# Undissociated screw dislocation in Si: Glide or shuffle set?

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In diamond and zinc blende crystals, the competition between glide and shuffle-set slips has been intensively studied. In particular, the undissociated screw dislocation in Si seen at low temperature about five years ago was generally believed to be shuffle set. In this letter, the authors have performed tight-binding and density functional theory calculations that show that a glide-set C core has lower energy than the shuffle-set A core after period-doubling reconstruction. Since the C core can cross slip between two glide-set planes, it satisfies all the experimental observations to date, and may play important roles in dislocation cross slip and ductile-to-brittle transition in these materials. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2236620]

When confined by pressure, silicon,[1] III–V compounds,[2] and even diamond[3] can plastically deform at room temperature ($T$) or lower. It was recently realized that the low-$T$ plasticity mechanism in the above materials could be very different from that at high $T$, because a shoulder appears in the measured temperature variation of the critical resolved shear stress $\tau_c$.[2] This poses additional question in the so-called glide-shuffle controversy[4] in these crystals, which possess two types of (111) planes for inelastic shear, widely separated shuffle set (blue in Fig. 1) and compact glide set (red). Historically, it was believed that the shuffle-set planes were favored for slip because only one bond needs to be cut as dislocations move through, in contrast to breaking three bonds across the glide-set planes, until transmission electron microscopy (TEM) revealed that specimen deformed at high-$T$ contains plenty of dissociated partial dislocations,[5,6] which can only exist on the glide-set plane.[7] Density functional theory (DFT) calculations[8] indicated that the shuffle-set dislocations indeed should have lower Peierls stress, but the glide-set dislocations have lower core energy[9] after dissociation and also smaller double-kink formation energies at low stresses.[4] The new TEM observations[1,2] show that at *low T*, long undissociated screw dislocations appear, which cross slip frequently. Suzuki *et al.*[2] and Koizumi *et al.*[10] proposed that these may be shuffle-set screw dislocations, centered at A and B in Fig. 1. Pizzagalli and Beauchamp then performed DFT calculations to show that the A core [Fig. 2(a)] has lower energy[11] than B, as well as C, which is a glide-set full screw dislocation.

In this letter, we show that based on extensive tight-binding (TB) and DFT calculations, the C core has lower energy than A after period-doubling reconstruction. This double-period C core structure is shown in Fig. 2(b). Since C can cross slip between two *glide-set* planes, it satisfies all the experimental observations to date. We believe that the C configuration, previously unstudied, may also play important transient roles in partial dislocation constriction and cross slip at high $T$, and perhaps ductile-to-brittle transition.[12]

The TB calculations were performed using the environment-dependent potential[13] that has been previously applied to study surface reconstruction and diffusion, and cluster geometries in silicon. One can easily model several thousand atoms with TB, which makes it a very powerful tool for scoping out possible low-energy configurations, that can be later verified by DFT.[14] We use the Vienna *ab initio* simulation package[15] (VASP) for DFT calculations, under the Perdew-Wang generalized gradient approximation[16] with ultrasoft pseudopotential.[17] The supercell we use in the DFT

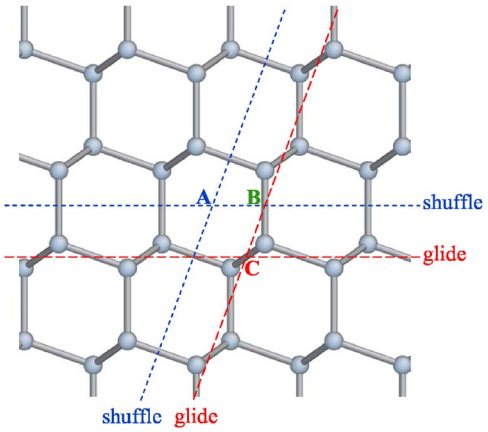


FIG. 1. Slip planes in Si and likely centers of undissociated screw dislocations.

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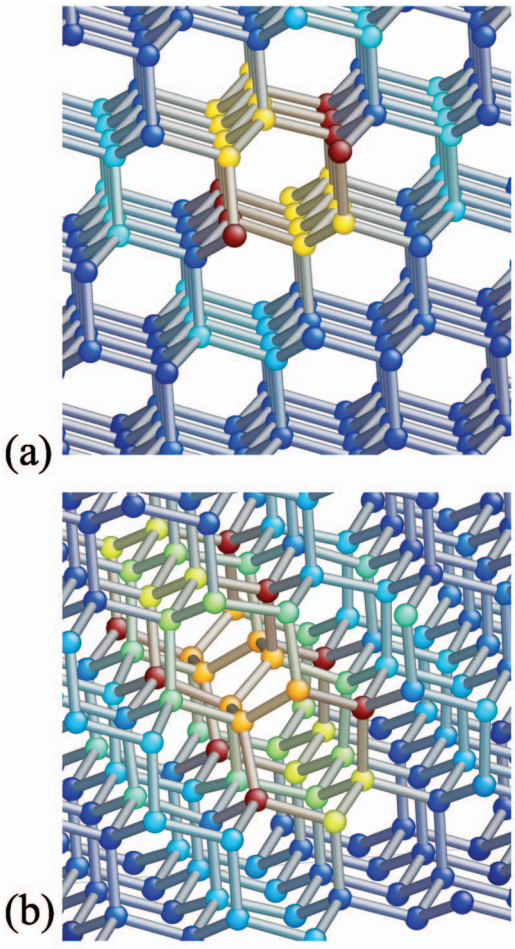


FIG. 2. (Color) DFT optimized (a) A core and (b) period-doubled C core configurations. The color of atoms represents the local atomic shear strain. (Ref. 23).

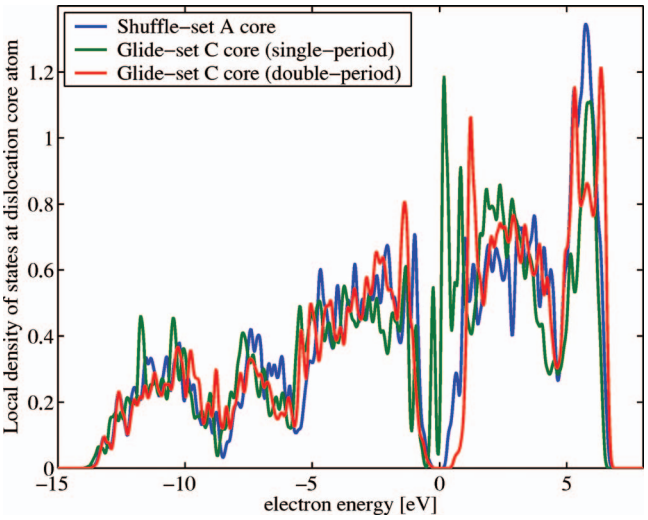


FIG. 3. (Color) Local electronic density of states inside A core, single-period and reconstructed C cores from TB calculations. The Fermi energy is at 0.

calculations is oblique, containing a screw dislocation dipole.[9] The most basic setup for the DFT calculations contains $12\times6\times4=288$ atoms, which has two unit cells in the Burgers vector direction. The **k**-point sampling is $1\times1\times8$ in such calculations, and the kinetic energy cutoff is 245 eV. Comparison of equilibrium properties with experiment is shown in Table I.

The single-period C core has a semimetallic chain of dangling bonds which introduces electronic states near the Fermi level, as one can see from Fig. 3 where local electronic density of states inside the dislocation cores is plotted. This chain of dangling bonds is susceptible to Peierls distortion,[18,19] leading to a period-doubling reconstruction along the chain [Fig. 2(b)] that opens up a wide band gap (Fig. 3).[20] We find that after the period-doubling reconstruction, the C core energy is lower than A by 0.16 eV/Å in TB and 0.14 eV/Å in DFT. In large-supercell TB calculations, we tried but did not find any longer-period reconstructions of C. We also looked for reconstructions of A [Fig. 1(a)] and B cores without success. The single-period A and B configurations appear to be the energy minima at the respective centers. The $(111)\langle1\bar{1}0\rangle$ Peierls stress for reconstructed C core is found to be ~6 GPa in DFT, in contrast to ~4 GPa for the A core.[11] Both are larger than the experimental $\tau_c(0\ \mathrm{K})$, estimated to be around $0.05G$ for III–V compounds and Si,[10] where $G$ is the $(111)\langle1\bar{1}0\rangle$ resolved shear modulus (61 GPa for Si). We make a general note that the Peierls stress calculated theoretically for long straight screws always exceeds the measured $\tau_c(0\ \mathrm{K})$ or $\tau_c(T)$ extrapolated to 0 K, in the case of bcc Mo, by a factor of 2 or more.[9] We attribute this to the explanation[21] that double kinks are not likely to be nucleated "homogeneously" on an infinite straight screw dislocation, but heterogeneously, such as near dislocation junctions, grain boundaries, and surfaces.

Core reconstruction is thus an important, if not decisive factor in the competition between glide and shuffle-set slips. Geometrically it appears that while the sparse bond density on the shuffle-set plane leads to lower Peierls stress, it also hinders possible core reconstruction which is favored at high bond density. So there is a systematic core energy[9] advantage to glide-set dislocations, irrespective of partial[20] or full dislocations. This reconstruction energy advantage may pertain to kink processes as well.

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TABLE I. Comparison of equilibrium properties of Si using the tight-binding potential (Ref. 13) and DFT with experiment. Ref. 22. [$a_0$: equilibrium lattice constant, $C_{11}$, $C_{12}$, $C_{44}$: cubic elastic constants, $G$: $(111)\langle\bar{1}10\rangle$ resolved shear modulus, and $K_s$: screw dislocation energy prefactor (Ref. 9)].

| | $a_0$ (Å) | $C_{11}$ (GPa) | $C_{12}$ (GPa) | $C_{44}$ (GPa) | $G$ (GPa) | $K_s$ (GPa) |
|---|---|---|---|---|---|---|
| Expt. | 5.432 | 167 | 65 | 81 | 61 | 64.27 |
| TB | 5.45 | 156.2 | 56.9 | 71.6 | 56.97 | 59.62 |
| DFT | 5.46 | 158.8 | 52.6 | 78.4 | 61.53 | 64.52 |

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