Effects of Dislocation Interactions: Application to the Period-Doubled Core of the 90° Partial in Silicon

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The elastic strain field of a dislocation is highly affected by nearby dislocations. The effects of dislocation-dislocation interactions on elastic energy and core structure are analyzed using a new and self-consistent method to apply periodic boundary conditions on unit cells containing dislocations. Local density functional theory on hydrogen terminated clusters is used to gauge the effects of long-range elastic fields on the core structure of the 90° partial in silicon. It is shown that the single and double period structures of this core are very close in energy, and that the structure adopted probably depends on the environment in which the dislocation is located. [S0031-9007(98)06362-5]

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Many physical properties characteristic of condensed matter are determined by one dimensional topological defects. An example is dislocations, which are responsible for plastic behavior. In semiconductors, dislocations also affect the electronic properties, so they have impact on device performance as well. Since the electronic level positions depend strongly on the arrangement of atoms and bonds in the dislocation cores, the electronic structure is intimately coupled to the core structure. Present knowledge regarding the atomic arrangement in dislocation cores primarily comes from computer simulations.

In a very recent Letter, Bennetto *et al.* [1] introduced a new period doubled structure for the 90° partial dislocation in silicon. This structure was found to be energetically favorable over the ordinary single period reconstruction. As in many of the recent theoretical papers on dislocations in silicon [2–5], they rely on the supercell approach using the quadrupole arrangement introduced by Bigger *et al.* [6]. In this current paper, a general and self-consistent method to construct unit cells containing dislocations will be introduced. Furthermore, the dislocation interaction effects introduced by periodic boundary conditions will be investigated. Finally, the relative stabilities of the double period (DP) and the single period (SP) structure of the 90° partial will be investigated. Notably, it will be shown that the relative stability of these structures is highly influenced by nearby dislocations, thus is very sensitive to the long-range elastic field. This is indeed not the case for the historically important problem about the relative stability between reconstructed and unreconstructed 90° partials [7–18].

The introduction of dislocations in a lattice changes the topology of the whole system, which in turn prevents one from characterizing the defect as a local perturbation in a more or less perfect lattice, as is usually possible for point defects. There exist short-range forces acting in the core region which tend to constrict it and a long-range elastic field which favors a wide core [19,20]. The structure of a dislocation core is thus determined by a balance between these two effects, and due to the long-range nature of the elastic field the dislocation should ideally be embedded in an infinite elastic medium.

Practically, a theoretical study of dislocations is restricted to a finite and relatively small number of unique atoms. There are two approximate methods that artificially represent the embedding in an infinite medium. The first is the cluster method, where a finite cluster surrounding the defect is constructed, and the second is the unit cell method [21], where an infinite superlattice of defects is formed by periodic boundary conditions.

The strength of the cluster method lies in its ability to treat an isolated defect. Here, all translational symmetry is destroyed, which implies that the electronic structure information is limited to a set of discrete levels. Cluster calculations suffer from problems with the cluster termination. First, surface atoms associated with dangling bonds give rise to levels in the fundamental gap. This problem may be circumvented by saturating the dangling bonds with hydrogen atoms. This method is reliable in calculating structures and dynamical properties of semiconductors and their defects [22,23]. Unfortunately the terminating hydrogen atoms interact strongly with states at the valence and conduction band edges which artificially enlarge the gap. The second problem associated with the cluster termination involves the problem of how the long-range elastic field should be included. Thus, it is difficult to simulate the embedding of the cluster in an elastic medium in a self-consistent manner.

The use of periodic boundary conditions has the advantage that the defect-surface interaction is replaced by a defect-defect interaction at a larger distance. In addition, the dislocations are embedded in an infinite elastic medium, since all atoms may respond to the elastic field. The disadvantages to this approach are, first, that it requires the sum of the Burgers vectors in the unit cell to be zero, since, otherwise, the elastic strain energy of the crystal would be infinite. Second, it introduces interactions between an infinite number of dislocations. This will, to

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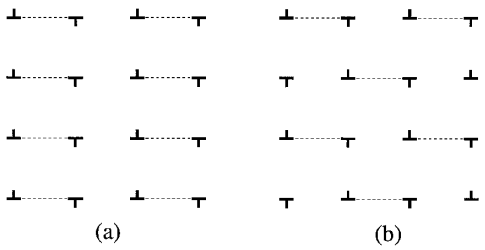

FIG. 1. In (a), an edge dislocation dipole is translated so that alternating tilt grain boundaries are formed. If the translation vectors are changed, a lattice of dislocation quadrupoles may be generated (b).

some extent, affect calculated results, especially if the unit cell is small. Increasing the number of unique atoms, as greater computing power will allow, will eliminate all of the problems for the unit cell approach.

While, in principle, periodic repetition of unit cells should eliminate uncertain surface effects, there has been a historical problem with matching the boundaries of a cell with its neighboring cells [21,24–27]. Bigger *et al.* [6] identified this problem to be due to grain boundaries generated when the unit cells are periodically repeated as in Fig. 1(a). They adopted a solution proposed by Heggie [28], generating a lattice of dislocation quadrupoles as in Fig. 1(b). By placing the dislocations of the quadrupole exactly symmetrically within the unit cell, a smaller cell containing only a dislocation dipole was constructed. This dislocation quadrupole method has been extensively used [2–5].

This leads to the first scope of this work, which is to determine a general and self-consistent way to construct unit cells containing dislocations. Our method avoids all of the problems with boundary mismatch, without restricting to a quadrupole arrangement. Thus, it will be shown that misfit at the cell borders is due only to an incorrect treatment of the periodicity and not due to the grain boundaries.

A general dislocation can be constructed as in Fig. 2; see, e.g., Ref. [29]. First, a closed curve C within the crystal, or an open curve terminating on the surface at both ends, is considered. The curve is not necessarily planar. Then a sense ξ is ascribed to the curve, and a cut along any simple surface A bounded by the line C is made. The line C becomes a dislocation line of Burgers vector $\mathbf{b}$ if, over the surface A, material

$$\delta V = -\mathbf{b} \cdot d\mathbf{A} \tag{1}$$

is inserted (if δV is negative, material is removed), and the surface on the negative side of the cut is displaced by $\mathbf{b}$ relative to the positive side. Afterwards, the material on both sides of the cut are rejoined, so the surface A is perfect again. The result is a pure line defect, which is the dislocation line C.

The strain displacement is left intact at the time of rewelding, but afterwards the medium is allowed to come to internal equilibrium. The resulting strain pattern is that of the dislocation characterized jointly by the boundary curve C and the Burgers vector $\mathbf{b}$.

In a crystal, the Burgers vector must generally be equal to a lattice vector in order that the rewelding process will maintain the crystallinity of the material. Such dislocations are called perfect. If the Burgers vector is not equal to a lattice vector, they are called imperfect, or partial, dislocations. These partial dislocations are always associated with stacking faults.

When the unit cell method is used, the final structure must be translation invariant. Then the above procedure must be done in a way that satisfies the symmetry requirements. Thus, the dislocations must be introduced simultaneously in every unit cell, so the final equilibrium structure is determined by the periodic arrangement of dislocations. The translational vectors of the superlattice should be taken from the final equilibrium structure. As a first approximation, they may be calculated from the translational vectors $\mathbf{c}_i$ of the starting unit cell, the surface cut A, and the Burgers vector $\mathbf{b}$. Before the dislocations are introduced, the translational vectors $\mathbf{c}_i$ of the supercells are given as linear combinations of the primitive translational vectors $\mathbf{a}_i$ of the crystal lattice. When the dislocations are introduced, the new translational vectors $\mathbf{c}_i'$ of the supercell are given by $\mathbf{c}_i' = \mathbf{c}_i + \Delta\mathbf{c}_i$, where by inspection $\Delta\mathbf{c}_i$ is found to be

$$\Delta\mathbf{c}_i = -\mathbf{b} \int_A \frac{\mathbf{c}_i \cdot d\mathbf{A}}{|\mathbf{c}_1 \cdot (\mathbf{c}_2 \times \mathbf{c}_3)|} . \tag{2}$$

When the final equilibrium structure is determined by the Keating potential [30], Eq. (2) is found to be exact.

The only defects introduced in the crystal are, as noted, the dislocations and for partials an additional stacking fault at the cut A. Therefore, there will never be problems with lattice mismatch at the cell borders, if the periodicity is taken into account in the manner described. This is in contrast to the conclusions drawn by Bigger *et al.* [6].

How does the elastic energy vary when the global dislocation pattern is changed at a fixed dislocation density? In order to answer this question, the 1024-atom unit cell shown schematically in Fig. 3 is used. Here, $L = 32a\sqrt{3/8} \approx 106$ Å, $D = 16a/\sqrt{3} \approx 50.2$ Å, and the thickness of the cell is $a/\sqrt{2}$, which is a single period of a 30°/90° partial dislocation. The lattice

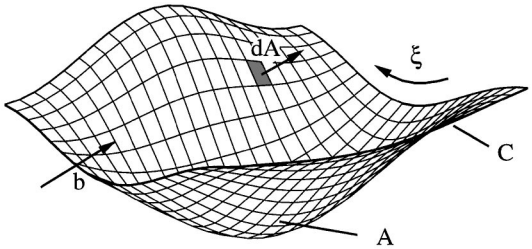

FIG. 2. A dislocation loop along the path C with Burgers vector $\mathbf{b}$.

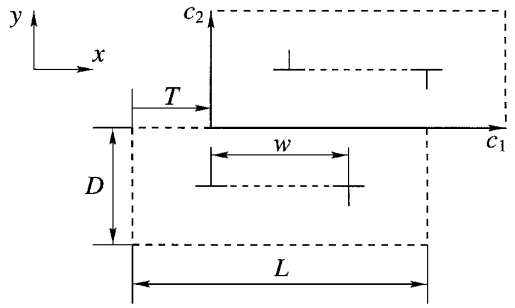

FIG. 3. A projection of the unit cell on the (110) plane. The x direction is in the $[\bar{1}12]$ direction of the underlying lattice, and y is in the $[1\bar{1}1]$ direction.

constant of silicon is $a = 5.431$ Å. The x direction is in the $[\bar{1}12]$ direction of the underlying lattice and y is in the $[1\bar{1}1]$ direction. A dislocation dipole of 90° partials is introduced in the cell in the way described. The partials are separated by an intrinsic stacking fault along the planar cut.

The global dislocation pattern is changed by varying the width w of the stacking fault, and by adding translations T to $\mathbf{c}_2$. These translations must be translation vectors of the silicon lattice in order to maintain the crystallinity. Furthermore, they must be perpendicular to $\mathbf{c}_1 \times \mathbf{c}_3$, since, otherwise, the volume is changed. These changes to the global dislocation pattern do not affect the average dislocation density in the crystal. The actual shape of the unit cell is, of course, arbitrary, as long as it covers the whole space once and only once when translated by linear combinations of $\mathbf{c}_1$, $\mathbf{c}_2$, and $\mathbf{c}_3$.

The elastic energy is calculated by the Keating potential [30], since this potential accurately reproduces the elastic constants. When the dislocation dipole is introduced in the unit cell defined by the vectors c_i, it is distorted by Δc_i, as described above. Eight different widths w of the stacking fault, ranging from $w = L/8 \approx 13.3$ Å to $w = 3L/4 \approx 79.8$ Å, are used. The width is, in principle, confined to the interval $0 \leq w \leq L$. If $w = 0$ or $w = L$, the elastic energy is zero. This is easily understood for the first case since no defect is introduced in the cell. When $w = L$, the dislocations annihilate with the dislocations in the neighboring cells. Therefore, this generates a dislocation-free material containing an array of infinite intrinsic stacking faults. The elastic energy for this case is zero, since the Keating potential does not give any stacking fault energy. This, in turn, means that the elastic energy as a function of w is symmetric about the maximum at $w = L/2$.

When the stacking fault width w is fixed, the global minimum in the elastic energy must be found by varying the translation T. Figure 4 shows the elastic energy of the cell as a function of T, for the eight different ribbon widths. The tilt grain boundary configuration [Fig. 1(a)] is generated when $T = nL$, where n is an integer, and the quadrupole configuration [Fig. 1(b)] is generated when $T = (n + \frac{1}{2})L$ and $w = L/2$. The minimum in the elastic energy is found when $T = nL$, i.e., in the tilt grain boundary configuration, for all ribbon widths. The quadrupole configuration is the structure with the largest elastic strain energy. The tilt grain boundary configuration is favored by 1.15 eV when $w = L/2$. This energy gain is the driving force behind grain boundary formation in real materials. The global effect on the elastic energy is independent of the dislocation core structure.

So far, only edge dislocation dipoles have been studied. If the dislocation dipole is of screw character, then the global energy minimum is found in the quadrupole configuration, contrary to the edge dislocations. Thus there is a fundamental difference in the interaction between screw dislocations on the one hand and between edge dislocations on the other. This difference can even be seen by elasticity theory [29], but the actual effects in a periodic defect structure are difficult to calculate.

Does the difference in elastic strain affect the core structure? To answer this question, the relative energy between the DP [1] and the SP reconstruction of the 90° partial in silicon is calculated on different global dislocation patterns. The elastic energy difference $E_{\mathrm{DP}} - E_{\mathrm{SP}}$ is determined by the Keating potential on the 1024-atom unit cell. The number of atoms in the cell is, of course, doubled for the double period structure. The energy difference varies smoothly when T is changed. The SP structure is favored by 4 to 18 meV/Å. This is in contrast to the result found by Bennetto *et al.* [1]. If the height of the unit cell is reduced to $D = 7a/\sqrt{3}$, forming a 488-atom cell, the variation in $E_{\mathrm{DP}} - E_{\mathrm{SP}}$ is reinforced. In this case, the tilt grain boundary configuration favors the SP structure by 30 meV/Å, and in the quadrupole configuration, which is not the global energy minimum structure, the DP structure is favored by 5 meV/Å. These calculations show that the result obtained by Bennetto

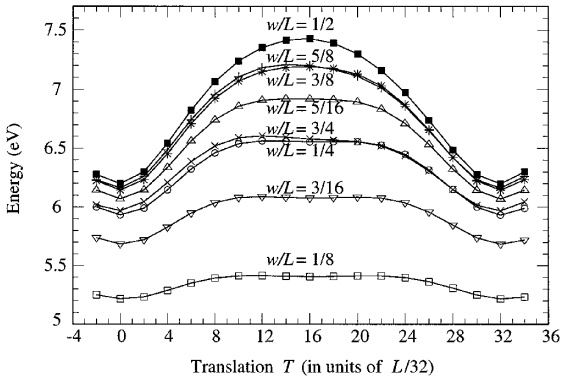

FIG. 4. The elastic energy of the 1024-atom unit cell, containing a dipole of 90° partial dislocations, as a function of the translation T. The different curves show the energy for cells where the stacking fault widths are $w = \frac{1}{8}, \frac{3}{16}, \frac{1}{4}, \frac{5}{16}, \frac{3}{8}, \frac{1}{2}, \frac{5}{8}$, and $\frac{3}{4}$, in units of L, defined in Fig. 3.

et al. might be an effect of their choice of unit cell, since the core energy is very sensitive to the dislocation interaction, especially when the unit cell is small.

In real silicon, a 90° partial, together with a 30° partial and a stacking fault, is the dissociation product of a perfect 60° dislocation. The experimental width of this ribbon is about 50 Å. Moreover, the dislocation density N is $N \approx 10^9$ cm^{-2} in deformed samples, compared with $N \approx 10^{12}$ cm^{-2} for the 1024-atom unit cell above. This means that the unit cell approach is uncertain because of both the high dislocation density and the interactions with dislocations of the wrong type. In order to clarify the situation, a local density functional (LDF) method is used on hydrogen terminated clusters containing a 90° partial. The cluster construction starts with the introduction of a dissociated 60° dislocation in a giant cylinder, containing about 8000 atoms per repeat distance $(a/\sqrt{2})$ of the dislocation. This dissociated dislocation consists of a 50 Å wide intrinsic stacking fault, bounded by one 30° and one 90° partial. This means that the 90° partial is located in a realistic environment. Since it is not feasible to treat this whole defect by *ab initio* methods, an initial relaxation is made using the bond charge model [31]. During this relaxation, the surface atoms of the cylinder are fixed at the positions given by elasticity theory. Finally, clusters containing up to 486 atoms around the 90° partial are generated from this relaxed structure.

These clusters are then used in the LDF calculations. During the LDF relaxation, the surface Si atoms are fixed at the positions determined by the bond charge model, in order to simulate the long-range elastic field. The result of these calculations is that the DP structure is favored by about 11 meV/Å. This is in agreement with Bennetto *et al.* [1], who used 96/192-atom unit cells in the quadrupole arrangement; however, the energy difference is 7 times smaller than their value of 79 meV/Å. On the other hand, if all atoms in the cluster, including surface atoms, are allowed to relax, the SP structure is energetically favored by 21 meV/Å. This again shows that the type of core reconstruction (SP or DP) of the 90° partial is sensitive to changes in the long-range elastic field.

This paper has shown that dislocation interactions are of great importance, even for the core structure. A new and self-consistent method is introduced for the application of periodic boundary conditions. Using *ab initio* LDF theory on clusters and the Keating potential on unit cells, it has been shown that the DP and SP structures of the 90° partial core are very close in energy, and that the structure adopted by the core probably depends on the environment in which the dislocation is located.

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