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The Core Structure and Energy of the 90° Partial Dislocation in Si

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Abstract: The 90° partial dislocation in Si is studied using a combination of Tersoff potentials and isotropic elasticity theory. Both periodic supercells and cylindrical cells are employed and the results compared. The dislocation core radius is extracted by fitting the results of atomic scale calculations to an expression for the elastic energy of the dislocation. The energy differences between two proposed reconstructions of the dislocation core are computed and found to depend systematically on the stress field imposed on the dislocation. It is suggested that hydrostatic stresses may introduce a core transformation.

keyword: Dislocation cores, dislocations in Si.

1 Introduction

A solid understanding of the properties of dislocations is essential to the successful modeling of mechanical properties in materials. The rapid increase in computational power in recent years has prompted substantial developments in simulating the large-scale behavior of dislocations [Kubin, Moulin, and Pirouz (1999); Schwarz (1999); Rhee, Zbib, Hirth, Huang, and de la Rubia (1998); Ghoniem, Tong, and Sun (2000); Faradjian, Friedman, and Chrzan (1999)]. However, the failure of continuum elasticity theory to describe a dislocation accurately at small distances obviates the need for a better picture of the dislocation core at the atomic level.

Dislocations in diamond cubic materials, and in Si in particular, have received much attention in recent years. In the $\langle 10\bar{1}\rangle\{111\}$ slip system of these materials, the predominant dislocations have Burgers vectors at 0° and 60° to the line direction, and these dislocations may dissociate into 30° and 90° partials. Most studies concentrate on the structure of the 90° partial [Bennetto, Nunes, and Vanderbilt (1997); Nunes, Bennetto, and Vanderbilt (1998); Valladares, Petford-Long, and Sutton (1999); Blase, Lin, Canning, Louie, and Chrzan (2000)], although some work on the 30° partial [Bulatov, Yip, and Argon (1995); Trinczek and Teichler (1993)] and on the perfect screw dislocation [Arias and Joannopoulos (1994)] is also reported.

The present work, too, focuses on the structure of the 90° partial dislocation in Si. In particular, the dependence of the relative stability of two possible reconstructions of the core on the stress field experienced by the dislocation is explored. Atomic scale calculations are performed using Tersoff potentials, employing both periodic supercells and cylindrical cells. Atomic scale calculations are interpreted, in part, using isotropic elasticity theory as a guide.

This paper makes three important points. First, a new method for extracting the core radius of an edge dislocation from atomic scale calculations employing periodic supercells is described in detail. The technique is employed to extract the core radius for the 90° partial dislocation in Si (as predicted by Tersoff potentials).

Second, it is demonstrated that both periodic supercells and cylindrical cells may be used to explore the relative stability of competing core structures. In fact, for large enough cells, supercells and cylindrical boundary conditions yield nearly identical results. Third, the energy difference between competing core structures for the 90° partial is stress state dependent, and the stress state dependence can be explored systematically using periodic supercells. This systematic stress dependence is demonstrated explicitly for applied shear and hydrostatic stresses.

The remainder of this paper is organized as follows. Section 2 introduces the 90° partial dislocation and two possible reconstructions for its core. An analysis of the relative stability of these two reconstructions is presented in

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section 3. Section 4 presents the results of applying pressure to the periodic dislocation array, and a discussion and conclusions are given in section 5.

2 Reconstructions of the 90° partial

In a diamond-cubic material such as Si, the unreconstructed core of the 90° partial dislocation viewed in the $\{111\}$ plane contains a zigzag chain of three-fold coordinated atoms [Fig. 1(a)]. In the late seventies, it was proposed by Hirsch (1979) and Jones (1980) that this core reconstructs by breaking the mirror symmetry along the dislocation line, restoring the fourfold coordination of the atoms in the core. This reconstruction, illustrated in Fig. 1(b) and commonly referred to as the single–period (SP) core, was assumed for many years to be the physically correct core structure.

A new core reconstruction (the double-period or DP core) was recently proposed by Bennetto, Nunes, and Vanderbilt (1997), in which alternating five- and seven-membered rings are formed, thus doubling the periodicity along the dislocation line [Fig. 1(c)]. Using periodic boundary conditions and a variety of energy calculation methods, the authors showed that the DP structure has a lower energy than the previously assumed SP structure. Other researchers, however, have questioned the generality of this result. Lehto and Öberg (1998) have argued that the relative stability of the two structures depends on the choice of unit cell used in the periodic boundary conditions, and calculations of Valladares, Petford-Long, and Sutton (1999) suggest that the difference between free energies of the SP and DP cores is insignificant at temperatures required for dislocation mobility in Si.

The present work explores in detail the effect of periodic boundary conditions on the relative energies of the two core structures. As Lehto and Öberg (1998) have noted, these energies are sensitive to the environment in which the dislocation is located. Here, that dependence is studied systematically. A recently developed method Blase, Lin, Canning, Louie, and Chrzan (2000) for performing the "Madelung-like" sum associated with the infinite arrangement of oppositely signed edge dislocations is applied. This procedure also yields the stress state imposed on the dislocations as a function of the unit cell parameters, as well as the elastic energy/supercell associated with the dislocation array. Total energies computed using Tersoff potentials are compared with the elastic energies predicted by isotropic elasticity theory to extract values for $\mu/(1-\nu)$, with μ the shear modulus and ν Poisson's ratio, and the core radius r_0 for the 90° partial dislocation in Si. The stress state dependence of the SP and DP core energy difference is then quantified through a series of calculations in which the unit cell for the periodic boundary conditions is varied.

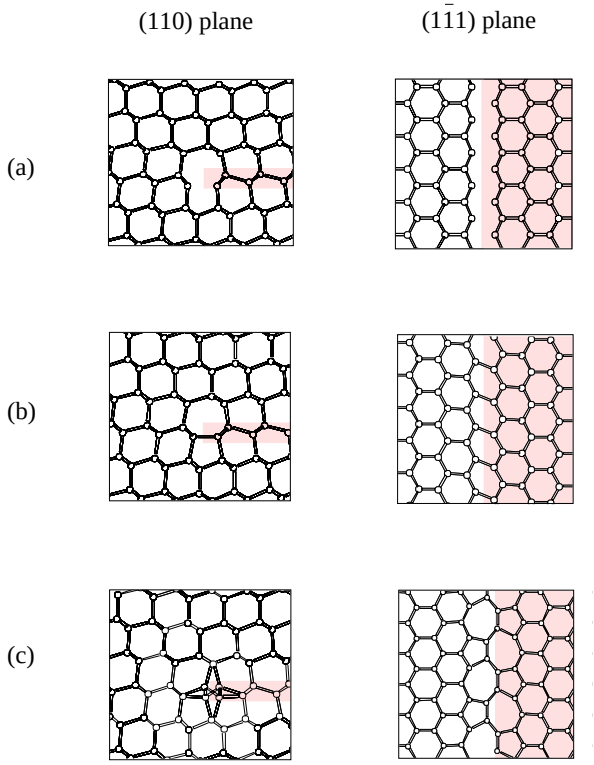

Figure 1 : Atomic structure of the 90° partial dislocation viewed from above the (110) and $(1\bar{1}1)$ planes: (a) unreconstructed, (b) single-period (SP) reconstructed, (c) double-period (DP) reconstructed. Shaded area indicates stacking fault.

3 Relative energies of the SP and DP core structures

3.1 Periodic boundary conditions

The choice of boundary conditions can have a significant effect on the observed results, and controversy remains as to the best methods for studying dislocation core structures. Two common approaches for boundary conditions are the "cluster" method and the method of periodic supercells. In the cluster method, a typical practice is to

generate initial positions of the atoms in a cylindrical cell surrounding the dislocation core within anisotropic elasticity theory, fix the positions of the atoms on the surface of the cylinder, and allow the remaining atoms to relax. While the cluster method is useful in that it allows the consideration of an isolated dislocation, it suffers from a sensitivity to the initial placement of the dislocation core and the necessity to treat in a special way atoms at the surface.

Periodic boundary conditions eliminate the difficulty of treating the surface atoms present in the cluster method, but introduce an infinite number of interactions between dislocations. When the supercell is small and the dislocations are thus very close together, extreme stress states may result. Moreover, each supercell must have a net zero Burgers vector to avoid a divergence in the elastic strain energy. These difficulties notwithstanding, the periodic supercell method has been the more popular for studies of the core structure and energy of the 90° partial in diamond cubic materials [Bennetto, Nunes, and Vanderbilt (1997); Nunes, Bennetto, and Vanderbilt (1998); Valladares, Petford-Long, and Sutton (1999); Arias and Joannopoulos (1994); Lehto and Öberg (1998)] and is the method applied for the majority of the work described in this paper.

3.1.1 Definition of parameters

The simplest possible supercell is a dipolar cell, containing two dislocations with opposite Burgers vector. The dimensions of the cell are defined by the unit vectors in the $(1\bar{1}1)$ plane of the perfect 12-atom orthorhombic cell: $\mathbf{a_1} = \frac{a}{2}[1\bar{1}\bar{2}]$, $\mathbf{a_2} = \frac{a}{2}[110]$, $\mathbf{a_3} = a[1\bar{1}1]$, where a is the lattice constant for Si, 5.43 Å. Adopting the notation of Bennetto *et al.*, the cell is assigned the parameters of length L, height D, dislocation separation w, and cell offset T. (See Fig. 2). For simplicity, all parameters are expressed as integers, with L, w, and T understood to be in units of $|\mathbf{a_1}|$ and D in units of $|\mathbf{a_3}|$.

Part of the controversy surrounding the discussion of periodic boundary conditions involves the choice of the parameters L, D, w, and T. As first noted by Bigger, McInnes, Sutton, Payne, Stich, King-Smith, Bird, and Clarke (1992), the value of the offset T requires some consideration in order to avoid a lattice mismatch at the cell boundaries. Previously, it was thought that this problem could be solved only by using a "quadrupolar" lattice, *i.e.* $T = L/2$, and several studies [Bennetto, Nunes, and Vanderbilt (1997); Nunes, Bennetto, and Vanderbilt (1998); Valladares, Petford-Long, and Sutton (1999)] have thus employed the quadrupolar lattice exclusively. However, Lehto and Öberg (1998) pointed out that this restriction is unnecessary. When two oppositely signed edge dislocations are introduced into a perfect solid and separated by a distance w, the top and bottom surfaces of the solid are displaced relative to each other by $b(w/L)$, where L is the width of the solid along the slip direction and b is the magnitude of the Burgers vector. Provided that the offset T is adjusted by this amount, there is only one additional restrictions (other than those imposed by the lattice periodicity itself) on L, D, w, and T. Specifically, the ratio T/L must be a rational number. (This limitation is not very restrictive.) This constraint insures that the assembly of dislocations may be treated as a collection of tilt boundaries, and avoids singularities in the elastic energy which would arise from introducing boundaries that are not pure tilt. Moreover, changing the values of these parameters affects the stresses and stress gradients experienced by a dislocation in the infinite lattice, and the energies observed are expected to depend on these stress states [Lehto and Öberg (1998)]. Thus, one may place the dislocation under a variety of stress states by simply changing the values of L, D, w, and T, and it is in this manner that the stress dependence of the relative

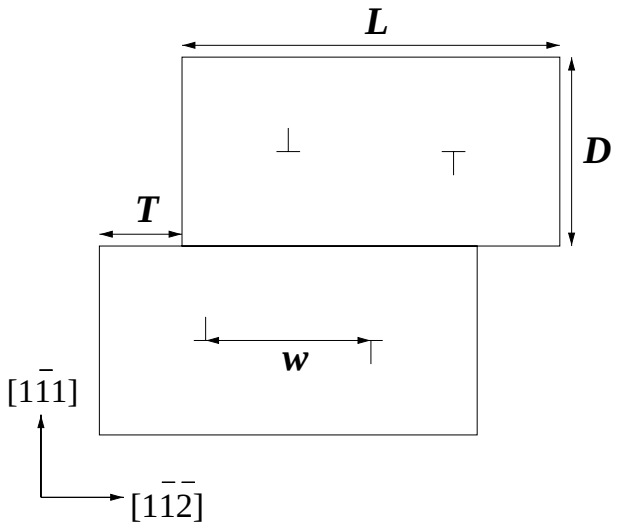

Figure 2 : Representation of two unit cells in the (110) plane. L is the width of the unit cell, D is the height, and w is the distance between dislocations in the cell. The offset T is also shown.

core structure may be quantified.

Each supercell employed in the periodic boundary calculations contains two dislocations of opposite sign in order that the total Burgers vector vanish, thus avoiding a divergence in the energy. It should be noted here that there are two possibilities for the SP reconstruction in a dipolar unit cell depending on whether the direction of mirror symmetry breaking is the same or the opposite for the two dislocations (See Fig. 3). Previous workers [Bennetto, Nunes, and Vanderbilt (1997); Valladares, Petford-Long, and Sutton (1999)] have quoted the average of the two distinctly different energies. However, the same sense reconstruction should always be higher in energy. In order to avoid spurious strains in the system, the bonds in the dislocation core must be angled such that the two "good" regions on either side of the stacking fault are shifted with respect to each other by an amount commensurable with the lattice spacing in the dislocation line direction. This places an artificial constraint on the cell which increases the energy. Because this constraint is not present in the opposite sense reconstruction, it is concluded that the opposite sense reconstruction gives the better estimate of the SP core energy, and all calculations considered here are performed with this configuration. (That this choice is physically reasonable is borne out by comparison with cylindrical cell calculations of the same energy difference. See section 3.2, below.)

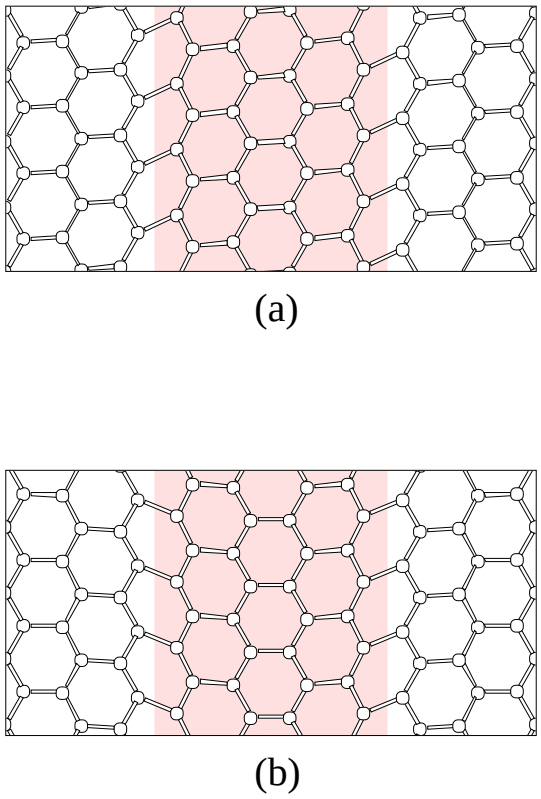

Figure 3 : Two possible cells for a dipolar, SP-reconstructed unit cell, viewed from above the $(1\bar{1}1)$ plane: (a) same-sense reconstruction and (b) opposite-sense reconstruction. Shaded region indicates stacking fault.

3.1.2 Stress field and energy of a periodic edge dislocation array

In order to explore how the relative energies of the SP and DP reconstructions depend on stress, it is necessary to sum the stress fields from an infinite number of dislocations. Since the stress field of a dislocation is proportional to $1/r$, where r is the distance from the dislocation, this sum is similar to a Madelung sum for an ionic crystal and must be handled carefully. The sum is found to converge rapidly when the periodic arrangement of dislocations is viewed as a 1-D stack of tilt boundaries, or linear arrays of dislocations. (See Fig. 4.) The stress field of a tilt boundary decays exponentially with the distance from the boundary [Hirth and Lothe (1992)]. The stress experienced by a single dislocation in a periodic array can then be expressed as the sum of the stress fields from all the tilt boundaries [Gulluoglu, Srolovitz, LeSar, and Lomdahl (1989)].

Similarly, the total elastic energy of the configuration is the sum of the self-energy of each tilt boundary [which depends on $\mu/(1-\nu)$ and the core radius r_0] and the work required to assemble the tilt boundaries in the presence of their stress fields [which depends only on $\mu/(1-\nu)$]. For a tilt boundary composed of edge dislocations located at $x = 0$ in the coordinate system of Fig. 4, the stress fields predicted from isotropic elasticity theory are [Hirth and Lothe (1992)]:

$$\begin{aligned}
\sigma_{xy} &= \sigma_0 2\pi X \\
&\quad \times(\cosh 2\pi X \cos 2\pi Y - 1) \\
\sigma_{xx} &= -\sigma_0 \sin 2\pi Y \\
&\quad \times(\cosh 2\pi X - \cos 2\pi Y + 2\pi X \sinh 2\pi X) \\
\sigma_{yy} &= -\sigma_0 \sin 2\pi Y \\
&\quad \times(\cosh 2\pi X - \cos 2\pi Y - 2\pi X \sinh 2\pi X) \qquad (1)
\end{aligned}$$

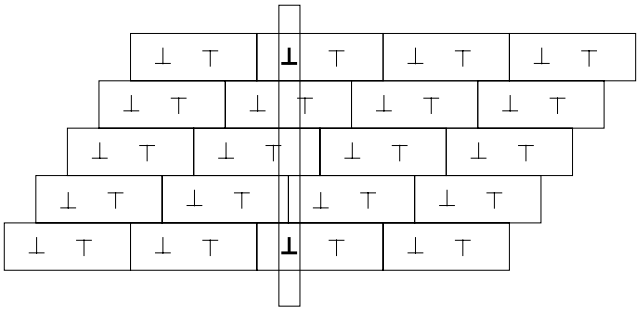

Figure 4 : A periodic array of dislocations considered as a 1-D stack of tilt boundaries, viewed in the (110) plane.

where

$$\sigma_0 = \frac{\mu b}{2d(1-\nu)(\cosh 2\pi X - \cos 2\pi Y)^2} \qquad (2)$$

and $X = x/d$, $Y = y/d$, where d is the distance between nearby dislocations in the boundary.

The self-energy of a tilt boundary is taken to be half the energy required to separate two equivalent boundaries of opposite sign from $x = r_0$ to $x = \infty$. With $Y = 0$ (the tilt boundaries are not shifted with respect to each other vertically), the shear stress σ_{xy} is

$$\begin{aligned}\sigma_{xy} &= \frac{\mu b}{2d(1-\nu)} \frac{2\pi X(\cosh 2\pi X - 1)}{(\cosh 2\pi X - 1)^2} \\ &= \frac{\mu b \pi}{2d^2(1-\nu)} \frac{x}{\sinh^2(\pi x/d)}. \end{aligned} \qquad (3)$$

The self-energy per dislocation per unit length is then given by [Hirth and Lothe (1992)]

$$\begin{aligned}E_{\rm self} &= \frac{1}{2}\int_{r_0}^{\infty} b\sigma_{xy}\, dx \\ &= \frac{\mu b^2}{4\pi(1-\nu)} [\eta_0 \coth \eta_0 - \ln(2\sinh \eta_0)] \end{aligned} \qquad (4)$$

where $\eta_0 = \pi r_0/d$.

The total eleastic energy of the collection of tilt boundaries includes both the self energy of the individual boundaries and the interaction energy between all the dislocations within the system. This energy can be computed as follows. One imagines that each of the boundaries is created at $x = \infty$, and then one computes the work required to bring the tilt boundary from $x = \infty$ to its final position. This work is merely the interaction energy between the newly created tilt boundary and all existing tilt boundaries. Calculation of the work requires that one compute the net stress on the boundary under consideration arising from *all* existing boundaries. Since the stress field of an individual tilt boundary decays exponentially with distance from the boundary, this net stress is computed readily using "brute force" summation.

The interaction energy (per dislocation per unit length) between two tilt boundaries separated by a distance x_0 and offset vertically by y_0 is, with $\zeta_0 = 2\pi x_0/d$, $Y_0 = y_0/d$, and $a = \cos 2\pi Y_0$,

$$\begin{aligned}\varepsilon(x_0, y_0) &= -\frac{\mu b^2 \pi}{d^2(1-\nu)} \int_{\infty}^{x_0} \frac{x(a\cosh 2\pi x/d - 1)}{(\cosh 2\pi x/d - a)^2} dx \\ &= \frac{\mu b^2}{4\pi(1-\nu)} \\ &\quad \times \left[\ln 2(\cosh \zeta_0 - a) - \frac{\zeta_0 \sinh \zeta_0}{\cosh \zeta_0 - a}\right] \end{aligned} \qquad (5)$$

for same-signed boundaries, and $-\varepsilon(x_0, y_0)$ for opposite-signed boundaries. One then computes the energy difference between configurations differing only in the number of added tilt boundaries. This difference converges rapidly to a constant, and allows computation of the elastic energy per unit cell.

The interaction energies depend directly on $\mu/(1-\nu)$, and the self energies depend on both $\mu/(1-\nu)$ and r_0. Hence the predictions of isotropic elasticity theory can be computed as a function of these parameters.

The above equation, which provides an expression for the elastic energy of a dipolar cell in terms of the parameters L, D, w, and T, now allows for the extraction of values of $\mu/(1-\nu)$ and r_0 for Si. Total energies are determined using Tersoff potentials [Tersoff (1988)] for various periodic configurations of dislocations in the single-period structure. These energies are then fit to the expression for the elastic energy with $\mu/(1-\nu)$ and r_0 as fitting parameters, assuming that both are independent of stress. (A successful application of this technique to analysis of *ab initio* results in diamond was presented by Blase, Lin, Canning, Louie, and Chrzan (2000).)

Three choices of unit cell in the SP reconstruction are employed: $L = 12$, $D = 3$; $L = 6$, $D = 2$; and $L = 6$, $D = 8$, in both the dipolar ($T/L = 0$) and quadrupolar ($T/L = 1/2$) arrangements, with w varied from 1 to $L-1$. The results of the fit are shown in Fig. 5, with $\mu/(1-\nu) = 70 \pm 17$ GPa and $r_0 = 0.67 \pm 0.05$ Å. The value for $\mu/(1-$

ν) is in agreement with both the experimental value of 87.1 GPa [Hirth and Lothe (1992)] and the Voigt average value predicted by the Tersoff potentials, 77 GPa. The core radius r_0 corresponds to $\alpha = b/r_0 \approx 3.3$, consistent with general expectations [Hirth and Lothe (1992)] and not too far from the result $\alpha = 4.08$ found by Trinczek and Teichler (1993); the discrepancy is likely due to the use of a different potential.

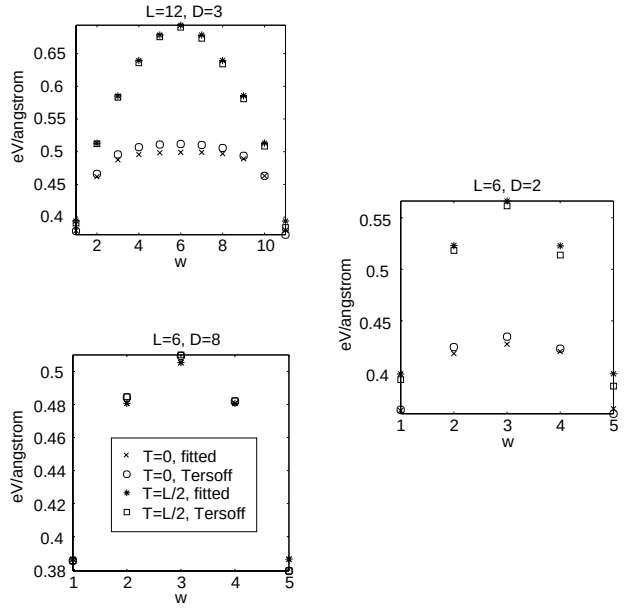

Figure 5 : Fits to isotropic elasticity theory of total energy calculations for the SP core from Tersoff potentials, using periodic boundary conditions for three different unit cells. Data are fit simultaneously, assuming $\mu/(1-\nu)$ and r_0 do not change with unit cell.

3.1.3 Stress dependence of the SP and DP core energies

The difference in core energies for the SP and DP reconstructions is now studied systematically. Most previous attempts at identifying the stable core structure [Bennetto, Nunes, and Vanderbilt (1997); Nunes, Bennetto, and Vanderbilt (1998); Valladares, Petford-Long, and Sutton (1999)] were restricted to a quadrupolar cell. While the stress field on a dislocation in this arrangement is indeed zero, it will be shown that the relative stability of the two core structures depends not only on the stress but also the stress gradients.

Indeed, there is much discussion of the proper choice of unit cell to predict the stable core structure for the considered dislocation (see, for example, Bigger et al. Bigger, McInnes, Sutton, Payne, Stich, King-Smith, Bird, and Clarke (1992)). The work of Lehto and Öberg demonstrating that the stable core structure may be stress dependent suggests that these initial arguments are misguided. There is not a single uniquely stable core structure for the dislocation in question. Rather, the dislocation core itself is deformable, and the stable structure of the dislocation may well depend on the imposed stress state.

The focus of the current work, then, is to explore the relative stability of the two core configurations as a function of imposed stress state. The exploration relies heavily on the use of periodic supercells. While this choice may not be optimal for some studies, it seems that *ab initio* total energy techniques are more easily applied using periodic supercells than, for example, considering a finite radius cylinder (which requires "capping" the surface bonds with H). Given the analysis above, it is possible to subject the dislocation cores to a broad variety of stress states merely by choosing a variety of periodic supercell configurations. The stress state imposed on the dislocations can be estimated using the isotropic elasticity theory analysis presented above. In this manner, the dependence of the energy difference on the dislocation environment can be quantified.

Fig. 6 shows the predicted difference in core energies, $E(\mathrm{DP}) - E(\mathrm{SP})$ as a function of the shear stress σ_{xy} for a large number of periodic supercells. Here $E(\mathrm{DP})$ and $E(\mathrm{SP})$ are energies per unit length per dislocation of the cells containing DP and SP cores, respectively. Since the elastic energies of the two unit cells are identical by definition, the considered difference can be equated to the difference in core energies of the two cores. The shear stress is varied for a given cell by changing w, which can range from 1 to $L-1$. The stresses thus obtained, as estimated by istropic linear elasticity theory for the cells under consideration, can be as large as 0.07μ, or almost 4 GPa. It is clear from the plot that although the DP core is more stable than the SP core for most stresses, in general the energy difference decreases with increasing σ_{xy}.

The lack of coincidence of the curves suggests that the relative stability of the two reconstructions depends on more than the shear stress. In fact, the diagonal stress components σ_{xx} and σ_{yy} and their gradients are also affected by the periodic arrangement of the dislocations. The two most outlying curves, corresponding to the

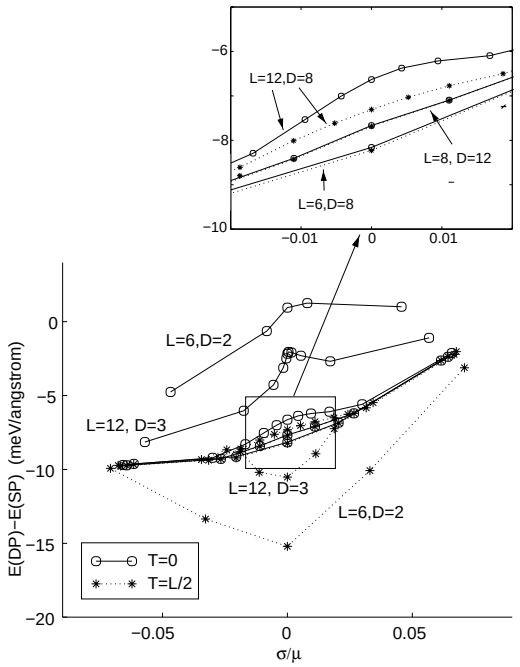

Figure 6 : Energy difference $E(\mathrm{DP}) - E(\mathrm{SP})$ for Si as a function of shear stress for various choices of unit cell. A negative number indicates that the DP structure is more stable.

smallest unit cell with dimensions $L = 6, D = 2$, have the largest diagonal stress components (for $w \neq L/2$, up to half the magnitude of the shear stress), whereas the cells $L = 6, D = 8$ and $L = 8, D = 12$ have the smallest diagonal components (down by a factor of 10^5 from the shear stress, over the range of w/L investigated). This suggests that (1) the small cells used by previous workers [Bennetto, Nunes, and Vanderbilt (1997); Valladares, Petford-Long, and Sutton (1999)] to determine the relative stability of the SP and DP cores may subject the dislocations to stress field conditions that drastically affect the observed value of the energy difference $E(\mathrm{DP}) - E(\mathrm{SP})$ and (2) the energy difference of the two cores may be sensitive to pressure such that under certain conditions the SP structure is to be the more stable core. In any case, it is clear, as Lehto and Öberg (1998) have pointed out, that the relative stability of the two cores is highly dependent on the environment in which the dislocation is located.

It is worthwhile commenting on the lack of symmetry between $\pm\sigma_{xy}$ in Fig. 6. Here, the positive shear stress is defined as the shear stress that pushes the partial towards the stacking fault. The asymmetry is present, quite simply, because there is no reason to expect a $\pm\sigma_{xy}$ symmetry: One side of the dislocation is bounded by a stacking fault, whereas the other borders the unfaulted crystal. Since the configuration of atoms clearly breaks $\pm$ symmetry, one expects that the energy difference between the cores will also break this symmetry.

3.2 Cylindrical boundary conditions

Given the number of degrees of freedom in choosing the periodic supercells, and the potential for the introduction of artifacts arising from choosing the same sense versus opposite sense reconstruction, it is wise to compare the periodic supercell calculations with those obtained using a cylindrical unit cell containing an isolated single dislocation. As a minimum check, it is reasonable to consider the case of zero applied shear stress, as this is the condition under which the periodic supercell calculations show the most significant dependence on the periodic supercell geometry.

The initial displacements of atoms within the cylindrical cell, which contains up to about 6000 atoms, are determined according to anisotropic elasticity theory, and the positions of atoms in an outer ring of thickness 5 Å are fixed. Relaxation of the core atoms is again performed using Tersoff potentials.

In the periodic cells, small changes in the initial positions of the dislocations (as defined by elasticity theory) are insignificant because all atoms are allowed to relax to the minimum energy configuration. In the cylinder, however, the initial position of the dislocation is important because it determines the displacements of the fixed outer atoms and thus affects the final energy. However, the attempt to treat a discrete atomic lattice with continuum elasticity theory introduces an ambiguity; a dislocation's position can only be defined to within an interatomic spacing. While one approach is simply to place the dislocation on the center axis of the cylinder, the lack of perfect radial symmetry about this axis at the atomic level suggests that the core energy of the relaxed configuration may be lower if the dislocation is displaced slightly from this axis. Further, there is no reason to assume that the optimal position for the dislocation is the same for the SP and DP structures.

In order to explore these issues more carefully, the following procedure is performed. The trial cylinder is

taken to have a radius of 20 Å and is periodic along the dislocation line direction. For each core reconstruction, the dislocation position is varied in increments of 0.1 Å along each direction within a circle of radius b, where b is the magnitude of the Burgers vector (about 2.2 Å). The resulting configurations are relaxed and the energies recorded. The energy differences associated with the placement of the core are found to be significant; changes in the core positions by less than 1 Å can shift $\Delta E = E(\mathrm{DP}) - E(\mathrm{SP})$, by as much as 5 meV/Å, which is on the order of ΔE itself. Since the change in elastic energy associated with the small change in position of the dislocation with respect to the outer ring of atoms is negligible, it is reasonable to choose the dislocation position at the point that minimizes the core energy for each structure. For the SP core, the optimal placement of the dislocation is found to be $x = -1.4$ Å, $y = -0.5$ Å, where the x-axis is in the $[1\bar{2}\bar{1}]$ direction and the y-axis is in the $[1\bar{1}1]$ direction. For the DP core, the optimal position is $x = 0.3$ Å, $y = -0.7$ Å.

As the radius of the cylinder is increased and surface effects become less significant, ΔE is expected to approach a value close to what is expected for an isolated (partial) dislocation in a bulk material. Fig. 7 plots ΔE as a function of cylinder radius, using the optimal positions for the SP and DP cores as determined above. The thickness of the outer cylinder of fixed atoms is kept constant at 5 Å; supplemental trials suggest that variations in this thickness are insignificant, especially as the cylinder radius is increased.

As the radius of the cylinder increases, ΔE approaches a value of approximately -6.8 meV/Å. This result is to be compared to the zero shear stress, or $w = L/2$, case in the periodic calculations shown in Fig. 6. Although this number varies among the choices of unit cell, it is reasonable to choose the points corresponding to the largest cells, in which the dislocations are the most isolated (albeit with separations on the order of tens of angstroms). The cells $L = 12$, $D = 8$ and $L = 8$, $L = 12$ show $E(DP) - E(SP)$ from -6.5 to -8 meV/Å. Thus, it can be concluded that the periodic supercell method gives results comparable to those from cylindrical cluster calculations in the case of an isolated unstressed dislocation, provided that the periodic cell is chosen judiciously.

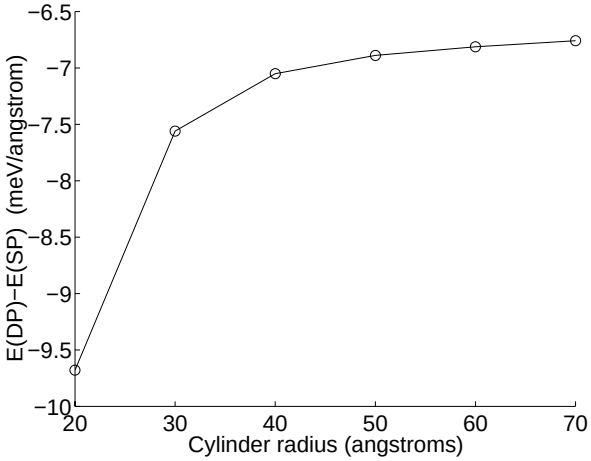

Figure 7 : Energy difference $E(\mathrm{DP}) - E(\mathrm{SP})$ for Si, calculated using Tersoff potentials and cylindrical boundary conditions, as a function of the cylinder radius.

4 Pressure calculations

The effects of the diagonal stress components σ_{xx} and σ_{yy} on the relative stability of the SP and DP cores, as discussed in section 3.1.3, suggest that one may be able to induce a transition where the SP core is more stable by applying a hydrostatic pressure to the periodic unit cells. This is accomplished in the following manner. A number of perfect diamond cubic cells are generated with lattice constants varying near the lattice constant $a = 5.43$ for Si. The energy of these unit cells, calculated using Tersoff potentials, is then tabulated and a cubic spline is fit to the E vs. V curve. Since $P = -\partial E/\partial V$, it is then possible to extract the lattice constant corresponding to a particular pressure. This lattice constant is then used to generate the dipolar unit cells, and the same analysis used in generating Fig. 6 is performed.

Fig. 8 shows the results of applying pressure to the $L = 6$, $D = 8$ cell, for which the diagonal stress components are normally very small. (The difference between the $T/L = 0$ and $T/L = 1/2$ curves is negligible on the scale of the plot.) As the diagonal stress components are increased, the curve moves up on the plot, indicating that the DP core is becoming less stable with respect to the SP core. For $P = 3$ GPa, the SP core appears to be more stable for all but the most extreme shear stresses.

For values of P of 5 GPa and above, the curves begin to take on a different shape. Examination of the relaxed core structures reveals that this is due to yet another tran-

sition; the SP core has transformed into a *symmetric* reconstruction, in which each atom along the core has three first neighbors and two further neighbors at a distance greater than the equilibrium bond length (See Figure 9). In this structure, found by Duesbery, Joos, and Michel (1991), the atoms are said to have "quasi-fivefold" coordination. The bonds across the dislocation core are longer in the quasi-fivefold coordinated symmetric core than in the four-fold coordinated asymmetric core.

Although Duesbery *et al.* found the symmetric reconstruction to be more stable using certain empirical potentials, it was later determined by Bigger *et al.* using more accurate *ab initio* techniques that the asymmetric reconstruction (Fig. 1(b)) is in fact more stable, and it is thus this reconstruction for the SP core that has been considered in the most recent literature. However, the inability of other empirical potentials to predict the correct SP reconstruction suggests that the transition seen here is similarly an artifact of the Tersoff potential and its limited range. For the cells under zero or low pressure, the symmetric reconstruction is metastable and transforms spontaneously to the unreconstructed core (Fig. 1(a)) which is significantly higher in energy than both the DP core and the asymmetric SP core. However, as the pressure is increased, the lattice constant and hence the average bond length decreases. When the lattice constant becomes small enough, more atoms may fall within the cutoff defined by the Tersoff parameters for Si, making the symmetric reconstruction (with five neighbors rather than four) more energetically favorable. Although it is clear that these calculations should be repeated using more accurate methods, the trend observed for the low pressure curves of Fig. 8 (if correct) suggests that the stable core structure may change from DP to SP upon application of an external pressure. If electronic states of the two cores can be identified so as to allow one to distinguish them experimentally, it may be possible to observe this transition directly.

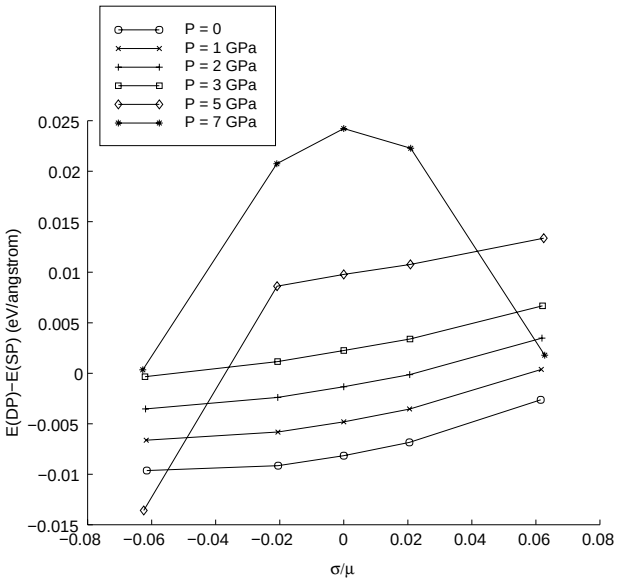

Figure 8 : Plots of $\Delta E = E(\mathrm{DP}) - E(\mathrm{SP})$ for the $L = 6$, $D = 8$ cell, with a hydrostatic pressure imposed. As the pressure is increased, the DP core becomes less stable with respect to the SP core.

5 Discussion and conclusions

In summary, the calculations presented here form an initial study of the deformation behavior of the core of the 90° partial dislocation in Si. Specifically, it is demonstrated that the deformation of the core leads to 1) a shear stress asymmetry in the difference in core energies between the DP and SP cores, and 2) the possibility of a shear and hydrostatic stress induced core transformation.

The shear-stress asymmetry may well be important, in so far as it suggests that the mobility of this partial may depend on the sign of the stress. The implication is that the magnitude of the dislocation velocity may depend on the sign of the applied stress, and whether or not the 90° partial is leading or trailing, much as is expected for dislocations in wurtzite materials [Maeda and Takeuchi (1996)].

The possibility of a stress induced core transformation may also have significant implications for the mobility of the dislocations. If dislocations move through the nucleation and lateral motion of kinks, then one might expect that both the double kink nucleation barrier and the the kink-migration barrier would depend on the structure of the core. Hence a proper theory of dislocation mobility must necessarily include the thermally-assisted formation of the unstable core phase, and reflect the changes in kink dynamics so expected. In addition, dislocation dynamics simulations, reflecting simple empirical mobilities may not capture the essential features of the dynamics of these dislocations.

Finally, it is noted that the atomic scale calculations reported here are computed using Tersoff potentials, and result in very small energy differences between the two core states. Though these energy differences are simi-

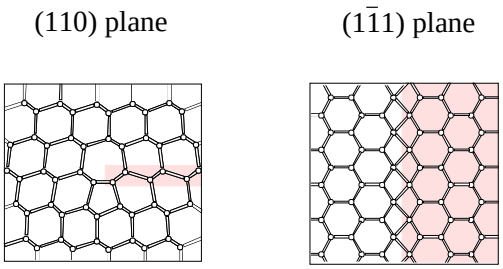

Figure 9 : Symmetric, quasi-fivefold coordinated reconstruction of the 90° partial dislocation viewed from above the (110) and $(1\bar{1}1)$ planes. Shaded area indicates stacking fault.

lar to those reported based on *ab initio* techniques, the energy differences are probably below the resolution of the potentials. Nevertheless, these calculations do suggest that further investigations, using more predictive total energy techniques are warranted. The calculations further establish the approximate size of a periodic supercell necessary to produce the required accuracy (2000 atoms). These calculations, while extremely numerically taxing, are, perhaps, within reach. Hence in the not too distant future, it will be possible to conduct studies of this sort using *ab initio* electronic structure total energy techniques.

In conclusion, this paper addresses three aspects concerning the study of edge dislocation cores. First, it is demonstrated in detail how one may use the isotropic linear elastic treatment of tilt boundaries to extract dislocation core radii from atomic scale calculations employing periodic supercells. Second, it is demonstrated how one can use linear isotropic elasticity theory to study systematically the dependence of dislocation core structures on imposed stress states. This demonstration suggests that similar calculations employing *ab initio* electronic structure techniques would be insightful. Third, it is suggested that applied shear stresses and hydrostatic pressures may induce a structural transformation in the core of the 90° partial dislocation in Si. A transformation of this type may impact the mobility of the dislocation substantially.

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