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Microscopic structure of the 90° and 30° partial dislocations in gallium arsenide

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Abstract

We performed a theoretical investigation on the atomic structure of {111} glide partial dislocations in gallium arsenide. The calculations were carried out using *ab initio* total energy methods, based on the density functional theory and the pseudopotential model. We addressed the microscopic structure of the 90° partial and the 30° partial dislocations. Our results show that the atomic configurations of the dislocation cores are similar to those proposed for the same dislocations in non-polar semiconductors. For the 90° partial, the double-period reconstruction is energetically more favourable than the single-period reconstruction. In addition, we computed the interaction of intrinsic defects with the dislocation cores.

1. Introduction

The mechanical properties of materials are generally controlled by the motion of dislocations [1]. Microscopic events, which happen inside the narrow region of the dislocation cores, determine the energetics of dislocation formation and their motion mechanisms, and can be directly correlated with a number of macroscopic properties [2, 3]. In zinc-blende semiconductors, perfect (60° and screw) dislocations move on the {111} planes, lying along ⟨110⟩ directions. These perfect dislocations generally belong to the glide planes and are dissociated into 30° and 9° partials. There has been a great effort, both theoretical [4–10] and experimental [11–13], to identify the core structure of these dislocations in semiconductors.

It is energetically favourable for perfect dislocations to dissociate into partials, with a stacking-fault ribbon forming between the two partials. In a III–V compound, such as gallium arsenide (GaAs), dissociation may generate three types of dislocation: an α dislocation, consisting of a 90° partial plus a 30° partial with the cores formed by column-V atoms; a β dislocation, consisting of a 90° partial plus a 30° partial with the cores formed by column-III

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atoms; and a dissociated screw dislocation, consisting of two 30° partials, one of each type. Obviously, the α/β distinction would not be present for a non-polar semiconductor. In their unreconstructed state, the dislocation cores contain dangling bonds as a result of the atomic deformations which generate the dislocations. In this scenario, core reconstruction (or bonding between atoms at the dislocation core) emerges naturally as a mechanism by which most of these dangling bonds can be eliminated. Core reconstruction should be energetically favourable in covalent materials, since the energy gain due to the pairing of the dangling orbitals is larger than the bond distortion energy in going from an unreconstructed configuration to a reconstructed one. The experimental data are consistent with the occurrence of core reconstruction, as evidenced by the fact that semiconducting materials have low concentrations of dislocation-related electrically active centres.

Here, we present a theoretical investigation on the structural properties of 90° and 30° partial dislocations in GaAs using *ab initio* total energy methods. We find that the stable core structures of both partials in GaAs are consistent with the configurations already identified in Si [4, 6, 10]. However, core reconstruction energies tend to be smaller in GaAs than in silicon (Si), as a result of bond ionicity. For the case of the 30° partial dislocation, we also investigated the electrically active centres resulting from unreconstructed sites in the dislocation core, with our results indicating that the formation energies of these centres in GaAs are lower than in Si. These results suggest the possibility of a higher concentration of electrically active centres in GaAs than in Si. Finally, we investigated the interaction of the intrinsic antisite defect As_{Ga} (EL2 centre) with the core of partial dislocations in GaAs. Our results show a strong segregation effect, with the As_{Ga} lowering its formation energy by about 1 eV at both reconstructed and unreconstructed sites of a β dislocation in GaAs.

2. Theoretical model

For the dislocation configurations considered in this investigation, simulations based on *ab initio* methods are computationally expensive. In order to perform such calculations, we devised a two-step procedure in which an initial relaxation of the atomic configurations was based on a classical potential [14, 15], and only a final relaxation was based on *ab initio* methods. In the initial relaxation step, the shape of the supercell was adjusted using the Parrinello–Rahman method [16], which reduces considerably the internal stresses generated by the dislocations. The output configurations were used as input to the final relaxation step in an *ab initio* procedure, based on the Hellmann–Feynman forces. The *ab initio* calculations [17] were performed in the density functional theory within the local density approximation framework. The Kohn–Sham equations were solved by the Car–Parrinello scheme with norm-conserving pseudopotentials [18]. The wavefunctions of the valence electrons were expanded in a plane-wave basis set, with a kinetic energy cut-off of ∼300 eV. The Brillouin zone was sampled by a set of two k-points along the dislocation direction [19]. This choice is justified by our previous experience with dislocation calculations using the cell geometries employed in this work [9, 10], and by the observation that the electronic charge distribution of the dislocation-related gap levels is delocalized only along the dislocation line. Geometric optimization of all the atomic structures was performed, allowing atoms to relax until the forces were smaller than 0.02 eV $Å^{-1}$.

We considered orthorhombic supercells, in which a dislocation dipole was introduced. This dipole consisted necessarily of an α and a β dislocation for both the 90° and the 30° partials. The dislocations in the cells were ∼13.4 Å apart, which is enough to prevent the core–core interaction. For most calculations, the supercells contained 192 atoms but, as discussed below, larger 288-atom cells were used in some calculations. The dimensions of these cells

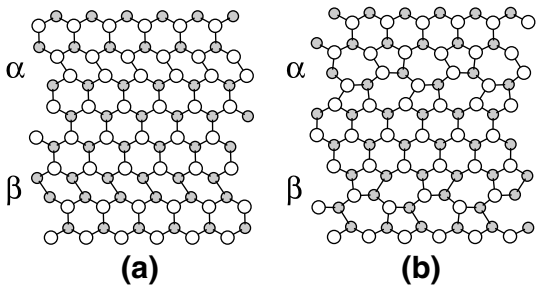

Figure 1. The atomic configuration in a {111} glide plane, with a 90° partial dislocation dipole (comprising an α and a β dislocation) lying along a ⟨110⟩ direction. The figure shows the core structures with (a) SP reconstruction and (b) DP reconstruction. Large and small circles represent atoms in the top (type V atoms) and in the bottom (type III atoms) of the glide plane, respectively. The figure only shows the intra-plane glide bonds.

are as follows: 9.7 Å in the {111} direction (corresponding to six double layers in the (111) stacking direction) and 26.8 Å in the $(11\bar{2})$ direction in the glide plane for all cells, and 15.6 Å (23.5 Å) along the $(1\bar{1}0)$ dislocation direction for the 192-atom (288-atom) cells.

3. Results

3.1. The 90° *partial dislocation*

Previous theoretical investigations have considered the core structure of a 90° partial dislocation in Si and in other non-polar semiconductors [4, 6, 7]. Figure 1 shows the two suggested configurations for the dislocation core of a 90° partial. For Si, a symmetry-breaking reconstruction of the core was initially proposed [4]. This has been commonly called the single-period (SP) reconstruction (figure 1(a)). More recently, a double-period (DP) reconstruction has been found to be energetically more favourable by as much as 70 meV $Å^{-1}$ than the SP one (figure 1(b)) [6]. This DP reconstruction is also energetically favourable for carbon and germanium [7]. In the case of GaAs, the core reconstruction is more complex, because there are two distinct dislocations (α and β) for which core reconstruction involves intra-core bonding which will generate As–As or Ga–Ga bonds.

Comparing the total energy of a configuration in which both (α and β) 90° dislocations have an SP reconstruction with the energy of a configuration in which both dislocations have a DP reconstruction, we found that the DP is favourable by 18 meV $Å^{-1}$. It is surprising that both the α core, full of As–As bonds, and the β core, full of Ga–Ga bonds, have the same stable configuration as the dislocation core in a non-polar semiconductor. However, the small energy difference between DP and SP reconstructions suggests that both configurations may be important for dislocation motion [20].

Bond lengths in a dislocation core with SP reconstruction ranged from 2.33 to 2.81 Å in the α dislocation and from 2.35 to 2.55 Å in the β dislocation. These values should be compared with the theoretical bond-length value of 2.40 Å for bulk GaAs. Still for the SP core, the bond-angle distribution for an α dislocation ranged from 83° to 145°, while the range was from 89° to 141° for the β dislocation. Therefore, the SP reconstruction leads to a wide distribution of bond angles and bond lengths in the core, in GaAs. The situation is very different for the DP reconstruction, where such distributions are much narrower. Bond lengths in a dislocation with DP reconstruction ranged from 2.34 to 2.64 Å in the α dislocation and from 2.34 to 2.50 Å in the β dislocation. Bond angles varied between 90° and 126° in the case of α dislocation and

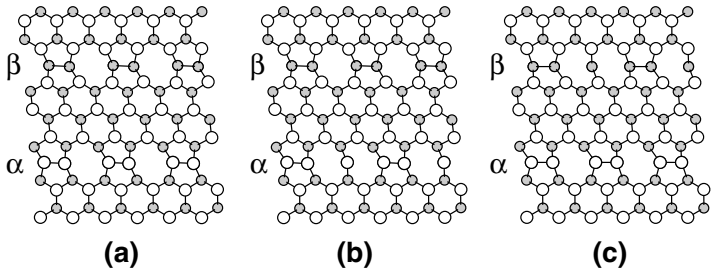

Figure 2. The atomic configuration in a {111} glide plane, with a 30° partial dislocation (α plus β). The figure shows the dislocation (a) with a reconstructed core, (b) with two α APDs and (c) with two β APDs. Large and small circles represent atoms in the top (type V atoms) and in the bottom (type III atoms) of the glide plane, respectively.

between 93° and 125° in the β dislocation. This is to be contrasted with the case of Si, where the average bond-length deviations are larger in the SP core, but with a slightly larger variation of bond angles in the DP core [7]. It appears that in the case of GaAs, a smaller strain energy is associated with both bond-length and bond-angle distortions in the DP core.

3.2. The 30° *partial dislocation*

For the 30° partial dislocation, there is only one known configuration for the reconstructed core. Figure 2 shows a glide plane containing the cores of an α and a β 30° partial dislocation. From our calculations, we found that the core reconstruction energy, or the energy required to break a core bond, is much larger for dislocations in Si than for α or β dislocations in GaAs [21]. While the reconstruction energy is 119 meV Å^{-1} (0.92 eV/reconstructed bond) for a 30° partial dislocation in Si, it is respectively 56 meV Å^{-1} (0.43 eV/reconstructed bond) and 73 meV Å^{-1} (0.56 eV/reconstructed bond) for 30°α and β partials in GaAs. These variations in the reconstruction energies are due to the fact that reconstruction involves bonding between atoms of the same species. As a result, there is an additional electrostatic repulsion between the core atoms in GaAs, which is not strong enough to prevent core reconstruction. Bond lengths inside the dislocation core ranged from 2.34 to 2.57 Å in the α dislocation and from 2.33 to 2.47 Å in the β dislocation. For the bonds in the dislocation core in Si, bond angles ranged from 92° to 124°, with an average of 108.8°. In the case of GaAs, the bond angles in an α dislocation varied between 87° and 125°, while those in a β dislocation varied between 86° and 122°, with average bond angles of 109.1° and 109.0° for α and β dislocations, respectively.

Although reconstruction is favourable, it is still possible that a few of the core atoms remain unreconstructed at finite temperatures (figures 2(b) and (c)). These centres are called antiphase defects (APDs), or reconstruction defects, and may generate electrically active centres in the gap. In a III–V compound, we defined an α APD and a β APD as the reconstruction defects in α and β dislocations, respectively [21]. We now consider the properties of an APD in GaAs as compared to an APD in Si. The APD formation energy is 0.82 eV in Si, while in GaAs formation energies are 0.36 and 0.44 eV for the α APD and the β APD, respectively. Most notably, for both Si and GaAs the APD energy scales with the respective core reconstruction energy, being around 80% of this quantity (when expressed in terms of reconstruction energy per bond). This provides a good agreement with a recent model, which suggested that dislocation activation energies should scale with the dislocation core energies [10]. Moreover, such low formation energies for α and β APDs would indicate that the concentration of electrically active centres should be considerably larger in deformed GaAs than in deformed Si. The bonds in an APD

are different from those in a reconstructed atom. In both Si and GaAs, the three neighbouring atoms of an APD relax inward and form a planar structure, with an average angle of 118°.

An important electrically active centre in crystalline GaAs is the so-called EL2 centre, which is described as an As atom replacing a Ga atom (i.e., an As antisite defect). We now discuss the energetics of this defect when occurring in the core of a 30°β partial dislocation in GaAs. A Ga atom of a β dislocation in a reconstructed configuration is bonded to three As atoms and to one Ga atom. This suggests that it should be energetically more favourable to replace a Ga core atom by an As atom in the dislocation core than in the crystal. To study the stability of this antisite defect in the dislocation core, we compared the total energy of a configuration with the As antisite in a crystalline-like position, the position furthest away from the dislocation inside the simulation cell, with the energy of a configuration with the As inside the core of a β dislocation. We find that there is a gain of 0.90 eV for the antisite defect to sit in a reconstructed configuration and 1.29 eV for the defect to stay in a β APD. Therefore, the concentration of arsenic antisite defects should be considerably larger in the dislocation core than in the crystalline environment.

4. Summary

In summary, we have investigated the structural properties of 90° and 30° dislocations in GaAs. The energies of core reconstruction and APDs were computed and compared to the same quantities in Si. The results indicate that the DP structure is more stable than the SP geometry in GaAs also. Moreover, our calculations suggest that the concentration of APDs in the dislocation cores should be higher in GaAs than in Si. In both materials the formation energy of an intrinsic antiphase defect scales with the respective reconstruction energy, and consequently with the activation energies for dislocation motion [10]. This lends further theoretical support to the idea that all of the energetics, and consequently the concentration of intrinsic defects in the dislocation cores, should follow some universal scaling law which correlates core reconstruction energies of dislocations with their activation energies. Our calculations also indicate that arsenic antisite defects should segregate to the dislocation core of a β dislocation, where their formation energies can be lowered by nearly 1 eV.

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