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Dissociation of screw dislocations in (001) low-angle twist boundaries: a source of the 30° partial dislocations in silicon

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ABSTRACT

The first experimental evidence for dissociation of grain boundary screw dislocations is presented for (001) low-angle twist boundaries in silicon. Using a combination of high-resolution electron microscopy and the weak-beam technique of transmission electron microscopy, it is found that the grain-boundary screw dislocations $(\mathbf{b} = \frac{1}{2}\langle 110\rangle)$ can dissociate in the (111) plane into two 30° partials, forming an intrinsic stacking fault, as do lattice screw dislocations of the glide set. On dissociation one partial dislocation stands off the grain-boundary plane. Some segments of the grain-boundary screw dislocations, however, may remain undissociated. An atomic model for the undissociated screw dislocation core, as well as a mechanism of its transformation into cores of individual 30° partials upon dissociation, are proposed on the basis of classical molecular dynamics simulations with an empirical interatomic potential. The model enables an understanding of the results of electron microscopy investigations.

§ 1. INTRODUCTION

Although grain-boundary screw dislocations in (001) low-angle twist boundaries in silicon have been studied experimentally since the late 1970s (Föll and Ast 1979), the atomic structure of their cores is not known as yet. Orthogonal networks of such screw dislocations occur in silicon on silicon systems manufactured using various silicon wafer bonding techniques (Benamara *et al.* 1996, Plössl *et al.* 1998). Like lattice dislocations, the grain-boundary screw dislocations lie along $\langle 110\rangle$ directions and have $\frac{1}{2}\langle 110\rangle$ Burgers vectors. In fact, Burgers vectors of these two types of dislocation do not exactly coincide, but their difference is vanishing for low-angle grain boundaries. However, there remains a question whether the atomic core structures of grain-boundary and lattice screw dislocations may be similar? As is known, in silicon with a dominant $\langle 110\rangle\{1\bar{1}1\}$ glide system, two sets of lattice dislocations can be conceived, depending on the glide plane position. Placing it between widely spaced $\{1\bar{1}1\}$ planes, one obtains the shuffle set (Shockley 1953, Read 1954a, b), while shearing between narrow spaced $\{1\bar{1}1\}$ planes results in the glide set (Hirth and Lothe 1982). Perfect dislocations of the glide set can dissociate into Shockley partial dislocations separated by an intrinsic stacking fault ribbon. This process is of

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fundamental importance for understanding dislocation mobility and plastic deformation in semiconductors. The purpose of this paper is to report recent high-resolution electron microscopy (HREM) and transmission electron microscopy (TEM) observations on the core structure and mobility of the $\frac{1}{2}\langle 110\rangle$ screw grain-boundary dislocations in silicon. Here we present direct electron microscope evidence that the grain-boundary screw dislocations forming (001) low-angle twist boundaries can dissociate intrinsically in $\{111\}$ glide planes into two 30° partials, as do the lattice screw dislocations of the glide set. On dissociation, one partial dislocation stands off the grain-boundary plane. Therefore, (001) low-angle twist boundaries can emit 30° partials into bulk silicon.

Computer simulation provides a powerful tool for atomic scale studies of twist boundaries in semiconductors. So far most simulations for silicon were focused on high-angle twist boundaries (Kohyama and Yamamoto 1994a, b, Keblinski *et al.* 1997a,b and references therein), which can not be described in terms of individual dislocations since their cores overlap. As far as low-angle twist boundaries are concerned, previous investigations for silicon (Phillpot and Wolf 1989) did not pay attention to the core structure of grain-boundary dislocations. Studies of high-angle twist boundaries can still give some insight into atomic structures of low-angle twist boundaries. As has been shown for face-centred cubic metals (Sutton 1982, Schwartz *et al.* 1985), there exists a decomposition of (001) twist boundary structures into structural units (Sutton and Balluffi 1995) of the ideal crystal (majority units) and structural units of the short period (001) $\Sigma = 5$ twist boundary (minority units). However, in order to make the decomposition complete, complementary units referred to as filler units have to be introduced. In terms of the dislocation model of grain boundaries, the minority units can be identified with the intersections of grain-boundary screw dislocations, between which the preserved structure is composed of majority units. Rows of filler units correspond to cores of these dislocations between dislocation intersections. Filler units are, however, not units of any (001) twist boundary. Their structure is not *a priori* known and thus is a matter of special modelling. Recently, a molecular dynamics (MD) study of an orthogonal screw dislocation network in Si was performed using a dislocation core model which enables preservation of maximum symmetry of dislocation intersections and overall the (001) twist boundary (Belov and Scheerschmidt 1999). This core model allows for covalent bonds parallel to the grain-boundary plane to be eliminated and is consistent with HREM and TEM observations on undissociated screw dislocations in (001) low-angle twist boundaries (Plössl *et al.* 1998). Here we present a new model which can explain the experimental data on dissociation of the grain-boundary screw dislocations. A MD simulation with an empirical many-body potential (Tersoff 1989) was performed to investigate the dislocation core structure before and after dissociation.

§ 2. Experimental

Both TEM and HREM were employed to investigate the dislocation structure of (001) low-angle twist boundaries produced by using the room-temperature bonding of Si(001) wafers. The bonding experiments were done in an ultra-high vacuum (UHV) system after appropriate cleaning and prebonding of commercial wafers of 100 mm diameter (Plössl *et al.* 1998). The twist misorientations between bonded wafers were in the range 0.3° to 3°. Depending on the structural details observed at the interface upon bonding, subsequently various annealing experiments were

performed with pieces of as-bonded wafers. The UHV bonding at room temperature may immediately result in covalent bonds between adhering (001) surfaces, which manifests in the formation of square networks of screw dislocations observed in the plane-view TEM images. In other cases, a similar strong bonding, however, without a discernible dislocation network occurs (Plössl *et al.* 1998). According to the cross-sectional HREM images (Plössl *et al.* 1998), there are no visible traces of the dissociation of the grain-boundary screw dislocations in the first case.

After annealing of the corresponding samples at temperatures between 750°C and 1200°C for various times, the proceeding development of the dislocation networks was observed. The TEM and HREM results presented here were obtained using a piece of an UHV-bonded wafer pair which was annealed at 1100°C for 24 h. Before annealing, dislocation networks were not observed in the plane-view TEM images of this bonded pair, and a higher electron transparency at the interface was found in the cross-sections by making use of HREM. Indications of an emerging grain-boundary screw dislocation network were recorded after a 1 h treatment at 850°C (Plössl *et al.* 1998). Plane-view TEM specimens were prepared as 25° cuts by final chemical thinning and cross-sections for HREM were made by the usual technique including Ar ion milling. Multi-beam diffraction contrast imaging conditions were used for plane-view investigations of the interfaces, as found the best for characterization of dislocation structures in low-angle twist boundaries (Föll and Ast 1979). The cross-sectional specimens were cut such as to allow electron transmission under high resolution imaging conditions near the mean ⟨110⟩ direction of the bonded crystals.

The following observations were made:

(a) An orthogonal network of $\frac{1}{2}\langle 110\rangle$ screw dislocations possesses a regular structure over large areas (figure 1(*a*)). Intrinsic stacking faults, indicating the grain-boundary dislocation dissociation, are visible in the cross-sectional HREM image (figure 2(*a*)). The periodicity of the stacking fault ribbons in figure 2(*a*) exactly corresponds to the spacing $D_d = 118$ Å between the screw dislocations in the plane-view TEM image, figure 1(*a*). According to figure 2(*b*), edge components of Burgers vectors of the partial dislocations have the opposite sign, which confirms that there are indeed two 30° partials. The intrinsic stacking fault of figure 2(*b*) comprises seven pairs of hexagonal rings, see figure 2(*c*). Thus, the partial separation can be estimated as 23.3 Å. This value is consistent with experimental data on dissociated screw dislocations in plastically deformed silicon (Gomez *et al.* 1975).

(b) The weak-beam image in figure 1(*b*), made for another dislocation network with the dislocation spacing $D_d = 420$ Å, demonstrates that some screw dislocations between intersections are completely dissociated, whereas most of the dislocations contain segments which show no apparent dissociation.

§ 3. Atomic models and computer simulation

The experimental data presented here imply that the grain-boundary perfect screw dislocation has an atomic core, a structure that makes possible its dissociation in $\{\bar{1}11\}$ planes. In order to investigate suitable core configurations at $T = 0$ K, an energy minimization simulation with the empirical many-body potential of Tersoff (1989) was performed. In simulations of grain boundaries or dislocations in Si, a

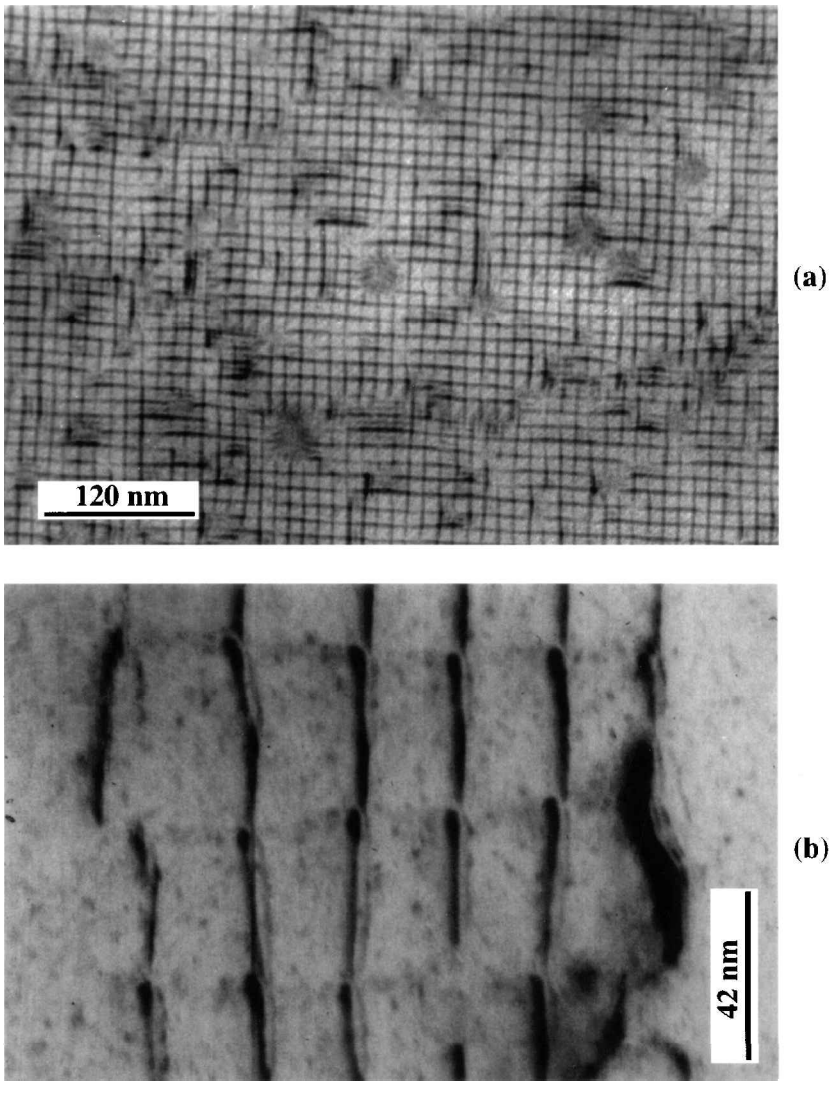

Figure 1. (*a*) Many-beam plane-view image of a screw dislocation network. The dislocation spacing is 118 A. (*b*) Weak-beam dark-field image (contrast reversed) of a square screw dislocation network. The dislocation spacing is 420 A. Incident beam direction is near ⟨111⟩. One set of dissociated screw dislocations is visible.

structural disorder may be expected in the form of either broken bonds or over-coordinated atoms. Therefore, the transferability of a potential to a wide class of structures becomes essential. The potential of Tersoff (T3) is known to reproduce the sequence of cohesive energies and structural properties of Si polytypes with different atomic coordinations, both used in the fitting database and beyond it, in reasonable agreement (Balamane *et al.* 1992) with the density-functional theory (DFT). Previous investigations (Duesbery *et al.* 1991, Belov and Scheerschmidt 1999) showed that, in contrast with the potential of Stillinger and Weber (1985), this potential function predicts the reconstruction for both 30° and 90° Shockley partials, with the reconstruction energies in fairly good agreement with DFT calculations (Bigger *et al.* 1992,

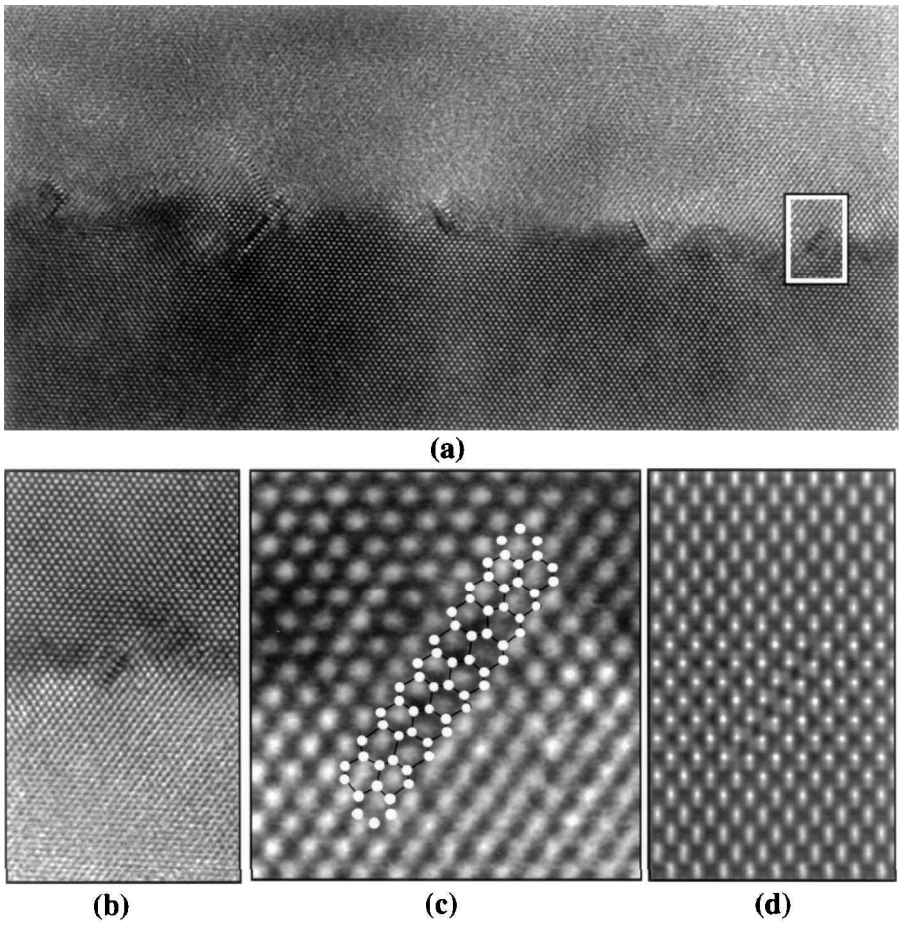

Figure 2. (*a*) Cross-sectional ⟨110⟩ HREM image of the twist boundary of figure 1 (*a*). (*b*) A selected area (enlarged) of figure 1 (*a*) with an intrinsic stacking fault ribbon bounded by two 30° partial dislocations. (*c*) Mapping of the atomic structure on the image 2 (*b*). (*d*) Simulated HREM image of a dissociated screw dislocation. Imaging conditions are specified by the electron beam energy $E = 200\,\text{kV}$, spherical aberration $C_s = 1.2\,\text{mm}$, the defocus value $\Delta = 50\,\text{nm}$ and the specimen thickness $t = 1.56\,\text{nm}$.

Csanyi *et al.* 1998, Justo *et al.* 1998). The novel potential function of Justo *et al.* (1998) reproduces the DFT reconstruction energies with the same accuracy as T3 (Belov *et al.* 1999). As a shortcoming of T3 one has to mention that 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 four-fold coordinated alternative of the diamond lattice. Therefore T3 may overestimate by approximately a factor of two the energy differences between the diamond lattice and other four-fold coordinated structures in silicon.

Perfect grain-boundary dislocations were investigated using the (001) $\Sigma = 401$ ($\theta = 5.7°$) twist boundary. It comprises two sets of $\frac{1}{2}\langle 110\rangle$ screw dislocations with the spacing $D_d = 38.4\,\text{Å}$. The computational cell contains a Si(001) slab of 20 atomic monolayers (~8000 atoms) with the grain boundary in the central plane and has dimensions $L_x = L_y = 76.8\,\text{Å}$ in the directions $x = [110]$ and $y = [\bar{1}10]$, respectively.

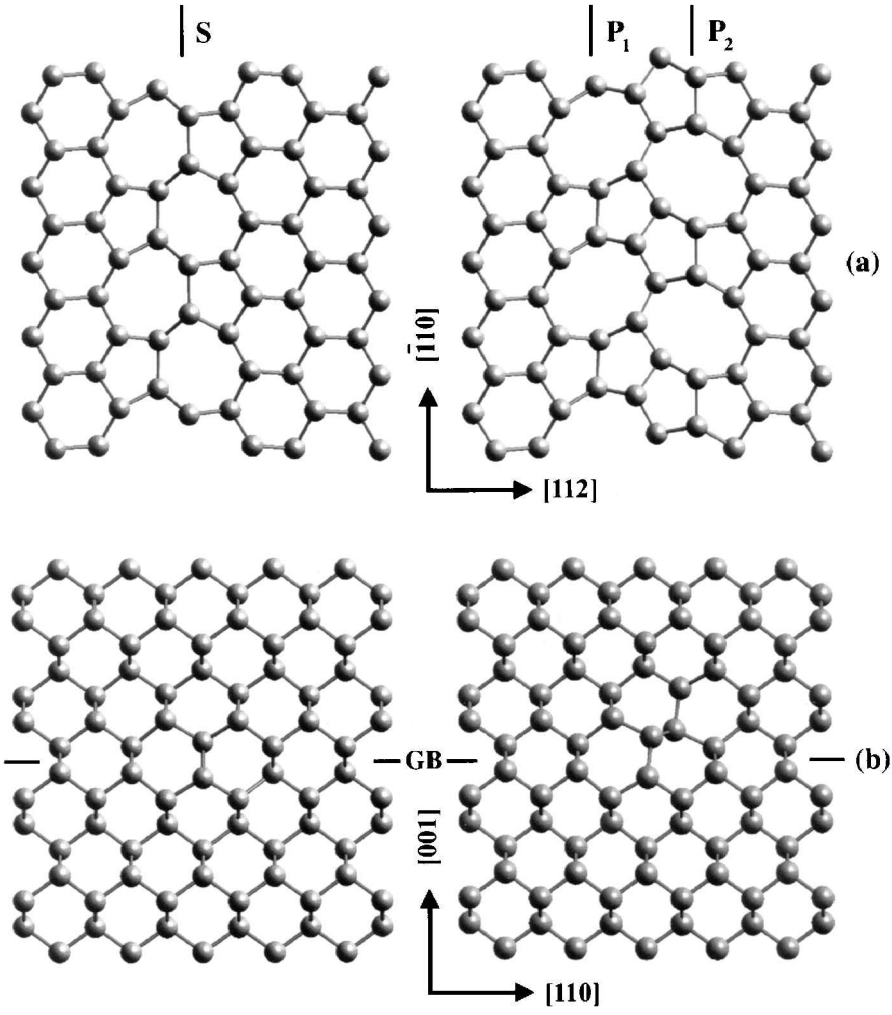

Figure 3._ (*a*) The atomic structure of the core of the perfect (left) and dissociated (right) $\frac{1}{2}\langle 110\rangle$ screw dislocation is shown in the projection onto the {111} plane. The line S indicates the dislocation position before splitting into two 30° partials. Positions of the partials are indicated by the lines P_1 and P_2, respectively. (*b*) The core structures of the perfect (left) and dissociated (right) dislocation are shown in the [110] projection.

Periodic boundary conditions were imposed in the grain-boundary plane. The energy minimization simulation was divided into three steps. First, the energy was minimized using constant-energy–volume MD with the Tersoff potential, with the atomic velocities being rescaled to remove the kinetic energy. At this step a screw dislocation network emerges; however, since the potential has a small cut-off radius, the energy minimum is not achieved (the same concerns the Stillinger–Weber potential as well) and there remains many broken bonds in the dislocation cores. Therefore, at the second step, dislocation cores are reconstructed to eliminate coordination defects and the grain-boundary core structure is further relaxed using the Keating (1966) potential. Unlike empirical potentials, for which bonds are only conceptual, the Keating potential enables the prescribed topology of the bond network to be

conserved in the course of a MD run. The outer atoms in this run are kept fixed. This procedure allows one to restore tetrahedral coordination of all atoms in the grain-boundary core, including dislocation intersections. At the third step, the structure was finally relaxed using the Tersoff potential.

In order to find the minimum energy structure, several conceivable reconstructions of the dislocation core were tested. Details of this analysis will be published elsewhere. The main result is that the energy minimum is achieved if the grain-boundary screw dislocations are reconstructed such as shown in figure 3(*a*). Unlike the reconstruction used in our previous study (Belov and Scheerschmidt 1999), the model of figure 3(*a*) contains bonds parallel to the dislocation line, which is a characteristic feature of the 30° partial dislocation. Figure 3(*b*) illustrates a possible transformation of the perfect dislocation core shown in figure 3(*a*) into cores of individual 30° partials. All atoms in the dislocation cores have four-fold coordination both before and after dissociation. The subsequent evolution of the configuration presented in figure 3(*b*), is the same as in the case of dissociation of the glide set screw dislocation into 30° partials.

§ 4. Discussion and conclusions

We have presented the first experimental evidence that high-temperature treatment can induce the grain-boundary perfect dislocations in a silicon (001) twist boundary to dissociate in $\{\bar{1}\bar{1}1\}$ planes into the 30° partial dislocations. Consequently, the grain-boundary dislocations exhibit similar mechanical behaviour with the perfect screw dislocations of the glide set. The ability of (001) low-angle boundaries to emit partials into bulk silicon can be important for applications.

The fact that the grain-boundary dislocations dissociate at 1100°C, by itself, is not surprising since it is well known that dislocations in Si become mobile at temperatures exceeding 800 K (Hirth and Lothe 1982, Louchet and George 1983). However, the dissociation also implies a suitable structure of their cores. Using empirical MD, we have found a core configuration which can be easily transformed into the cores of 30° partials.

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