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Structural and electronic properties of 90° dislocations in silicon nanorods: A first-principles calculation☆

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ABSTRACT

Dislocation as a topological line defect plays a key role in electronic devices made of crystalline silicon (Si). In this work, using the first-principles calculations we have systematically investigated the atomic structures and electronic properties of 90° dislocation in Si nanorods, including the cases of glide and shuffle perfect dislocations, as well as single-period and double-period reconstruction partial dislocations. Our results show that the dislocations strongly influence the valence and conduction bands near the Fermi level, inducing a narrower band gap. Especially for glide and double-period reconstruction dislocations, the transition from indirect gap of bulk Si to direct gap is achieved. The analysis of the band structures and partial charges reveals the existence of defect levels in the band gap. More interestingly, the defect level of shuffle dislocation crosses the Fermi level, resulting in one-dimensional metallic chain along the dislocation line, which can be related to experimental observations.

1. Introduction

As a topological line defect, dislocation in semiconductor silicon (Si) can act as recombination centers for charge carriers in Si-based electronic devices. The performance and reliability of them can be strongly influenced by dislocations. Si has a covalently bonded diamond cubic lattice corresponding to two interpenetrating fcc lattices, one of which is displaced by $\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right)$ with respect to other. The primitive-unit-cell vectors is $1/2\langle 110\rangle$. Thus, the perfect dislocation Burgers vectors are the same as those in fcc lattice. The perfect $1/2\langle 110\rangle$ dislocations can lie on narrowly and widely separated $\{111\}$ planes, respectively. These dislocations are named as glide and shuffle dislocations, respectively, by Hirth and Schockley [1,2]. In contrast with glide dislocation, there are dangling bonds approximately normal to $\{111\}$ planes in the core region of shuffle dislocations [3,4].

Theoretical investigations of dislocation in semiconductors Si were begun by Hornstra who modelled the perfect 60° shuffle dislocation [5]. Ray and Cockayne investigate the dissociation of glide dislocations in silicon using the weak-beam method of electron microscopy [6]. Furthermore, $1/2\langle 110\rangle$ glide dislocations were found to be dissociated into two Schockley partial dislocaions connected by an intrinsic stacking fault (ISF) to lower formation energy [7]:

$$1/2\langle 110\rangle \rightarrow 1/6\langle 211\rangle + \mathrm{ISF} + 1/6\langle 12\bar{1}\rangle. \quad (1)$$

The distance between the two partial dislocations is 75 ± 6 Å for edge dislocations and 41 ± 6 Å for screw dislocations, respectively [6]. Joos et al. firstly determined the core structure and the mobility of dislocations in Si using the Peierls-Nabarro model [8–10]. However, the reconstruction of the dislocation core is not taken into account. Tight binding and classical Keating-model calculations indicate that single period (SP) and double period (DP) reconstructions of 90° dislocations can lower the energy of symmetric partial core structure [11–13]. Moreover, the full reconstruction is also supported by the low density of dangling bonds obtained by electron paramagnetic resonance (EPR) measurements.

Based on the reconstructed dislocation core, the segregations of As and Fe to the dislocation cores in Si are studied using first-principles methods [14,15]. In order to cancel the long-range stress and strain fields of the individual partial dislocations, the supercell contains a dislocation dipole of partial dislocations. Kveder et al. presented a model to describe the recombination of minority carries at decorated dislocations with transition metal impurities in Si [16–18]. Bigger et al. shown that SP dislocation has a lower energy than the unrelax configuration that can be directly attributed to the electronic structures of the dislocations with only shallow electronic states [19]. The structures and

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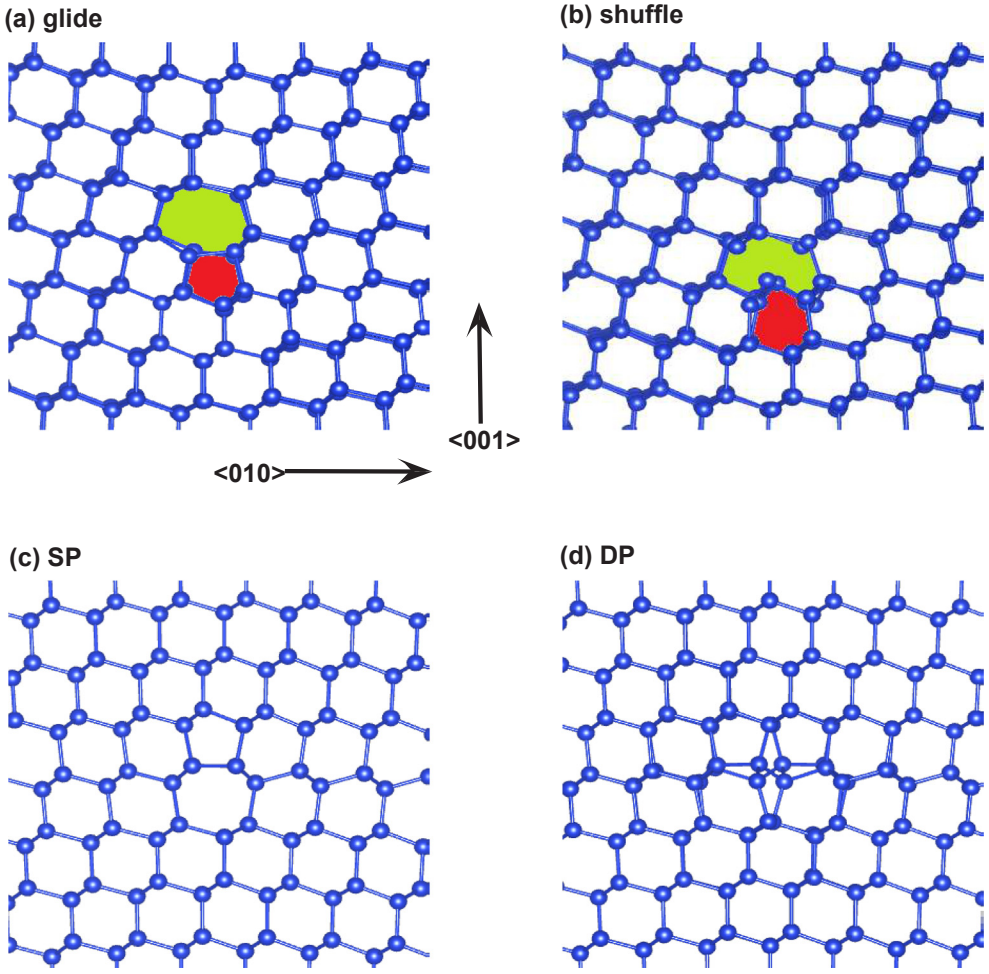

Fig. 1. The core structures of 90° (a) glide, (b) shuffle, (c) SP, (d) DP dislocations.

energies of formation of antiphase defects on the SP partial dislocation have been studied by Valladares et al. and the antiphase defects are associated with states in the gap [20–22]. The reconstructed atomic structure of the 90° partial dislocations in GaAs was investigated by Park [23,24]. The defect states of the SP and DP in GaAs are mid-gap and shallow, respectively [23,24]. The atomic and electronic structures of 60° perfect dislocations in CdTe is also investigated by Kweon et al. [25]. Therefore dislocations in Si, although studied since many years, are still subjects of strong interests. Especially, that the behavior of electrons is affected by the long-range stain fields of dislocation plays an important role in designing the semiconductor devices made of Si. However, their electronic states are far to be completely understood. In this paper, we carry out first-principles calculations to mainly focus on the structural and electronic properties of 90° glide and shuffle perfect dislocations, and SP and DP partial dislocations in Si. Our results for electronic band structures and partial charges show that the dislocations in Si strongly influence the carriers in valence and conduction bands near the Fermi level, giving rise to abundant physics which can be observed in related experiments. Our theoretical study would be important for various applications in the design of Si-based devices.

2. Computational method

We perform the first-principles calculations using the Vienna ab initio Simulation Package (VASP) based density functional theory [26–28]. The core-valence interactions are treated by the projector augmented wave (PAW) pseudopotentials [29,30]. The exchange-correlation potential is chosen as generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) formalism [31]. A plane-wave-basis set with kinetic-energy cutoff of 400 eV has been used. The full Brillouin zone(BZ) is sampled by $15 \times 15 \times 15$ Monkhorst-Pack grid in self-consistent calculations of bulk Silicon. Atom positions were relaxed until the remaining forces acting on the atoms were less than 10^{-2} eV/Å. Considering the periodic features along the line of dislocation, we construct nanorods to simulate the isolated dislocation in bulk silicon using periodic boundary conditions within a supercell approach. The long-range elastic stress and strain fields of dislocations make it challenging to simulate dislocations using small periodic supercells, which are treatable by electronic structure calculations. A rectangular supercell with a single dislocation with Burgers vectors perpendicular to dislocation line is a suitable atomic representation for such a dislocation profile. We use supercells containing 360 Si atoms for glide dislocation and 358 Si atoms for shuffle dislocation, which are found to be sufficiently large to obtain the correct configurations dislocation core. It is known that dislocation cores can undergo reconstructions along the dislocation line. For the partial 90° dislocation, there exist at least two different core configurations, such as the SP and the DP reconstruction. We still employ nanorodes to simulate the reconstructed dislocation, and the supercells with 216 and 432 Si atoms are used for SP and DP reconstruction, respectively. For nonperiodic