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Atomic simulation of the dynamic properties for a double period structure with 90° partial dislocation in Si

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ABSTRACT

The dynamic properties of a double period (DP) structure with a 90° partial dislocation were investigated by atomic simulation methods in Si. By the use of molecular dynamics (MD) method, the motion sequences of kinks and reconstruction defect (RD) of DP structure were obtained. Based on the conjugate gradients (CG) results and tight-binding (TB) potential, the formation energies E_f of kinks were computed. In addition, the migration barriers W_m of kinks were also calculated via nudged elastic band (NEB) method with TB potential. The results show that E_f is smaller than W_m, which means that the migration barrier of kink dominates the motion of DP structure. According to the activation energies of short dislocation segments (2.17 eV) and long dislocation segments (1.61 eV), we predict that the experimental results may be between these two values.

1. Introduction

It is well known that 90° partial dislocation is one of the most important dislocations in Si. It is not only related to the plastic deformation behavior, but also concerned with the electronic and optical properties of micro-electro devices [1,2]. In Si, this dislocation orientates along ⟨1 1 0⟩ direction and glides in the {1 1 1} plane. The unreconstructed core of 90° partial dislocation has higher energy and dangling bonds. To lower the energy and eliminate the dangling bonds, it reconstructs by breaking the mirror symmetry normal to the dislocation line, enabling threefold-coordinated atoms to bond and form the fourfold coordinated stable structure [3,4]. In this way, two different reconstructions

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and the reconstruction defect (RD) exist in the core. The RD is also known as soliton [5] or antiphase defect (APD). One of the traditionally accepted structure is the single period (SP) reconstruction, which retains the same periodicity $b = 1/2\langle 1\ 1\ 0\rangle$ as the crystal lattice [3,4]. Many works have been done about the mobility of 90° partial dislocation, by calculating the formation energy E_f and migration barrier W_m of kinks in SP structure [2,6–9]. Moreover, the dynamic properties of RD in SP structure (SP-RD) have also been explored, which shows that RD can migrate rapidly along the dislocation line and acts as nucleation centers for double kinks [10,11]. Recently, Bennetto et al. discovered a new double-period (DP) reconstruction and demonstrated the corresponding atomic structure of kinks [12]. To distinguish these defects from SP structure, we simply denote the left kink and right kink of DP structure as DP-LK and DP-RK, respectively. This new structure is found to be lower in energy than SP structure regardless of whether the empirical interatomic potential, tight-binding or density-functional theory (DFT) was used [12]. This structure retains fourfold coordination for every atom and can be derived from the SP structure by inserting alternating kinks. Although both of them are fully reconstructed, the DP structure is preferred because it is able to reduce the local bond strains near the core [13]. In addition, Valladares et al. considered the free energies of the SP and DP structure, which found that the core structure of 90° partial dislocation is dominated by the DP reconstruction at all temperatures up to the melting point of Si [14]. However, up to now, the studies of the mobility of 90° partial dislocation have only been concerned with the SP structure [2,6–9]. For the dynamic properties of DP structure, little work has been done.

According to the model of Hirth–Lothe, the migration of dislocation occurs by nucleation and migration of kinks and is controlled by the activation energy Q [15]. Thus, the activation energy Q of DP structure is composed of the kink formation energy E_f and migration barrier W_m [15]. For long dislocation segments

$$Q = E_f + W_m \tag{1}$$

For short dislocation segments

$$Q = 2E_f + W_m \tag{2}$$

In this work, the atomic simulation methods are adopted to study the dynamic properties of DP structure. First, the molecular dynamics (MD) method is employed to explore migration processes of kinks and RD in this structure. Furthermore, we compute the formation energies E_f of kinks. The migration barrier W_m is obtained by using the climbing image nudged elastic band (NEB) [16] method. Finally, the activation energies of long and short dislocation segments are calculated.

2. Computational methods and models

A comprehensive study of dislocation kink structure and dynamics would require the use of very large models, for which hardly can be handled by DFT method. Although the MD method together with empirical potential can deal with tens of thousands of atoms for a long time period, the accuracy of energy calculation is still questionable in view of thermal fluctuation and potential reasons. Thus, the MD method was just used to explore the migration processes of kinks and RD of DP structure. In addition, the environment-dependent interatomic potential (EDIP) [17], which can be used to describe both 90° partial dislocation and 30° partial dislocation [18], was chosen in the calculations. To ensure the accuracy of energy results, the tight-binding (TB) [19] was adopted in the energy (E_f and W_m) calculations.

The simulations were performed under the NPT ensemble and the time step is 1 fs. Moreover, the periodic boundary conditions (PBC) were applied in the three directions of the model. Before each calculation, positions of all atoms were initially relaxed by the conjugate gradients (CG) algorithm until the force acting on each atom was less than 0.01 eV/Å.

In order to use the PBC in the calculations, two DP structure with opposite Burger vectors was introduced in a model. The sketch view of the straight DP structure, DP-LK and DP-RK dipole models in the (1 1 1) plane are shown in Fig. 1. It can be seen that the appearances of kinks do not change the stacking fault area among the dislocations. In MD simulations, the three vectors of DP-LK and DP-RK