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Atomic structures of dislocation intersections at (001) low-angle twist and shear boundaries in silicon

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ABSTRACT

The first atomistic simulations of orthogonal networks of screw dislocations in silicon have been performed to investigate the core structures of dislocation intersections. Structural models for the dislocation intersections are proposed and examined by the classical molecular dynamics method with the empirical interatomic potential of Tersoff. The screw dislocations ($\mathbf{b} = \langle a/2 \rangle \langle 110 \rangle$) are assumed to be undissociated, according to experimental data on atomic structures of the synthetic low-angle Si/Si(001) twist boundaries. It is found that cores of the dislocation intersections are formed by closed characteristic groups of atoms (extended point defects). The structure of these defects depends on the fact whether the screw dislocation arrays generate a twist or a shear boundary. The former has a well-defined energy minimum, with the characteristic groups having the point-group symmetry 222 (D_2). The latter is found to exhibit a degeneracy in the number of local energy minima, corresponding to non-symmetrical characteristic groups with a different coordination of atoms.

§ 1. INTRODUCTION

Up to now, most atomistic computer simulations of grain boundaries in semiconductors have focused on high-angle grain boundaries as systems far from equilibrium and exhibiting unusual structural and electronic properties (Kohyama and Yamamoto 1994a,b and references therein). In silicon and germanium, the atomic structures of two geometrical extremes—high-angle tilt and twist boundaries—are in fact essentially different (Sutton and Balluffi 1995). The cores of most of the experimentally observed tilt boundaries are formed by suitable structural units invariably comprising only fourfold coordinated atoms. Thus boundary structures with a well-defined energy minimum prevail. The twist boundaries generally exhibit a higher structural disorder (various coordination defects) than do tilt boundaries (Kohyama and Yamamoto 1994b). The most distinctive feature that distinguishes them from tilt boundaries is a large degeneracy in the number of local energy minima (Tarnow *et al.* 1990). Low-angle grain boundaries have not been considered particularly, because they can be described by periodic dislocation arrays or networks (Hirth and Lothe 1982); since the spacing between the dislocations is large enough to prevent overlapping of their cores, atomic structures of such grain boundaries can be

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understood from those of individual dislocations. In turn, dislocation modelling in semiconductors is a traditional and well-elaborated area of computer simulations, which nowadays 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. What is, however, missing in this picture of a low-angle grain boundary is that 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 little has been done in modelling atomic structures of dislocation intersections in covalently bonded crystals. Using empirical potentials, Mostoller *et al.* (1994) carried out a molecular dynamics (MD) study of an orthogonal network of Lomer dislocations at the Ge/Si(001) interface. The intersections of Lomer dislocations were found to be formed by closed characteristic groups of fourfold coordinated atoms (extended point defects), which retain some symmetry elements of the perfect diamond lattice and resemble the structural units typical of high-angle tilt grain boundaries in germanium and silicon.

Here we report results of the first MD simulation of an orthogonal network of $(a/2)\langle 110\rangle$ screw dislocations in silicon. Unlike the Lomer dislocation networks, this system is not *a priori* expected to comprise only fourfold coordinated atoms at the dislocation intersections. In general, like high-angle twist boundaries, the system can represent a higher level of microscopical complexity. The present study was encouraged by a considerable interest in the atomic and electronic structures of the Si/Si(001) interfaces manufactured using the Si-wafer bonding technique. The screw dislocation networks constitute the twist component of such synthetic interfaces. They occur due to an angular misfit between bonded wafers and possess a very regular structure over large areas (Benamara *et al.* 1996, Plössl *et al.* 1998). Two orthogonal sets of screw dislocations can produce not only a pure twist boundary; if the Burgers vector in one set changes to the opposite direction, a pure shear boundary occurs. We have performed a comparative study of both cases.

§ 2. Model and potential

We consider 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). The spacing $D = 10b$ 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 fifth-order predictor-corrector algorithm of Gear was employed in the integration scheme with a time step of 0.5×10^{-15} s. The computational cell $L_x \times L_y \times L_z$ contains a Si(001) slab of 20 atomic monolayers (~8000 atoms) 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, y and z. However, the dimension L_z in the direction $z = [001]$ was chosen sufficiently large to keep the slab surfaces free. Two pairs of screw dislocations (along the x and y axes) were introduced in the central plane of the slab using displacement fields of infinite periodic arrays of screw dislocations in an anisotropic elastic medium (Hirth and Carnahan 1992). An important feature of the model accepted in this study for the dislocation network is that the dislocation lines are displaced by $\pm b/2$, with $b = 3.84$ Å, at the

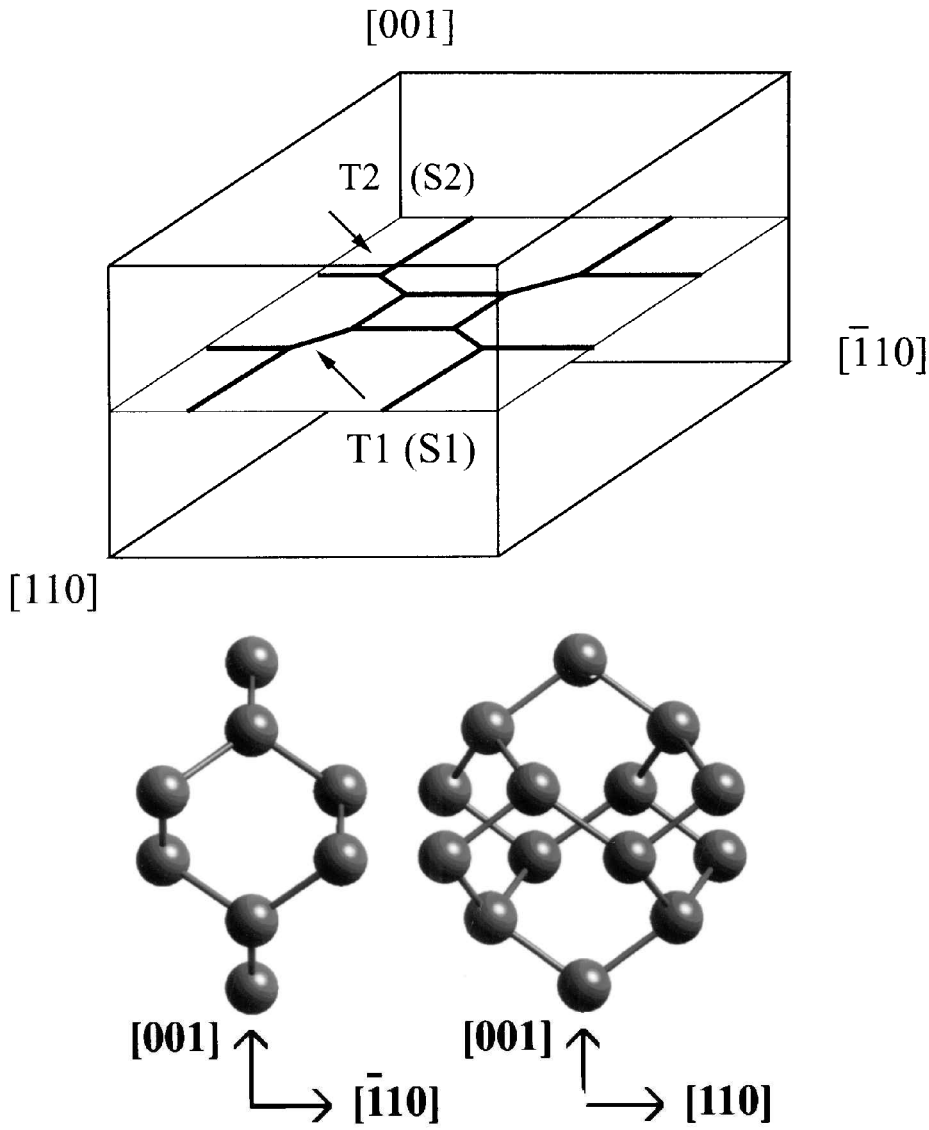

Figure 1. (*a*) A Si(001) slab with two pairs of $\langle a/2\rangle\langle 110\rangle$ screw dislocations in the central plane. Intersections T1 and T2 (S1 and S2) correspond to a twist (a shear) boundary. (*b*) The structure of an individual screw dislocation core is shown in the [110] and the [$\bar{1}$10]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

points of their intersections, as shown in figure 1. Owing to this shift, the core structure remains invariant along the dislocation line. Consequently, there must be, at least, two structurally different types of intersection displacing one dislocation in the opposite direction, with the total shift vanishing within the computational cell. The periodicity of the dislocation network in the xy plane is thus equal to $2D$. This is the reason why the computational cell has to contain, at a minimum, two pairs of screw dislocations.

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 transmission electron microscopy (TEM) and high resolution electron microscopy (HREM) data regarding the dislocation structures of the (001) low-angle twist boundaries fabricated by using the room-temperature Si-wafer bonding in ultra-high vacuum. There are regular orthogonal networks of $(a/2)\langle 110\rangle$ screw dislocations in the plane-view TEM images. Although the elastic energy would decrease drastically upon the splitting of these screw dislocations into 30° partials, no visible traces of the dissociation were observed in the cross-sectional HREM images either after bonding or after thermal treatment at 850°C (Plössl *et al.* 1998). At the same time, intrinsic stacking faults indicating the perfect dislocations splitting into the partials were detected (R. Scholz, 1998, private communication) 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 figure 1, was assumed as the starting point of our considerations.

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 of principal value. We model the atomic interaction in silicon using the empirical many-body potential of Tersoff (1989). 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 the density functional theory. The structural properties of some polytypes not included in the database, such as *bc*-8 and β-tin, are described by the Tersoff model much better than are their energies (Balamane *et al.* 1992). Recently, it has, however, been claimed (Justo *et al.* 1997) that this empirical model 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. Surprisingly, this conclusion was based on the results of MD studies of Duesbery *et al.* (1991), in which the Tersoff potential was not used. Instead, another potential of the same functional form but with a different set of parameters was employed. As was already shown by DFT calculations (Bigger *et al.* 1992) of two reconstructions of the 90°-partial dislocation core, this parametrization, indeed, could not be recommended for dislocation modelling. In contrast to the statement of Justo *et al.* (1997), our own MD tests demonstrated that the Tersoff potential predicts the reconstruction for both Shockley partials, with the reconstruction energy of $0.36\,\mathrm{eV}/b$ of the 30°-partial being in reasonable agreement with the DFT value of $0.43\,\mathrm{eV}/b$. The reconstruction energy of $0.86\,\mathrm{eV}/b$ of the 90°-partial is even in better agreement with the DFT value of $0.87\,\mathrm{eV}/b$ than the corresponding value of $0.80\,\mathrm{eV}/b$, obtained with the novel empirical model of Justo *et al.* (1997, table 5). To facilitate comparison with the results of other studies, our tests were performed using a quadrupolar dislocation lattice as described by Bigger *et al.* (1992), however, with a larger period.

However, one shortcoming of the Tersoff potential has to be pointed out. This model overestimates by a factor of two the difference of the cohesive energy of the *bc*-8 phase from the diamond cubic crystal, more strongly discriminating this

fourfold coordinated alternative of the diamond lattice. Our DFT studies (Belov *et al.* 1998b) of a special (001), 90° twist boundary in Si, which like *bc*-8 has only fourfold coordinated atoms and moderate bond-angle distortions (Belov *et al.* 1998a), confirmed this tendency of the Tersoff model to overestimate by approximately a factor of two the energy differences between the diamond lattice and other fourfold coordinated structures in silicon.

§ 3. Results and discussion

It is well known that low-angle twist and shear boundaries behave differently at the mesoscopic-scale level. The former satisfy the Frank criterion (Hirth and Lothe 1982) and their stress fields rapidly vanish at distances of about D away from a twist boundary, whereas the latter produce long-range stress fields. According to our MD simulations, they demonstrate different structural features also at the atomic-scale level: in the structure of the dislocation intersections.

(i) *Twist boundary.* In this case both intersections, T1 and T2, possess a well-defined energy minimum. They are formed by symmetrical characteristic groups of atoms (illustrated in figure 2), which have the same point-group symmetry 222 (D_2) as the core structures of individual screw dislocations, shown in figure 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 Å to 2.62 Å and, in addition, one atom at the distance $a_c = 2.53$ Å, as shown in figure 2. This coordination defect results from the compression of the T1 group along a twofold symmetry axis lying in the twist boundary plane. It is difficult to conclude unambiguously whether the compression is a feature of the real dislocation structure or of the Tersoff potential. In particular, the structure optimization performed using a valence–force potential (Stoneham *et al.* 1988) eliminates this coordination defect, with the distance a_c increasing to as large as 3.14 Å. The valence–force potentials, however, are not reliable for the defect modelling. 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. Similar (or even larger) values of the bond-angle variations have been obtained by a tight-binding method (Kohyama and Yamamoto 1994b) for relaxed atomic configurations of the (001) $\Sigma = 5$ large-angle twist boundaries with fourfold coordinated atoms. This appears to indicate that the Tersoff model fairly well describes the angular forces within this range of bond angles. As is known, an inadequate description of angular forces at large bond angles is a common shortcoming of the modern empirical potentials (Balamane *et al.* 1992).

(ii) *Shear boundary.* Only one intersection, S1, was established to have a well defined energy minimum in this case. Unlike T1 and T2, it is formed by a characteristic group of atoms with the point-group symmetry $\bar{4}$ (S_4), as illustrated in figure 3. All atoms in S1 retain the fourfold coordination with the bond-angle and bond-length distortions varying, respectively, from

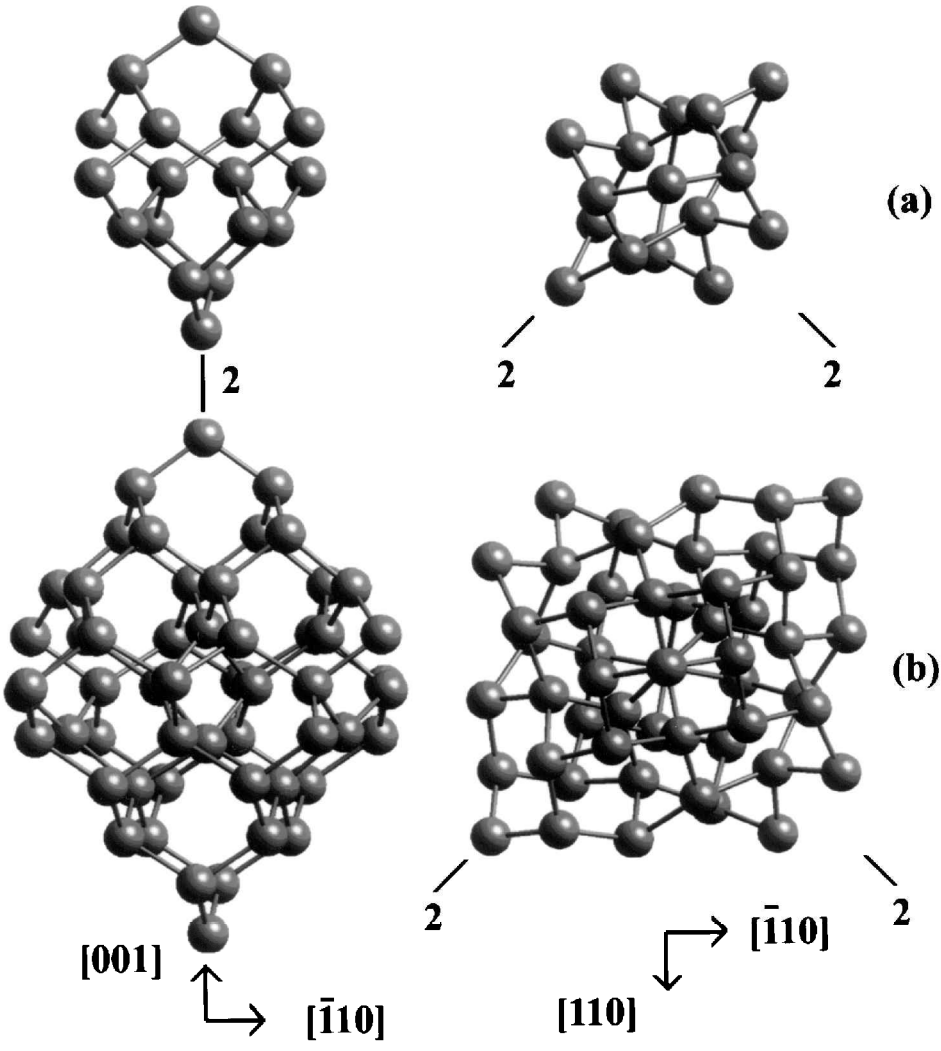

Figure 2. Structural models of the screw dislocation intersections in the case of a twist boundary. Characteristic groups (*a*) T1 and (*b*) T2 are shown in the [110] (left) and the [001] (right) projection. The symbol 2 denotes twofold symmetry axes.

-36.4° to $+37.9^\circ$ and from -1.2% to $+11.8\%$ It is more important that, in contrast to S1, the complementary intersection S2 represents a higher level of microscopic complexity. This intersection was found to exhibit 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. A detailed analysis of their structural features will be given elsewhere. Figure 3 illustrates a non-symmetrical group S2 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 four metastable configurations with various coordination defects was

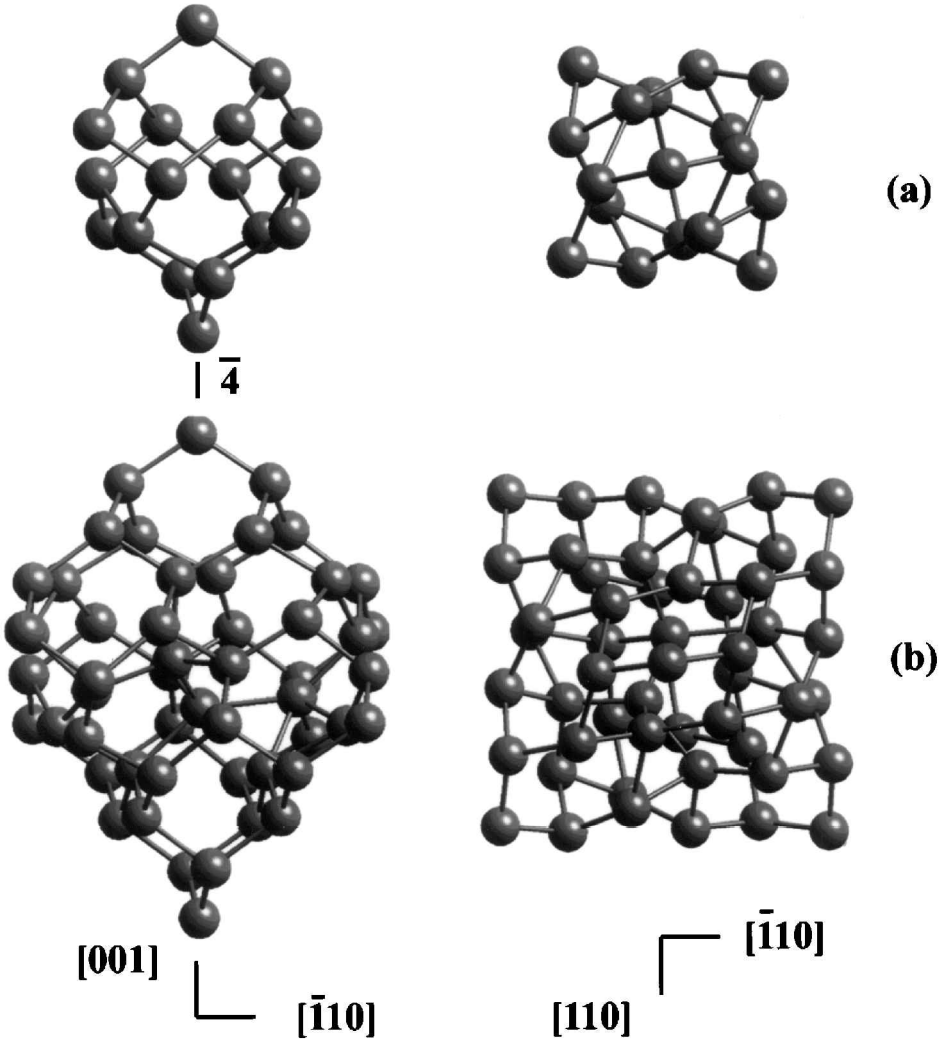

Figure 3. Structural models of the screw dislocation intersections in the case of a shear boundary. Characteristic groups (*a*) S1_and (*b*) S2 are shown in the [110] (left) and the [001] (right) projection. The symbol 4 denotes an improper fourfold symmetry axis.

revealed for S2. The difference of their energies from the structure of figure 3 does not exceed 0.4 eV/intersection. Stable symmetrical configurations for S2 with both under- and overcoordinated atoms were also found.

§ 4. Conclusions

We have performed the first atomistic study of orthogonal networks of perfect screw dislocations in silicon, with the main emphasis focused on the atomic structures of their intersections. Models of minimum structural disorder are proposed on the basis of molecular dynamics simulations for the cores of the intersections. Previous investigations of the (001) low-angle twist boundaries (Phillpot and Wolf 1989) in Si did not pay attention to the core structures of the grain boundary

dislocations. Among atomistic studies of low-angle twist boundaries in other crystal structures, the modelling of a (001) $\Sigma = 85$ twist boundary in Cu (Schwartz *et al.* 1985) has to be mentioned. The atomic structure of screw dislocation intersections was described in terms of structural units of a (001) $\Sigma = 5$ twist boundary.

The classical method used in the present study does not provide an insight into the electrical properties of low-angle twist boundaries in silicon. However, taking into account the similarity between structural properties of the screw dislocation intersections and the (001) $\Sigma = 5$ large-angle twist boundaries (Kohyama and Yamamoto 1994a), one can expect a similarity between their electrical properties. The density of the intersections in networks varies with the misorientation as $(\theta/b)^2$, being 4.0×10^{11} cm^{-2} for $\theta = 1.4^\circ$. This value fairly well correlates with the density of positive charges 10^{11} cm^{-2} (Plössl *et al.* 1998) measured by the spreading resistance method (Benamara *et al.* 1996) for a twist boundary of this misorientation. Therefore, the structural disorder due to the dislocation intersections may have a considerable impact on the electrical properties of low-angle twist boundaries.

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