

4H-SiC Screw Dislocations and Their Electronic Structures

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Abstract

Geometrical and electronic structures of several kinds of threading screw dislocations (TSDs) in 4H-SiC have been obtained with using first-principles calculations on massively parallel computers. The results suggest that a non-nanopipe TSD can coexist with other TSDs that have relatively smaller radius nanopipes. All the TSDs that we have examined have been found to have energy gaps of 0.4-0.6 eV.

1. Introduction

SiC is a wide-bandgap semiconductor material applicable to power devices which are used under higher voltages. SiC is known to have many kinds of polytypes, which have different stacking sequence with a same structure element. Above all, the 4H type has attracted quite much attention. The SiC substrate is known to have several kinds of defects, while the effects of those defects on device performances are not determined yet. Dislocations, e.g., threading screw dislocations, are also important defects. Harmful defects should be reduced as much as possible, but details of each kind of defects are not known. We focus here on TSD, which is one of the representative dislocations. To analyze the structures and the electronic states of TSDs, we performed the first-principles calculations.

2. Computational Method and Calculation Models

For the calculations, we used the PHASE code, which has been developed and tuned for massively parallel computers by IIS, Univ. of Tokyo and NIMS. PHASE is based on the density functional theory and the pseudopotential schemes with a planewave basis set for expanding wavefunctions and charge densities. The cut-off energy for the planewave basis set is 16 or 25 Rydberg and LDA is used for the exchange-correlation terms.

We have prepared the models in each of which two anti-parallel screw dislocations with their burger's vectors being $[0001]$ and $[000\bar{1}]$ are arranged in a checkered pattern to fulfill the periodic boundary condition. Unitcells of our

TSDs are expressed as $(n\vec{a}, n\vec{a}/4 + n\vec{b}/2 + \vec{c}/2, \vec{c})$, where n is an integer and $\vec{a}$, $\vec{b}$ and $\vec{c}$ are unit cell vectors for 4H-SiC. Atoms around the dislocations are removed in cylindrical shapes as shown in Fig. 1 or not removed. The radii of the cylinders (r_c) are varied from 0.05 to 0.95 nm (Fig. 2). Two-fold coordinated atoms are completely removed from the inner walls of the nanopipes, i.e. the cylindrical shape holes. To see the interactions between TSDs, the unitcell size is varied from $n=16$ to 56. The number of atoms in the unitcell is $4n^2$, if the holes are not removed.

3. Results and Discussions

Non-nanopipe TSDs form Si-Si bonds after geometry optimization (Fig. 3). In smaller unitcells of $n=16$ and 24, the smallest nanopipes changed to cracks (Fig. 4). In the other nanopipe TSDs, surface atoms on the inner nanopipe walls keep three-fold coordinated states (Fig. 5). Fig. 6 shows the formation energies per one TSD for all the TSDs. Formation energies are almost the same for any size of nanopipes except for those changed to cracks. This suggests that TSDs without nanopipe and those with small-radii nanopipes can coexist.

All the TSDs examined here have an energy band gap of 0.4~0.6 eV, as shown in Fig. 7, in spite of the strong stress around TSDs. This is because those stresses were released due to the reconstruction of the bondings around TSDs. As a result, around TSDs, Si-Si bondings and C-C bondings exist along with normal Si-C bondings.

The energy gap of TSDs may come from its surfaces. The inner surface of the nanopipes consists of $[11\bar{2}0]$ and $[1\bar{1}00]$ surfaces, as shown in Fig. 2. Table 1 shows the surface energies and energy gaps of those surfaces. Smaller energy gaps of TSDs than the surfaces may come from the strained surfaces of TSDs.

4. Conclusions

We examined the geometries and electronic structures of TSDs with various sizes of nanopipes and found that they can coexist and have an energy gap of about 0.5 eV.

Acknowledgements

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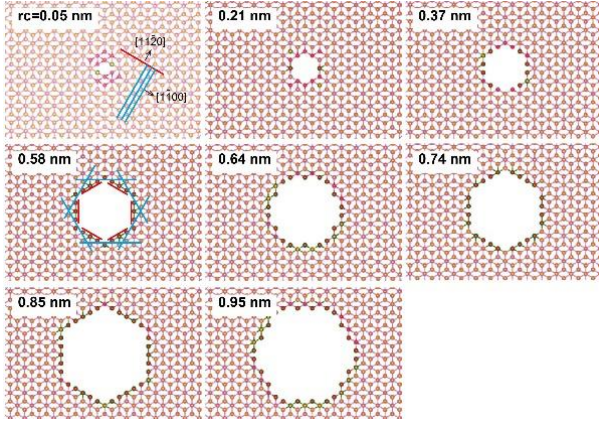


Fig. 2 The (0001) cross-sections of the nanopipe TSDs. Three-fold coordinated Si and C atoms are colored in red and green.

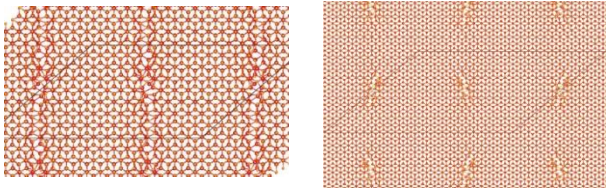


Fig. 4 Cracks changed from nanopipe TSDs in smaller unitcells, $n=16$ (left) and 24 (right).

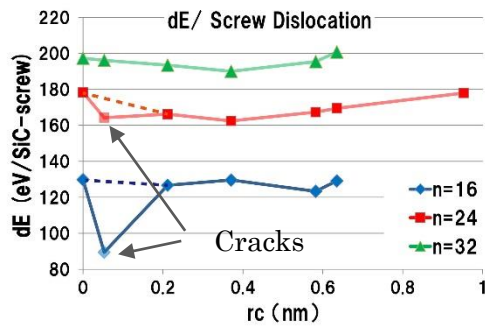


Fig. 6 Formation energies of TSDs.

Table 1 Surface energies and energy band gaps of 4H-SiC surfaces.

Surface	Surface energy (eV/Angstrom ²)	Energy gap (eV)
[11 $\bar{2}$ 0]	0.190	1.0
[11 $\bar{1}$ 0]	0.201	0.8

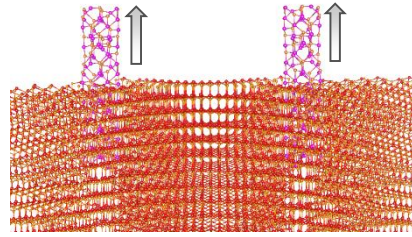


Fig. 1 Two cylindrical shape holes are remove.

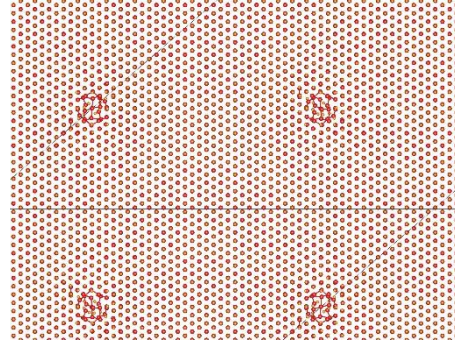


Fig. 3 Geometry optimized non-nanopipe TSDs. Si-Si bonds are connected.

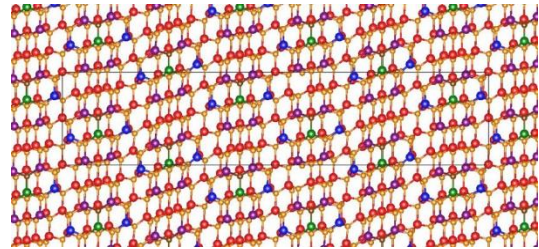


Fig. 5 An inner wall panorama of a nanopipe of the TSD ($rc=0.63$ nm). The most inner Si atoms are green, and the second ones are blue.

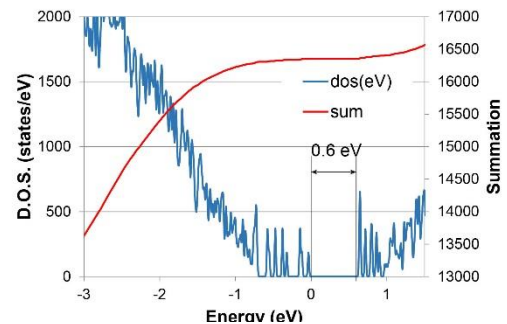


Fig. 7 Density of states of the TSD, in which $rc=0.05$ nm and $n=32$.