phys. stat. sol. (a) **171**, 159 (1999)

Subject classification: 61.72.Ji; 61.72.Lk; 68.35.Dv; S5.11

Extended Point Defect Structures at Intersections of Screw Dislocations in Si: A Molecular Dynamics Study

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(Received September 29, 1998)

Molecular dynamics computer simulations have been employed with the Tersoff interatomic potential to examine the atomic structure of $(a/2)\langle 110\rangle$ screw dislocations forming regular two-dimensional arrays in silicon. The main attention is focused on the atomic configurations of dislocation intersections. The dislocations are assumed to be undissociated, following HREM observations on the low-angle (001) twist boundaries produced by silicon wafer bonding in ultrahigh vacuum. It is shown that cores of the dislocation intersections are formed by closed characteristic groups of atoms (extended point defects). The symmetry of these defects strongly depends on the fact whether the screw dislocation arrays generate a twist or a shear boundary.

1. Introduction

Advances of wafer direct bonding [1] as a joining technique in electronics and micromechanics invoked extensive experimental research of interface defects in bonded wafers [2, 3]. Special attention was paid to the Si/Si(001) system, since a (001) silicon wafer remains a material most widely used in the wafer bonding technology. The most important techniques to investigate the bonded interfaces are transmission and high resolution electron microscopy (TEM, HREM) as well as theoretically empirical molecular dynamics (MD). Interfaces obtained by direct bonding of the silicon wafers show typical features of low-angle grain boundaries [4].

TEM plain-view observations [2, 3] revealed square networks of $(a/2)\langle 110\rangle$ screw dislocations resulting from a twist misorientation of wafers upon bonding. As regards the core structure of these grain boundary dislocations, it is not yet understood. Atomistic simulation is a suitable tool to investigate the interfacial defects at an atomic-scale level. Nowadays the modelling of dislocations in semiconductors is a well-elaborated area of computer simulations, which employ a wide range of approaches: from empirical interatomic potentials to *ab initio* electronic structure calculations using the density functional theory (DFT) and modern norm-conserving pseudopotentials. However, the traditional core structure modelling of individual dislocations is insufficient for understanding important details of the atomic structure of low-angle grain boundaries. Cores of the dislocations strongly interact at the points of their intersections. This effect can considerably modify the dislocation core structures and influence the electronic properties of low-angle grain boundaries containing more than one set of dislocations. So far

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little has been done in modelling atomic structures of dislocation intersections in covalently bonded crystals. Using empirical potentials, Mostoller *et al.* [5] carried out a molecular dynamics (MD) study of an orthogonal network of Lomer dislocations at the Ge/Si(001) interface. According to [5], the intersections of Lomer dislocations are formed by closed symmetrical groups of atoms (extended point defects called dreidls), which resemble the structural units typical of high-angle tilt grain boundaries in germanium and silicon [6]. Among atomistic studies of dislocation networks in other crystal structures, the modelling of a low-angle (001) $\Sigma = 85$ twist boundary in Cu [7] has to be mentioned. The atomic structure of perfect screw dislocation intersections in [7] was described in terms of structural units of a high-angle (001) $\Sigma = 5$ twist boundary.

Here we present results of a MD simulation of orthogonal networks of $(a/2)\langle 110\rangle$ screw dislocations in silicon. Intersections of individual right-handed screws were investigated by simulating a low-angle twist boundary. In turn, to analyze intersections of individual right- and left-handed screws, a pure shear boundary was used.

2. Simulation Methods

The proper choice of an interatomic potential is a corner stone of any atomistic simulation. In simulations of extended bulk defects such as grain boundaries or dislocations in covalently bonded solids a structural disorder may be expected in the form of broken bonds and overcoordinated atoms. Therefore, the transferability of a potential to a wide class of structures becomes especially important. We model the interatomic interaction in silicon using the empirical many-body potential of Tersoff [8]. It reproduces the sequence of cohesive energies of Si polytypes with different atomic coordinations, both used in the fitting database and beyond it, in reasonable agreement with DFT [9]. As a shortcoming of this empirical model Justo et al. [10] noted that it fails in predicting the correct structure for reconstructed cores of Shockley partial dislocations. In particular, it does not yield the reconstruction for the 30°-partial dislocation and provides a value for the reconstruction energy of the 90°-partial in very poor agreement with the density-functional theory. This conclusion was likely based on the results of MD studies of Duesbery et al. [11], in which the original Tersoff potential was not used. Our own MD studies demonstrated that the Tersoff potential [8] predicts the reconstruction for both Shockley partials, with the reconstruction energy of the 30°-partial dislocation being in a reasonable agreement with the DFT value (see Table 1). We used a quadrupolar dislocation lattice as described in [12], however, with a larger period.

We simulate periodic networks consisting of two sets of $(a/2)\langle 110\rangle$ screw dislocations (along the $[110]$ and $[\bar{1}10]$ directions, respectively, of the perfect reference lattice). In the case of a twist boundary, both sets of dislocations are right-handed screws. A shear

Table 1

Reconstruction energy (in eV/b) of partial dislocation cores in Si calculated using empirical potentials of Stillinger and Weber (SW) [13], Justo et al. (JU) [10], Tersoff (T3) [8], as well as DFT (according to [10])

	DFT [10, 12]	SW [11]	JU [10]	T3 (this work)
90°-partial	0.87	–	0.80	0.86
30°-partial	0.43	0.81	0.45	0.36

boundary comprises one set of right-handed and one set of left-handed screws. The spacing $D = 10b$, where $b = 3.84$ Å, between dislocations in each set corresponds to either the twist angle $\theta = 5.7^\circ$ of a twist boundary or the shear strain $\varepsilon = 0.1$ of a shear boundary. The minimum energy structures of both grain boundaries were obtained using constant-energy-volume MD, with the velocities being rescaled to remove the kinetic energy. The computational cell $L_x \times L_y \times L_z$ contains a Si slab of 20 monolayers stacked along the [001] direction ($\approx$8000 atoms in the cell) and has dimensions $L_x = L_y = 20b$ in the directions $x = [110]$ and $y = [\bar{1}10]$, respectively. Periodic boundary conditions were imposed along the axes x and y, whereas the slab surfaces were kept free. Two pairs of screw dislocations (along the axes x and y) were introduced in the central plane of the slab using displacement fields of infinite periodic arrays of screw dislocations in an anisotropic elastic medium [14].

The elasticity theory does not provide an insight into the atomic positions within the dislocation core. Therefore, our choice of the initial positions of atoms in this region was based on HREM data regarding the dislocation structures of Si/Si(001) interfaces fabricated by the room temperature Si-wafer bonding in ultrahigh vacuum [2]. While there are regular orthogonal networks of $(a/2)\langle 110\rangle$ screw dislocations in the plane-view TEM images, no visible traces of the dissociation into 30°-partials were observed in the cross-sectional HREM images both upon bonding and after thermal treatment at 850 °C [2]. At the same time, intrinsic stacking faults indicating the perfect dislocations splitting into the partials were detected indeed [15] after annealing at 1100 °C. The periodicity of the stacking fault ribbons exactly corresponds to the spacing between the screw dislocations observed in the plane-view TEM images before annealing. Therefore, the simplest model for the core of a perfect $(a/2)\langle 110\rangle$ screw dislocation, illustrated in Fig. 1, was accepted in our considerations.

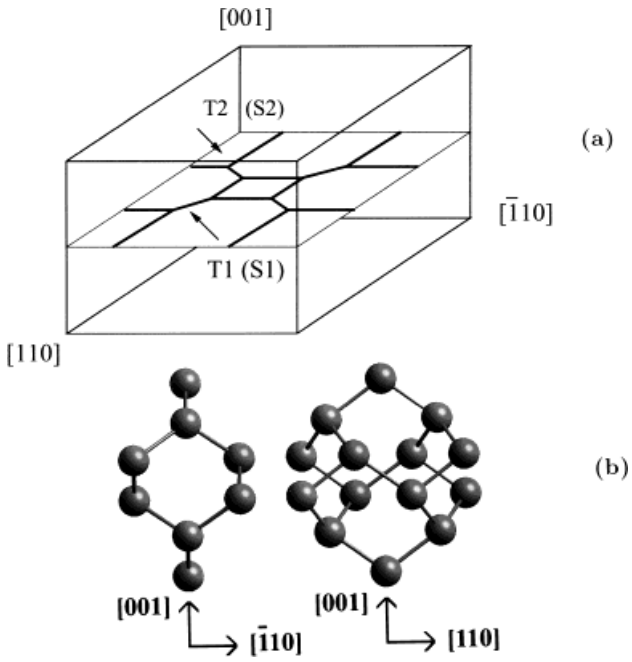

Fig. 1. a) A Si(001) slab with two pairs of $(a/2)\langle 110\rangle$ screw dislocations in the central plane. Intersections T1 and T2 (S1 and S2) correspond to a twist (a shear) boundary. b) The structure of an individual $(a/2)$ [110] screw dislocation core is shown in the [110] and the [$\bar{1}$10] projection

3. Discussion of Results

According to our MD simulations, intersections of right-handed screws and intersections of right and left-handed screws possess very different atomic structures.

(i) Twist boundary. A relaxed atomic structure of the twist boundary is shown in Fig. 2. It has a period $2D$ and therefore there are two types of an intersection, T1 and T2. They are formed by symmetrical characteristic groups of atoms (illustrated in Fig. 3), which have the same point-group symmetry 222 (D_2) as the core structures of individual screw dislocations, shown in Fig. 1. Most of the atoms forming the T1 group remain fourfold coordinated, in spite of large bond-angle distortions: from $-31.8°$ to $+42.6°$. The bond-length distortions are also large, ranging from -1.4% to $+11.4\%$. There are, however, two fivefold coordinated atoms. Each of them has the conventional fourfold coordinated environment with four neighbours at distances from 2.38 to 2.62 Å and, in addition, one atom at the distance $a_c = 2.53$ Å, as shown in Fig. 3. It is difficult to conclude unambiguously whether this coordination defect is a feature of the real dislocation structure or of the Tersoff potential. In particular, the structure optimization performed using the code Cerius3.2, which employs the Keating valence-force field, eliminates this defect, with the distance a_c increasing to as large as 3.14 Å. The complementary intersection T2 is formed by a more complicated atomic group. It comprises only fourfold coordinated atoms, but the bond-angle and bond-length distortions are large, ranging from $-28.9°$ to $+32.8°$ and from -1.8% to $+7.6\%$, respectively.

(ii) Shear boundary. In this case, among two types of an intersection, S1 and S2, only the intersection S1 is formed by a symmetrical characteristic group of atoms. Unlike T1

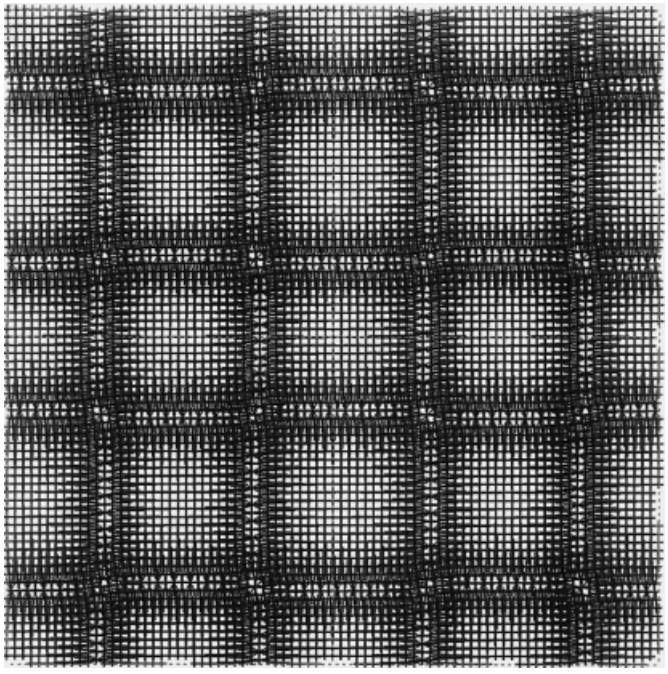

Fig. 2. The relaxed atomic structure of an orthogonal network of $(a/2)\langle 110\rangle$ screw dislocations. The case of a twist boundary

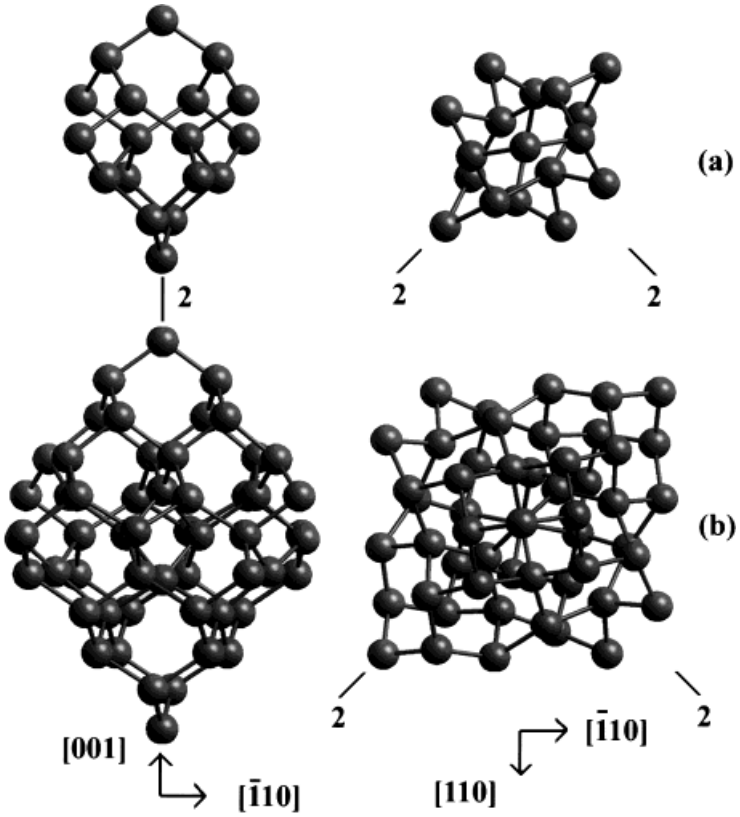

Fig. 3. Structural models of the screw dislocation intersections in the case of a twist boundary. Characteristic groups a) T1 and b) T2 are shown in the [110] (left) and the [001] (right) projection. The symbol 2 denotes twofold symmetry axes

and T2, its point-group symmetry is $\bar{4}$ (S_4), as illustrated in Fig. 4. All atoms in S1 retain the fourfold coordination with the bond-angle and bond-length distortions varying, respectively, from $-36.4°$ to $+37.9°$ and from -1.2% to $+11.8\%$. It is more important that, in contrast to S1, the complementary intersection S2 exhibits a large degeneracy in the number of local energy minima corresponding to a variety of non-symmetrical characteristic groups with a different coordination of their atoms. Fig. 4 illustrates a non-symmetrical group $S2_0$ corresponding to the minimum energy structure found in our simulations. The group contains two atoms of wrong coordination (three and five, respectively) and one dimer-like bond parallel to the twist boundary plane. In addition, a set of non-symmetrical metastable configurations with various coordination defects was revealed for S2, see Fig. 5. Symmetrical metastable configurations for S2 with both under- and over-coordinated atoms were also found. Table 2 lists values of the supercell energy (with respect to the minimum energy structure) for different structural models of S2. We remind that there are two intersections of the S2 type in the supercell. The existence of the large number of energy minima found in our simulations for a low-angle shear boundary resembles the phenomenon

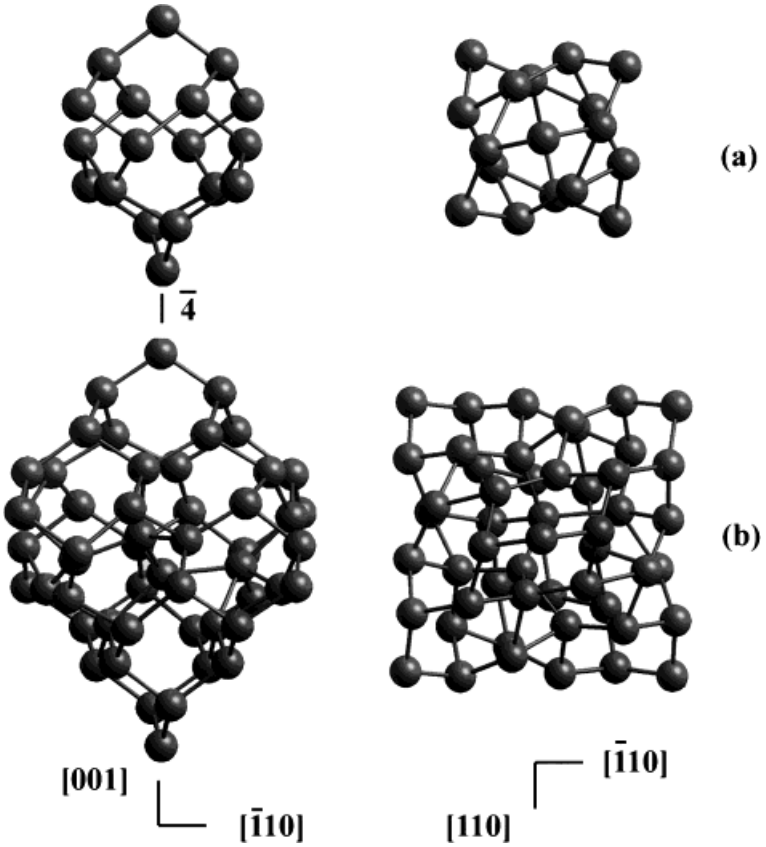

Fig. 4. Structural models of the screw dislocation intersections in the case of a shear boundary. Characteristic groups a) S1 and b) S2 are shown in the [110] (left) and the [001] (right) projection. The symbol $\bar{4}$ denotes an improper fourfold symmetry axis

Table 2

Energy of the supercell (with respect to the minimum energy structure) with a shear boundary depending on an atomic configuration of the intersection S2. In the column for coordination defects, the numbers of three-coordinated (dangling bond (DB)) or five-coordinated defects (floating bond (FB)) defects in the intersection are listed

configuration	supercell energy ΔE (eV)	coordination defects
$S2_0$	0.00	DB: 1, FB: 1
$S2_1$	0.30	FB: 4
$S2_2$	0.42	FB: 5
$S2_3$	0.55	DB: 1, FB: 5
$S2_4$	0.72	FB: 6
$S2_5$	2.32	no defects
$S2_6$	4.44	FB: 2

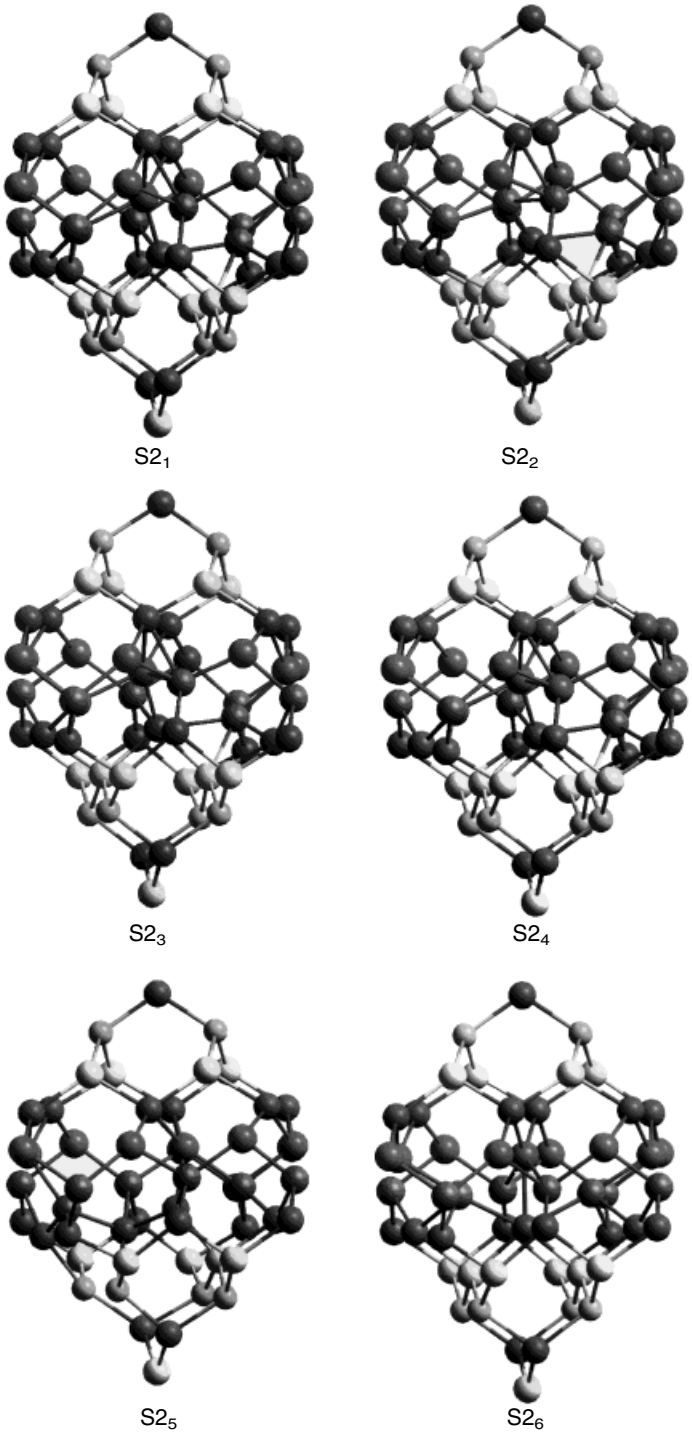

Fig. 5. Atomic structures of metastable configurations of the intersection S2

previously reported for a high-angle (001) $\Sigma = 5$ twist boundary in Ge [16] and Si [17]. However, in the last case the degeneracy was associated with different translational states of the twist boundary.

4. Conclusions

In the course of molecular dynamics simulations of the regular two-dimensional arrays of $(a/2)\langle 110\rangle$ screw dislocations in silicon, new closed symmetrical defect structures have been generated. Such extended point defect structures occur at the intersections of the orthogonal screw dislocations and possess a considerably higher structural disorder than the individual dislocations do. The structural disorder may have a significant impact on the electrical properties of dislocation networks. The density of the intersections in networks varies with the misorientation as $(\theta/b)^2$, being 4.0×10^{11} cm^{-2} for $\theta = 1.4°$. This value fairly well correlates with the density of positive charges 10^{11} cm^{-2} [2] measured by the spreading resistance method for a twist boundary of this misorientation.

Acknowledgement A.Yu. Belov is grateful to INTAS for partial financial support through the project N 96-0363.

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