n_6 sixfold rings along $[110]$ (as viewed in projection along $[1\bar{1}0]$) were constructed by classical simulations using the Stillinger-Weber (SW) po-

tential.⁶ A few calculations were also done with the Tersoff potential,⁷ which gave no significant changes in the structural results.⁸ Two half-planes were removed at separations corresponding to $n_6=1-5$ in large rectangular samples, and these samples were annealed and their energy minimized to form a $\pm(a/2)[110]$ edge dislocation dipole. Parallelograms that could be periodically repeated in the fashion described by Bigger *et al.*⁴ were excised from the larger rectangular ones to give a series of samples with 32, 72, 128, 200, and 288 atoms. These were annealed and minimized at constant pressure with the SW potential using the Parrinello-Rahman method.⁹ *Ab initio* local-density-approximation (LDA) calculations were then done at constant volume, using the computer code CETEP (Ref. 10) (Cambridge-Edinburgh Total Energy Package), adapted to run on the ORNL Intel Paragon computer. At the time these calculations were done, this machine had 512 nodes with 32 MB/node and a peak performance of 35 G-flops.

Figure 1 shows a projection of the 128-atom unit cell

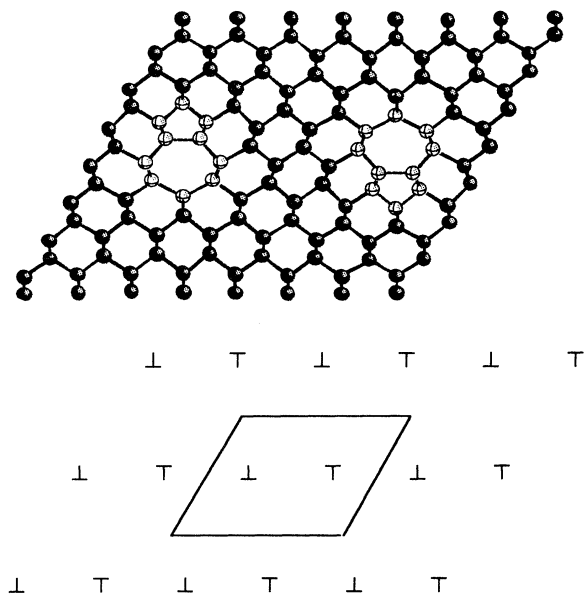


FIG. 1. $[1\bar{1}0]$ projection of a 128-atom unit cell for the edge dislocation dipole (top), and a portion of the 2D dislocation lattice showing the unit cell (bottom).

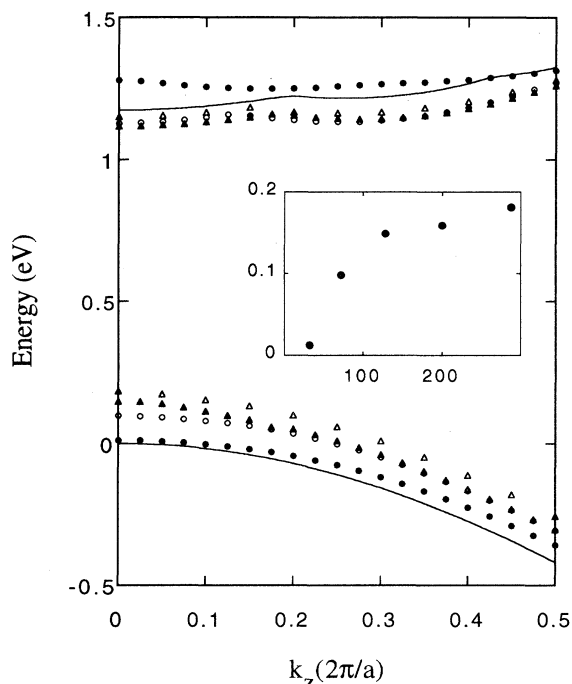


FIG. 2. Energies of the top valence and bottom conduction bands along k_z for edge dislocation dipoles in Si for unit cells of 32 (closed circles), 72 (open circles), 128 (closed triangles), and 288 (open triangles) atoms, compared to the perfect crystal (continuous curves). The inset shows the energies of the top of the valence band at the Γ point for all of the unit cells and separations.

with a three-ring separation between the two dislocations of opposite Burgers vectors, and a general picture of the dislocation lattice viewed along the dislocation direction. The sample size increases from 32 to 288 atoms as the separation increases from one to five sixfold rings, with the number of layers along the dislocation line held constant at 2, the minimum required for periodic boundary conditions.

The *ab initio* calculations were done with a plane-wave energy cutoff of 8 Ry. The convergence criteria imposed were that the forces on any atom are less than 0.1 eV/\AA , and that the energy change in the final cycle is less than 0.0001 eV/atom . The calculations included two special \mathbf{k} points [$\mathbf{k}=(0,0,\frac{1}{8}), (0,0,\frac{3}{8})$] in the Brillouin-zone (BZ) sums for all of the samples. With different sample sizes, one expects the quality of the BZ sums for the same number of \mathbf{k} points to be better for the larger systems, and it is inappropriate to use the same reference bulk crystal energy for the strain-energy calculations. To remove this possible source of error, we have calculated the reference crystal energy with the same \mathbf{k} -point sampling as in the dislocation lattice from perfect bulk unit cells identical to the dipole unit cells except for the presence of the dislocations.

It is well known that LDA calculations give values for the valence-conduction-band energy gaps that are too small. To investigate the effects of the dislocations on the electronic structure, we therefore turned to the tight-binding method, using the sp^3s^* model of Vogel, Hjalmarson, and Dow,¹¹ which gives acceptable values for the band gaps in the group-IV and III-V semiconductors. Atomic coordinates were taken from the samples relaxed in the LDA. Figure 2 shows the dispersion of the top valence- and bottom conduction-band states along the dislocation direction for the 32–288-atom samples. The main effect of the dislocations is to push the top of the valence band into the gap of pure bulk Si, and this effect is enhanced as the dipole separation increases. At the Γ point, the shift in the top of the valence band changes from 0.01 eV at the one-ring separation to 0.18 eV for the five-ring separation. As shown by the inset in Fig. 2, relatively little change occurs in going from three- to five-ring separations. The charge density for the topmost valence band in the 288-atom unit cell is plotted in Fig. 3. The charge density is concentrated at the apexes of the 5-fold rings in the cores where the bonds are most compressed and the bond angle is the smallest.

We have also done tight-binding calculations for a

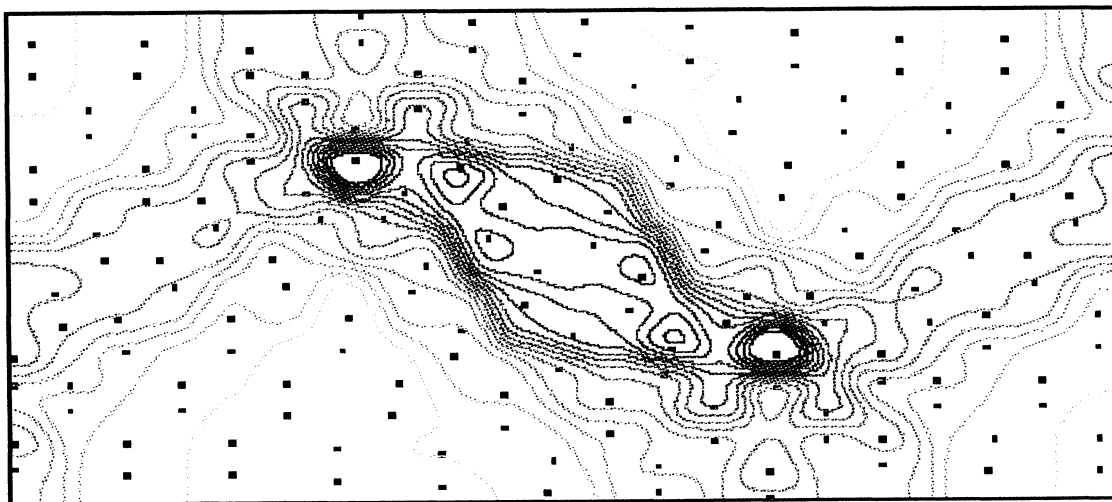


FIG. 3. Charge-density contours for the top valence band for the 288-atom unit cell.

much larger sample of 648 atoms corresponding to a separation of eight rings or 34.5 Å, with the structure obtained by relaxation with the SW potential. For the 288-atom unit cell, the energies of the top of the valence band found after classical and *ab initio* relaxation differ by only 4 meV, which gives some confidence that the relaxation predicted classically gives a reasonable basis for electronic structure calculations. The shift of the valence-band maximum into the gap for the 648-atom unit cell at Γ is 0.17 eV, consistent with Fig. 2.

For the dipole lattices, the maximum changes in bond lengths in the core (%) vary from (+5.8, -3.3) for the 32-atom unit cell to (+8.3, -3.8) for the 288-atom cell, and the changes in bond angles from (+16.8, -10.2) to (+18.0, -12.3). Despite these relatively large distortions, all atoms remain tetrahedrally coordinated, with no dangling bonds. The enhancement of the band-edge shifts correlates well with the increasing localization of the structural distortions in the dislocation cores.¹² We

have found similar but weaker behavior for the 90° partial, as expected since the strain should vary to first order with the magnitude of the dislocation's Burgers vector. Here, to determine the structure, we used the Tersoff potential which Bigger *et al.*⁴ showed gives good agreement with *ab initio* results for a 64-atom unit cell. Calculations were done for unit cells of 64, 144, and 400 atoms, with dipole separations of 13.3, 20.0, and 33.3 Å or three, five, and nine rings. The upward shifts of the top of the valence band at Γ are 0.07, 0.104, and 0.103 eV, respectively; Bigger *et al.* also show a shift of about 0.07 eV for the 64-atom sample relaxed in the LDA. The maximum changes in bond lengths increase by modest amounts from (4.2, -1.8) to (4.4, -2.0), and in bond angles from (23.8, -13.7) to (24.1, -14.1) in going from the 64- to 400-atom systems.

For a planar array of dislocations interacting according to linear elastic theory, the energy per unit length can be written in the form¹³

$$E = K_c \sum_{\mathbf{r}} |\mathbf{b}(\mathbf{r})|^2 - (K/4\pi) \sum'_{\mathbf{r}, \mathbf{r}'} \{ \mathbf{b}(\mathbf{r}) \cdot \mathbf{b}(\mathbf{r}') \ln(|\mathbf{r} - \mathbf{r}'|/r_c) - [\mathbf{b}(\mathbf{r}) \cdot (\mathbf{r} - \mathbf{r}')][\mathbf{b}(\mathbf{r}') \cdot (\mathbf{r} - \mathbf{r}')]/|\mathbf{r} - \mathbf{r}'|^2 \}, \quad (1)$$

where K_c is a core energy coefficient, r_c is the core radius, $\mathbf{b}(\mathbf{r})$ is the Burgers vector for the dislocation at position \mathbf{r} , and K is the appropriate elastic constant.¹⁴ For the dipole lattice shown in Fig. 1, the energy per unit cell in the dipole lattice can be shown to be

$$E_0 = 2\{K_c b^2 + (Kb^2/4\pi)[\ln(d/r_c) - 1 + S_0/2]\}, \quad (2)$$

where $S_0 = -0.59$ arises from the second sum in Eq. (1) excluding terms in the same unit cell, and depends only on ratios of unit-cell parameters that are constant for our set of (unrelaxed) samples.

Figure 4 shows the calculated strain energies per unit length as a function of dipole separation for both the *ab initio* and classical simulations. The symbols are the calculated values, and the curves are fits to the form predicted by elastic theory in Eq. (2). The figure demonstrates that the logarithmic dependence on separation extends downward to even the smallest separation of one ring.

To determine the core energies, some value for the core radius r_c must be assigned. Analysis of the classical results indicates that it is a reasonable assumption to treat the ten atoms in the linked fivefold plus sevenfold rings as the dislocation core. From inspection of Fig. 1, it is apparent that this core structure spans six layers with a spacing of $a/4$ along $y = [001]$, so a radius that includes the top and bottom atoms of the ten but not atoms in the layers immediately above and below is $r_c = 6(a/4)/2 = 1.06b = 4.1$ Å. The core energies $E_c = K_c b^2$ (eV/Å) and elastic constants K (10^{12} dyn/cm²) determined from the fits then are (1) *ab initio* $E_c = 0.75, K = 0.72$; and (2) classical $E_c = 0.83, K = 0.72$. For comparison, the experimental value for K is 0.90, so our calculated value is in reasonably good agreement with experiment.

To summarize, we have used a combination of *ab ini-*

tio, tight-binding, and classical methods to study the properties of $(a/2)\langle 110 \rangle$ dislocation dipoles in Si. A relatively deep shift of the valence-band edge of 0.18 eV into the bulk Si band gap is found to be associated with the core of a perfect edge dislocation. In the core, the atoms retain tetrahedral coordination, so this effect is not due to

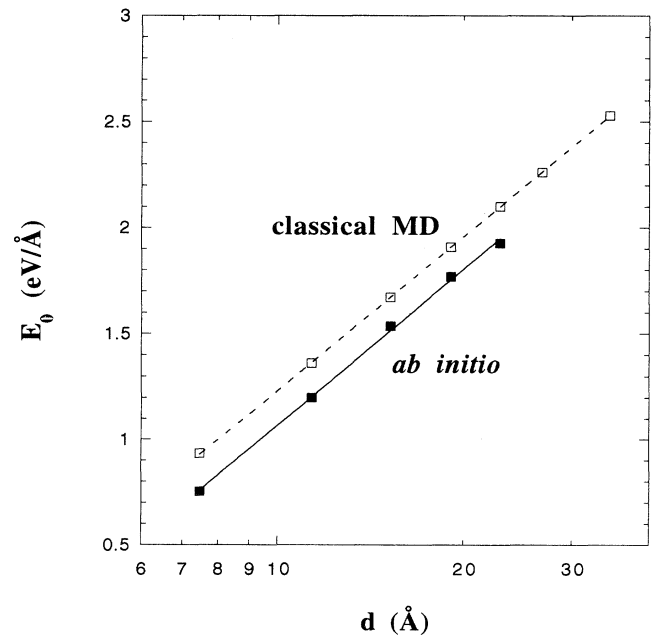


FIG. 4. Calculated strain energies per unit length of the edge dislocation dipoles. In the classical simulations, results for larger unit cells of 392 and 648 atoms are included.

the presence of dangling bonds, but instead appears to be associated with the compressed bonds in the core. In order to observe this effect, the system needs to be large enough that dislocation interactions do not dilute the strain concentration at the cores. In addition, the strain energies for all samples exhibit a logarithmic dependence on separation consistent with linear elasticity. The core energy of the $\langle 110 \rangle$ perfect edge dislocation is $E_c \sim 0.8$ eV/Å.

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*Present address: Molecular Simulations Limited, 240/250 The Quorum, Barnwell Road, Cambridge CB5 8RE, UK.

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