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The equilibrium structures of the 90° partial dislocation in silicon

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Abstract

We consider the free energies of the single-period (SP) and double-period (DP) core reconstructions of the straight 90° partial dislocation in silicon. The vibrational contributions are calculated with a harmonic model. It is found that it leads to a diminishing difference between the free energies of the two core reconstructions with increasing temperature. The question of the relative populations of SP and DP reconstructions in a single straight 90° partial dislocation is solved by mapping the problem onto a one-dimensional Ising model in a magnetic field. The model contains only two parameters and is solved analytically. It leads to the conclusion that for the majority of the published energy differences between the SP and DP reconstructions the *equilibrium* core structure is dominated by the DP reconstruction at all temperatures up to the melting point. We review whether it is possible to distinguish between the SP and DP reconstructions experimentally, both in principle and in practice. We conclude that aberration corrected transmission electron microscopy should be able to distinguish between these two core reconstructions, but published high resolution micrographs do not allow the distinction to be made.

1. Introduction

Since silicon has a face centred cubic lattice, perfect dislocations lie on {111} slip planes and have $\frac{1}{2}\langle 110\rangle$ Burgers vectors (Hirth and Lothe 1982). They lie primarily along $\langle 110\rangle$ directions because of the existence of deep $\langle 110\rangle$ Peierls valleys which are a consequence of the strong covalent nature of bonding in this material. In general these dislocations are of either pure screw or 60° character. However, since silicon has a two-atom basis (i.e. the diamond cubic structure), there are in fact two distinct positions for the slip planes and thus two different sets

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of dislocations with identical Burgers vectors, known as the shuffle and glide sets (Hirth and Lothe 1982). Electron microscopy experiments have shown that dislocations in silicon are in general dissociated and glide in this extended configuration (Ray and Cockayne 1971, Gomez *et al* 1975, Gomez and Hirsch 1977). Both the screw and 60° dislocations belonging to the glide set can dissociate into pairs of partial dislocations bounding an intrinsic stacking fault ribbon. The screw glide dislocation dissociates into two 30° partial dislocations whereas the 60° glide dislocation dissociates into one 90° and one 30° partial (Hirth and Lothe 1982). These partials have Burgers vectors of the form $\frac{1}{6}\langle 112\rangle$. The screw and 60° shuffle dislocations, on the other hand, can only dissociate into partials bounding an intrinsic stacking fault if there is a row of either vacancies or interstitials associated with one of the partials (Hornstra 1958). Most of the evidence indicates that the dislocations found in plastically deformed silicon belong to the glide set (Olsen and Spence 1980, Anstis *et al* 1981, Northrup *et al* 1981, Hirsch 1985) and because of this both the 90° and 30° glide partials have received much attention. However, it should be noted that recent deformation experiments on silicon at low temperatures and with confining pressures have revealed undissociated perfect dislocations of different characters (Rabier *et al* 2000).

Both partials are believed to undergo reconstruction of their cores to eliminate unsaturated bonds and restore fourfold coordination to all atoms. This belief is consistent with the relatively low density of unpaired spins found by electron paramagnetic resonance (EPR) experiments in silicon (Hirsch 1985). The challenge to theory and simulation has been to suggest possible reconstructions of the dislocation cores that are consistent with the experimental observations. In this paper we consider only the 90° partial.

The core reconstruction of the 90° partial has been studied since the late 1970s. A consensus was beginning to form that the reconstruction proposed independently by Hirsch (1979), Jones (1979) was correct. In this reconstruction there is a displacement that breaks the mirror symmetry normal to the dislocation line, enabling threefold coordinated atoms in the unreconstructed core (figure 1(a)) to come together and bond. In this way two degenerate reconstructions exist, one for each sense of the mirror symmetry breaking displacement, and all atoms are fourfold coordinated in the core. This core reconstruction is shown in figure 1(b). The symmetry breaking displacement does not alter the translational symmetry along the dislocation line, which retains the same periodicity as the crystal lattice, i.e., $\frac{1}{2}\langle 110\rangle$. Following Bennetto *et al* (1997), we shall refer to this structure as the single-period, or SP, reconstruction.

Another core reconstruction was proposed by Duesbery *et al* (1991). In this structure the mirror symmetry is not broken and the atoms on either side of the dislocation line move towards each other so that each core atom will have as a result three nearest neighbours plus two more neighbours at a somewhat greater distance. For any given core atom, these two neighbours are the two closest atoms across the dislocation line. This reconstruction is known as the quasi-fivefold reconstruction. However, Bigger *et al* (1992) carried out first principles simulations of the 90° dislocation with full ionic and electronic relaxation in the local density approximation (LDA) and with periodic boundary conditions, and their results indicated that the quasi-fivefold configuration was higher in energy by 0.23 eV Å^{-1}. More importantly, they found that the quasi-fivefold structure was metastable and that it transformed to the SP configuration as soon as it was perturbed slightly, rendering the SP reconstruction the more likely structure.

Bennetto *et al* (1997), however, discovered a new core reconstruction for the 90° partial with double the periodicity along the dislocation line. Following Bennetto *et al*, we refer to this structure as the double-period, or DP, reconstruction. The DP structure retains fourfold coordination for every atom. They found that it had a lower potential energy (at 0 K) than the SP structure regardless of whether they used an empirical interatomic potential, tight binding

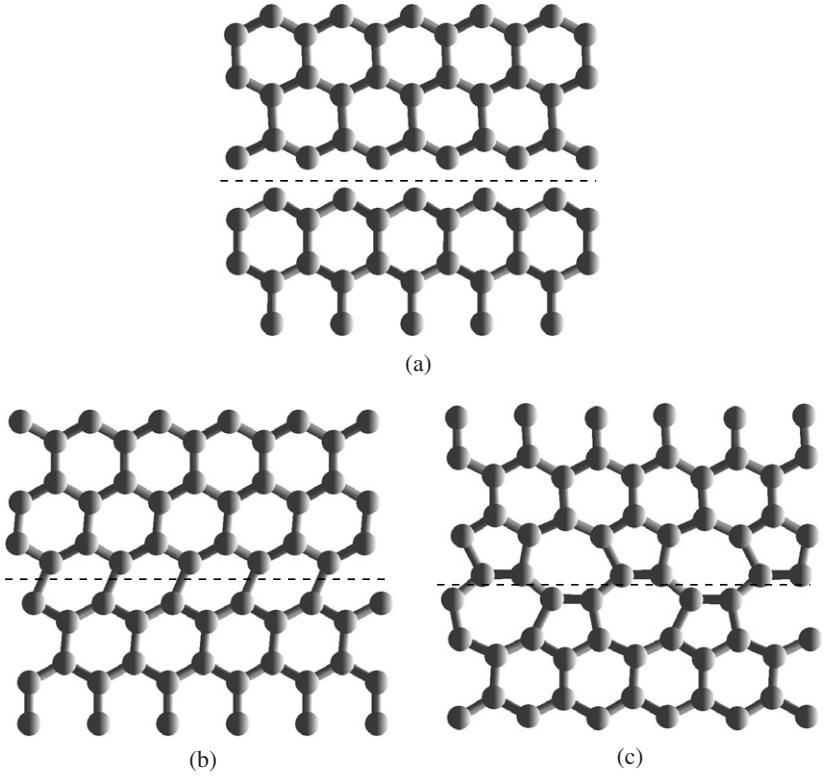

Figure 1. Core structure of the 90° partial looking down on the (111) slip plane. The dislocation (along the broken line) is lying in the $[1\bar{1}0]$ direction. (a) Unreconstructed core. (b) SP reconstruction. Note how the bonding breaks the mirror symmetry normal to $[1\bar{1}0]$ that existed in the unreconstructed core. (c) DP reconstruction. The mirror symmetry normal to the dislocation line is again broken in this case. In both the SP and DP reconstructions all atoms are fourfold coordinated.

or a first principles density functional (LDA) calculation. Based on their density functional simulations they obtained an energy difference of 0.079 eV $Å^{-1}$. We note that Bigger *et al* (1992) imposed periodic boundary conditions with only a single period along the dislocation line. Therefore, configurations with more than one crystal period along the dislocation were suppressed in their work. The DP structure is shown in figure 1(c). This structure also breaks the mirror symmetry normal to the dislocation line and as in the case of the SP structure there are two degenerate structures which are mirror images of each other. However, due to the period doubling we have an equivalent structure to that shown in figure 1(c) which can be obtained by a translation of the whole structure by one single period along the dislocation line (and the same for the mirror image structure). In this way we have a total of four degenerate reconstructions (Bennetto *et al* 1997).

Recently, another structure called the extended DP structure has been proposed for 90° partials in $Ge_{0.35}Si_{0.65}$ in an attempt to explain certain experimental findings (Batson 2000). However, we do not consider this structure in the present study for the reasons given below. In what follows, we focus on the SP and DP core reconstructions and address the question of the roles they play in the structure of the 90° partial dislocation in silicon.

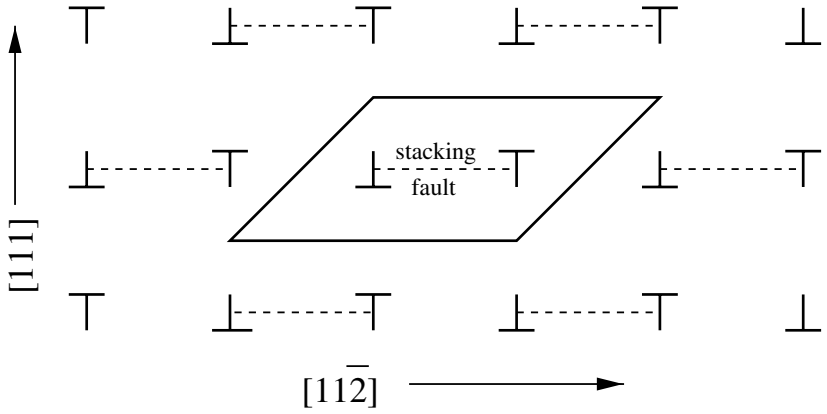

Figure 2. Schematic view of the type of cell employed in our simulations. It contains a dislocation dipole and when repeated periodically it generates a quadrupolar lattice of dislocations. The cell is shown looking along the dislocation lines.

2. Simulation method

We have employed supercells and periodic boundary conditions. We have considered two 512-atom oblique cells, each containing two 90° partials with opposite Burgers vectors separated by a ribbon of intrinsic stacking fault (i.e., a dislocation dipole). The cells were identical to each other except that in one case the dislocations forming the dipole had the SP structure while in the other they had the DP structure. The obliqueness was such that when repeated periodically the cells generated a quadrupolar array of dislocations (Bigger *et al* 1992). In the slip plane the cells were $\frac{4}{2}[11\bar{2}]$ by $\frac{8}{2}[1\bar{1}0]$ and their height was $\frac{4}{3}[111]$. Figure 2 shows a schematic view of the type of cell used in our simulations.

To describe the atomic interactions we have used the Tersoff potential (Tersoff 1986). The parameter set employed is the one appearing in Tersoff (1988). Apart from being fitted to the equilibrium bond length and bulk modulus of the diamond structure, this parameter set has also been fitted to reproduce more accurately the three elastic constants of bulk silicon as well as the phonon frequencies at high symmetry points inside the Brillouin zone (Tersoff 1988). The improved description of these quantities means that the potential is able to take proper account of the dislocation elastic fields and it is suitable for calculating normal modes of vibration. Also, Bigger *et al* (1992) showed that this parameter set gives results in good overall agreement with their *ab initio* calculations of the energetics of the quasi-fivefold and SP structures, which other parameter sets and interatomic potentials were not able to do. Thus, the Tersoff potential with this parameter set is appropriate for the present study.

3. Energy differences of dislocation structures

We have confirmed that the DP structure has a lower potential energy than the SP structure at 0 K. Using the Tersoff potential we find that the DP structure is lower in energy by 0.032 eV Å^{-1}. As noted by Bennetto *et al* (1997) there is a significant difference in the total energy of the periodic cell depending on whether the senses of the reconstruction of the SP case are either identical or opposite. We have obtained the same result: if the reconstruction sense is the same (opposite) then the DP structure is more stable by 0.044 (0.020) eV Å^{-1}. This is at first a curious result because the structures of the two reconstruction senses of the SP core are related

by the plane of broken mirror symmetry normal to the dislocation line. We have identified the existence of a dipolar line of force associated with the SP core parallel to the dislocation line and passing through the atoms at the ends of the reconstructed bonds. The dipole is reversed when the reconstruction sense is reversed. There are different elastic interaction energies between periodic arrays of dipolar lines of force of the same and opposite senses. This is the origin of the difference in the total energies of the periodic cells containing identical and opposite reconstruction senses of the SP core. Since the difference arises from either attractive or repulsive elastic interaction energies between the dipolar lines of force, one should average the values obtained with the same and opposite reconstruction senses to obtain the best estimate for the energy difference between the SP and DP structures of an isolated dislocation line. Bennetto *et al* (1997) reached the same conclusion but without specifying the origin of the difference in energies between the same and opposite reconstruction SP cells. A more detailed discussion of the dipolar lines of force associated with SP 90° partials can be found in Valladares and Sutton (2005). Our value of 0.032 eV Å^{-1} was therefore obtained by averaging as we have just described. Two possible reconstruction senses also exist for the DP case but in that case we have found, again in agreement with Bennetto *et al* (1997), that the difference in energy is negligible.

First principles simulations on the SP and DP structures have been performed by Bulatov *et al* (2001) using supercells and by Lehto and Öberg (1998) using clusters. The former study indicates that the DP structure is more stable than the SP structure by 0.05 eV Å^{-1}. In the latter 486-atom clusters containing a single dislocation were employed, and the results indicate that either the SP or DP structure may be marginally more stable (by 0.021 or 0.011 eV Å^{-1} respectively), depending on the boundary conditions imposed on the clusters. The first value is obtained by relaxing all surface atoms, while the second value is obtained by fixing the atoms of the surface at the positions determined by the elastic field. They considered the elastic field of a 90° partial and a 30° partial at a separation of 50 Å simulating the elastic field of a dissociated 60° perfect dislocation. These isolated dislocation cluster simulations suggest that the energy difference is smaller than the LDA value obtained by Bennetto *et al* (1997), and our results support this view. They also suggest that there is a significant contribution to the SP–DP energy difference from the elastic field, and this is consistent with our identification of a dipole line of force at the SP core, which is associated with a long range elastic field (Valladares and Sutton 2005).

In table 1 we have summarized results for the energy difference between the SP and DP structures at 0 K excluding the zero-point energy. We take the average of the results obtained with the same and opposite reconstruction senses to be the most physically meaningful of those obtained with periodic boundary conditions.

4. Free energy differences of dislocation structures

4.1. Free energies and normal modes

Dislocations in silicon become mobile at temperatures in excess of 800 K (Louchet and George 1983). Given that the potential energy difference between the core structures at 0 K is so small, this raises the question of whether the free energy difference at 800 K is even smaller, so that both reconstructions should exist. We present results that indicate that the free energy difference at 800 K is indeed smaller than the internal energy difference at 0 K.

To estimate the free energy we have used the harmonic approximation for the vibrational degrees of freedom (Sutton and Balluffi 1995):

$$F = E_{\mathrm{P}} + kT \sum_n \ln\left(2\sinh\left(\frac{\hbar\omega_n}{2kT}\right)\right), \tag{1}$$

Table 1. Energy differences in eV Å^{-1} at 0 K (excluding zero-point energy) between SP and DP structures computed by Keating, Tersoff, tight binding (TB) and density functional theory (DFT) descriptions of atomic interactions. Superscripts (1), (2), (3) and (4) refer to Bennetto *et al* (1997), Bulatov *et al* (2001), Lehto and Öberg (1998) and this work respectively. The top three rows are results obtained with periodic boundary conditions with (a) 192, (b) 576, (c) 96 and (d) 512 atoms in the unit cell, with the two partials in each unit cell having either the same or opposite reconstruction senses (except for Bulatov *et al* (2001) (c), who do not specify the relative reconstruction sense). The 'average' is the average of the results for same and opposite reconstruction senses, except again for Bulatov *et al* (2001). The cluster calculations were carried out on clusters of 486 atoms either with the surface atoms fixed in position (e) or relaxed (f).

$E_{SP} - E_{DP}$	Keating$^{(1)}$	Tersoff$^{(4)}$	TB$^{(1)}$	DFT$^{(1)}$	DFT$^{(2)}$	DFT$^{(3)}$
Same reconstruction sense	0.047$^{(a)}$ 0.011$^{(b)}$	0.044$^{(d)}$	0.096$^{(a)}$ 0.059$^{(b)}$	0.102$^{(a)}$		
Opposite reconstruction sense	0.007$^{(a)}$ 0.003$^{(b)}$	0.020$^{(d)}$	0.056$^{(a)}$ 0.051$^{(b)}$	0.055$^{(a)}$		
Average	0.027$^{(a)}$ 0.007$^{(b)}$	0.032$^{(d)}$	0.076$^{(a)}$ 0.055$^{(b)}$	0.079$^{(a)}$	0.050$^{(c)}$	
Cluster						0.011$^{(e)}$ −0.021$^{(f)}$

where E_P is the potential energy at 0 K, the ω_n are the phonon angular frequencies and the sum is over all normal modes of the system. The potential energy for both reconstructions was obtained from the Tersoff relaxed cells. Using these relaxed structures we obtained the frequencies of the normal modes at a number of k-points in the Brillouin zone by diagonalizing the dynamical matrix associated with each structure. The k-point sets used were chosen according to the scheme of Monkhorst and Pack (1976). Although different sets were used, it turned out that our cell size was sufficiently large that the free energy was converged to within 0.03% with just the Γ point.

4.2. Results

The difference, ΔF, between the free energies (in eV Å^{-1}) of the SP and DP structures is shown in figure 3. The broken lines show the results for the same (upper curve) and opposite (lower curve) reconstruction senses of the SP core. The solid line is the average of the two, which we take to be the most physically significant for the reasons described above. The free energy difference decreases as the temperature increases. At 0 K the internal energy difference is reduced from 0.032 to 0.029 eV Å^{-1} by the zero-point energy. At 800 K the free energy of the SP structure is only 0.023 eV Å^{-1} greater than that of the DP structure. These energies suggest that at 800 K, where $kT = 0.069$ eV, both reconstructions might exist when the dislocation is created. We consider this possibility more carefully in the next section.

5. Equilibrium structure of the 90° partial at a finite temperature

5.1. The 1D Ising model

The 1D Ising model consists of a one-dimensional chain of N spin $\frac{1}{2}$ s in an external magnetic field, each spin interacting only with its two nearest neighbours (Huang 1963). The energy of

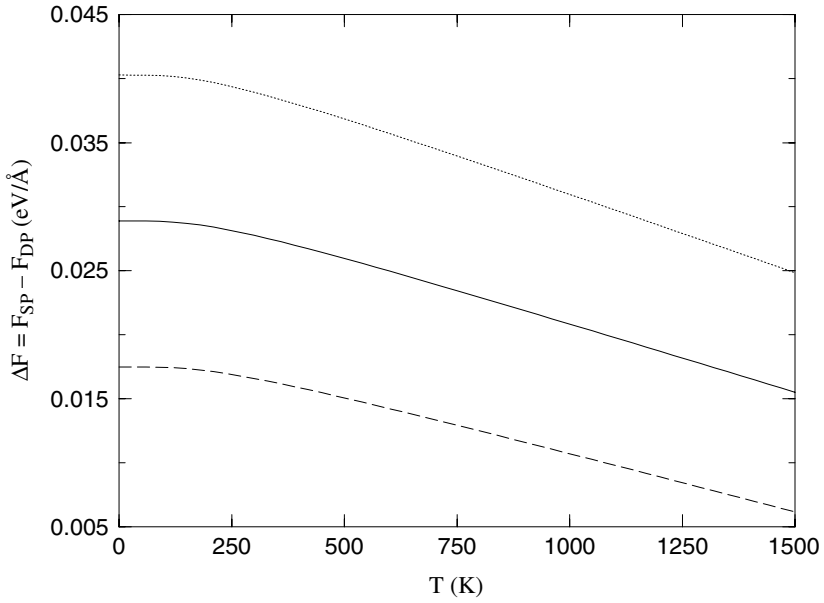

Figure 3. Difference ΔF between the free energies per unit length of the SP and DP structures as a function of temperature (1 eV Å^{-1} = 1.602 nN). The upper curve is for the two partials having the same reconstruction sense while the lower curve is for the two partials having opposite reconstruction senses. The solid curve is the average of the upper and lower curves.

the system is given by

$$E_{\mathrm{I}} = -J \sum_{k=1}^{N} s_k s_{k+1} - B \sum_{k=1}^{N} s_k, \tag{2}$$

where s_k corresponds to the kth spin and can take the values 1 (up) or -1 (down), J is a parameter associated with the interaction energy between spins s_k and s_{k+1}, B is the external magnetic field and the sums are over all spins, with the condition $s_{N+1} = s_1$. We see that E_{I} is the sum of the energies of the individual spins in the magnetic field plus the sum of the interaction energies between neighbouring pairs of spins.

Using this expression we can find the canonical partition function by summing over all possible states of the system, and from the partition function all thermodynamic quantities can be found, like the free energy per spin or the magnetization per spin, for example (Huang 1963).

5.2. Mapping the SP–DP problem onto the 1D Ising model

The SP–DP problem can be mapped onto the 1D Ising model in a magnetic field (Finnis 1999). Let us divide a single 90° partial dislocation into segments of length one DP period. These segments correspond to the spin $\frac{1}{2}$ s of the Ising model. If the kth segment has the DP structure then s_k is equal to 1, and if it has the SP structure then s_k is equal to -1. The energy of the segment will depend on the structure it adopts. Let us call E_{SP} and E_{DP} the energies of any given segment depending on whether it has the SP or DP structure, respectively. The difference between these two energies corresponds to the difference in the energies of an individual spin in the external magnetic field depending on whether it is up or down. The quantity analogous to the interaction energy between pairs of spins is the interfacial energy between SP and DP

segments. In this case, however, we have only an interfacial energy term when the two segments have different structures, since there is no interface between segments with the same structure. This is in contrast to the Ising model, in which we always have an interaction energy between pairs of spins no matter whether they are parallel or antiparallel. With this, the energy of the dislocation is given by

$$E_{\mathrm{SP-DP}} = -\sum_{k=1}^{N} I_k s_k s_{k+1} - B\sum_{k=1}^{N} s_k, \tag{3}$$

where

$$B = \frac{E_{\mathrm{SP}} - E_{\mathrm{DP}}}{2} \tag{4}$$

and

$$I_k = I_{\mathrm{SP-DP}}(1 - \delta_{s_k s_{k+1}}), \tag{5}$$

$I_{\mathrm{SP-DP}}$ being the interfacial energy between SP and DP segments.

The energy in this case is the sum of the energies of the different segments, with either the SP or DP structure (with the zero of energy halfway between E_{SP} and E_{DP}), plus the sum of the interfacial energies between SP and DP segments only. With s now standing for segment, the state of the system is defined by s_k equal to 1 (DP) or -1 (SP), $k = 1, \ldots, N$. One reason for considering segments of length one DP period is that the two opposite sign complexes forming one period of the DP structure (when they are at the minimum separation possible) will not in general be degenerate and hence we do not expect to be able to split E_{DP} evenly among the two different half DP periods.

5.3. Analytic expressions

Using (3)–(5) we have found the canonical partition function by the transfer matrix method (Yeomans 1992), and from this the following thermodynamic quantities. As $N \longrightarrow \infty$, the free energy per dislocation segment is given by

$$\frac{F}{N} = -kT \ln\left\{\cosh\left(\frac{B}{kT}\right) + \left[\cosh^2\left(\frac{B}{kT}\right) - \left(1 - \exp\left(-\frac{2I_{\mathrm{SP-DP}}}{kT}\right)\right)\right]^{\frac{1}{2}}\right\}. \tag{6}$$

The quantity analogous to the magnetization per spin is given by

$$\langle s\rangle = \frac{\sinh\left(\frac{B}{kT}\right)\left\{1 + \left[\cosh^2\left(\frac{B}{kT}\right) - \left(1 - \exp\left(-\frac{2I_{\mathrm{SP-DP}}}{kT}\right)\right)\right]^{-\frac{1}{2}}\cosh\left(\frac{B}{kT}\right)\right\}}{\cosh\left(\frac{B}{kT}\right) + \left[\cosh^2\left(\frac{B}{kT}\right) - \left(1 - \exp\left(-\frac{2I_{\mathrm{SP-DP}}}{kT}\right)\right)\right]^{\frac{1}{2}}}. \tag{7}$$

This last quantity indicates how much of the dislocation is, on average, SP reconstructed and how much is DP reconstructed, at temperature T. More precisely, if p_{SP} and p_{DP} are the fractions in equilibrium of the total length with the SP and DP structures respectively, then

$$p_{\mathrm{SP}} = \frac{1 - \langle s\rangle}{2} \tag{8}$$

and

$$p_{\mathrm{DP}} = 1 - p_{\mathrm{SP}}. \tag{9}$$

These four expressions depend on two parameters, namely, $B = (E_{\mathrm{SP}} - E_{\mathrm{DP}})/2$ and $I_{\mathrm{SP-DP}}$. If we know their values, we can obtain the above quantities at any temperature T, and in particular we will know the equilibrium structure of the 90° partial.

5.4. Calculation of the parameters B and I_{SP-DP}

As discussed above, we have obtained a value of 0.032 eV Å^{-1} for the energy difference between the SP and DP structures. For segments of length one DP period $B = (E_{\mathrm{SP}} - E_{\mathrm{DP}})/2 = 0.123$ eV.

In order to calculate the interfacial energy $I_{\mathrm{SP-DP}}$, we have constructed two cells identical in size and shape to those considered so far except that the length along the dislocation line was doubled. Each pair of dislocations had the SP structure over half its length and the DP structure over the other half. The halves with the SP structure were directly opposite each other on either side of the stacking fault, and hence the DP halves as well. In one cell both dislocations had the same reconstruction sense (for both the SP and DP halves) while in the other they had opposite reconstruction senses. Each cell, therefore, contained four SP–DP interfaces. We relaxed these two 1024-atom cells again using the Tersoff potential. If we sum the energies of the two 512-atom cells containing just the SP and the DP structures respectively, for the cases of same and opposite reconstruction sense, and if we subtract this sum from the energy of the corresponding sense 1024-atom cell containing both the SP and DP structures, then this difference will be four times the SP–DP interfacial energy for these two cases of relative reconstruction sense.

For the opposite reconstruction sense we obtain a value of 0.094 eV whereas we obtain -0.174 eV for the same reconstruction sense. The negative value in the latter case arises from the moments of force associated with the dipolar lines of force of the SP core when the reconstruction sense in the 1024-atom cell is the same. This is analogous to the case of negative formation energies of complexes and antiphase defects on the SP structure when one has the same reconstruction sense for the two partials in the cell, as explained in Valladares and Sutton (2005). The only meaningful value is the positive one and therefore we have $I_{\mathrm{SP-DP}} = 0.094$ eV.

5.5. Results and discussion

At 0 K, we have $\langle s \rangle = 1.0$, and hence $p_{\mathrm{SP}} = 0.0$ and $p_{\mathrm{DP}} = 1.0$. That is, the whole dislocation has the DP structure as expected. The free energy per dislocation segment is $F/N = -(E_{\mathrm{SP}} - E_{\mathrm{DP}})/2 = -0.123$ eV, which is just the energy of a DP segment, since, as we have mentioned above, the zero of energy lies halfway between E_{SP} and E_{DP}.

At 800 K, where $kT = 0.069$ eV, we have $\langle s \rangle = 0.996$ and this gives $p_{\mathrm{SP}} = 0.002$ and $p_{\mathrm{DP}} = 0.998$. The equilibrium structure, therefore, is overwhelmingly DP, with only 0.2% of all segments having the SP structure on average. For the free energy per dislocation segment we obtain $F/N = -0.123$ eV, for the accuracy we are working with, indicating that at this temperature the configurational entropy contribution is negligible. For temperatures close to the melting point, say 1450 K ($kT = 0.125$ eV), we have $\langle s \rangle = 0.925$ and thus $p_{\mathrm{SP}} = 0.038$ and $p_{\mathrm{DP}} = 0.962$. The structure is still overwhelmingly DP although now the fraction of segments having the SP reconstruction has increased to 3.8%. For the free energy we obtain $F/N = -0.127$ eV. The configurational entropic contribution is starting to become more important. We see that for the values of the parameters we have employed the structure is essentially DP from 0 K all the way to the melting point.

The first principles cluster calculations of Lehto and Öberg (1998) give as one of their results -0.021 eV Å^{-1} for the energy difference per unit length between the SP and DP reconstructions. With this value we have $B = (E_{\mathrm{SP}} - E_{\mathrm{DP}})/2 = -0.081$ eV. If we use this value along with the value we have obtained for $I_{\mathrm{SP-DP}}$ from our calculations we have the following. At 800 K, $\langle s \rangle = -0.985$ and it follows that $p_{\mathrm{SP}} = 0.992$ while $p_{\mathrm{DP}} = 0.008$. Now

the structure is essentially SP, with only 0.8% of all segments having the DP reconstruction. For the free energy per dislocation segment we obtain $F/N = -0.081$ eV, which is just the energy of a segment with the SP structure, with respect to our zero of energy. Again, the configurational entropy contribution at this temperature is negligible. For these parameter values, the structure is virtually pure SP from 0 K to the melting temperature.

With the interfacial energy $I_{\mathrm{SP-DP}} = 0.094$ eV we conclude that the dislocation core is overwhelmingly SP or DP reconstructed if the difference in energy per unit length of these two reconstructions is 0.01 eV Å^{-1} or more. However, since all the values for this energy difference reported in the literature except for the one quoted above indicate that DP is more stable than SP by 0.01 eV Å^{-1} or more (see table 1), this would seem to indicate that the equilibrium structure of the 90° partial is DP at any temperature. The energy difference per unit length between the two reconstructions has to be of the order of 0.001 eV Å^{-1} to have significant amounts of both structures in equilibrium at temperatures $T > 0$ K.

Recently, another spin model has been proposed independently to study the relative populations of the SP and DP structures on the 90° partial in silicon (Beckman and Chrzan 2003). To each dislocation site they assign two spin variables which in conjunction give a total of six possible values for any given site. Five energy parameters are required to describe all possible interaction energies between adjacent sites. In spite of its complexity the model is not able to take into account all possible defect structures, as the authors themselves state. On the other hand it allows configurations which have been proven to be unstable and hence not to exist, such as kinks on the SP partial with the same reconstruction sense on either side (Valladares *et al* 1998). Nevertheless, their model reaches the same conclusion as our two-parameter analytic treatment above; whenever there is an energy difference between the SP and DP reconstructions of greater than 0.058 eV Å^{-1} the core will be more than 99% populated by the lower energy configuration at all temperatures up to the melting point.

Although the *equilibrium* structure of the 90° partial is determined by the above model, the actual structure of 90° partials may be determined by the processes by which new dislocation segments are generated, for example, at a Frank–Read source. The resulting structures may differ from those determined by equilibrium thermodynamics. Together with the SP and DP free energies presented in section 4, the barriers associated with the generation of new SP and DP segments will determine the relative populations of these two structures. We might expect the generation of SP segments to be easier than that of DP segments since there are fewer atoms involved because the core is narrower. In this case 90° partial dislocations could have the SP reconstruction in appreciable amounts in reality.

6. Review of experimental observations

Although the SP and DP structures differ primarily through the period doubling along the dislocation line, there are differences in the atomic structures of the cores viewed in projection along the dislocation line. These differences are shown in figures 4(a) and (b), where we can see the greater width in the $[11\bar{2}]$ direction of the DP core. This can be seen by looking at the dumb-bells of atoms lying in the slip plane. The orientations of the dumb-bells change owing to the formation of the stacking fault. The change of orientation occurs in one $\frac{1}{4}[11\bar{2}]$ spacing in the SP core and two $\frac{1}{4}[11\bar{2}]$ spacings in the DP core. Therefore, the question arises as to whether, in principle, high resolution electron microscopy (HREM) can distinguish between these core structures by aligning the electron beam parallel to the dislocation line. To address this question HREM image simulations were performed in Valladares *et al* (1999) with the electron beam aligned parallel to a pure SP and a pure DP dislocation ⟨110⟩ core direction.

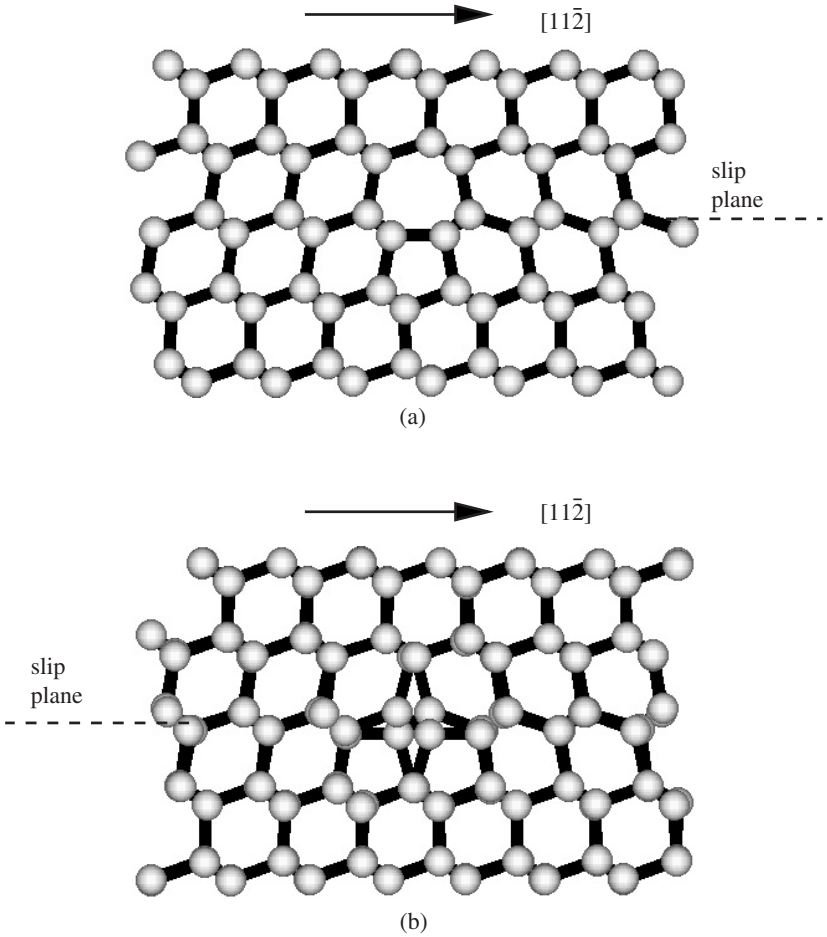

Figure 4. Core structure of the 90° partial viewed along the dislocation line (⟨110⟩ direction) for (a) the SP reconstruction and (b) the DP reconstruction.

It was concluded that provided the resolution was high enough one could distinguish between the pure SP and pure DP structures through the existence of an additional dumb-bell of intermediate orientation in the image of the DP core. We have carried out an extensive search of published HREM images of the 90° partial in Si (Olsen and Spence 1980, Bourret *et al* 1983, Barry and Alexander 1987, Elkajbaji and Thibault-Desseaux 1988). In all, however, the resolution was invariably insufficient to detect the orientation of the dumb-bells. Nevertheless, the use of an aberration corrected objective lens in a high resolution electron microscope may provide the required resolution to distinguish the orientation of the dumb-bells, and hence settle the matter.

Recently, other methods have been suggested for determining the structure of 90° partial dislocations, which consist in obtaining coherent convergent beam electron diffraction patterns or STEM images and intensities (Spence and Koch 2001), but to our knowledge no experimental results have been published yet.

⟨110⟩ STEM images have been obtained, however, for 90° partials in $Ge_{0.35}Si_{0.65}$ (Batson 2000). As we commented in the introduction, a different structure called the extended DP

structure was proposed in order to explain these images as well as electron energy loss spectroscopy (EELS) results. In this structure the dislocation core is four times wider than the SP core and it contains three crossed dumb-bells side by side in the slip plane plus an extra pair of crossed dumb-bells above the slip plane when viewed in projection along the ⟨110⟩ direction (for comparison, the DP core has only one pair of crossed dumb-bells as seen in figure 4(b)). HREM images of dissociated 60° dislocations in silicon viewed normal to the stacking fault (Kolar *et al* 1996) show that the concentration of kinks is higher on 90° partials than on 30° partials. If the same is true for $Ge_{0.35}Si_{0.65}$ then the 90° partial observed by Batson may be occupying two or even three adjacent Peierls valleys, which might explain the greater apparent width of the cores he has observed. The existence of kinks on both the SP and DP reconstructions and their effect on STEM images and EELS spectra has not been considered yet. For these reasons we have not studied the extended DP structure.

7. Conclusions

In this paper we have sought to establish the structure of the straight 90° partial dislocation in silicon. We have mapped the problem onto a 1D Ising model in a magnetic field in which each spin represents either a DP segment or two SP segments. The Ising model has just two parameters and it has an analytic solution. The parameter B is half the difference in self-energies of two SP segments and one DP segment. The parameter I_{SP-DP} is the interfacial energy between a DP segment and two SP segments. We obtained a value of $I_{SP-DP} = 0.094$ eV. If the value of $|B|$ is greater than 0.225 eV the core is more than 99% populated by the lower energy reconstruction at all temperatures. This reflects the relatively minor contribution, at temperatures up to the melting point, to the free energy of the dislocation line from the configurational entropy of mixing SP and DP segments. There does appear to be a consensus that $|B|$ is greater than 0.05 eV, although there is considerable variation on by how much. We conclude that at all temperatures up to the melting point the *equilibrium* structure of the straight 90° partial dislocation is dominated by the DP reconstruction. In reality equilibrium thermodynamics may not be the decisive factor if the core structure is determined by activation barriers for creating SP and DP configurations when the dislocation is formed. We hope aberration corrected transmission electron microscopy observations of the core structure viewed along the dislocation line will be carried out to settle this matter.

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