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First Principles Calculations of As Impurities in the Presence of a 90° Partial Dislocation in Si

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We investigated the interaction of As impurities with a 90° partial dislocation in Si. The calculations show that As atoms segregate to the dislocation core. The most stable site for the As atom is at the stacking fault side, which is favorable by 0.26 eV as compared to an As atom in a crystalline position. There is no charge transfer from the As impurity to the dislocation core when the impurity is far from it. The segregation of the impurity can be understood mainly due to structural effects. This result let us conclude that the experimentally observed negatively charged dislocations are due to impurities trapping at the core of the dislocation and not charge transfer from impurities away from the dislocation.

Keywords: First principles calculations; As impurities; Dislocation in Si

I. INTRODUCTION

Dislocations in semiconductors, in the presence of impurities, have attracted considerable interest, mainly due to their influence on the electronic properties of the material which affect the fabrication and operation of electronic devices. Dislocations can form and move during the device operation being detrimental to device performance. The understanding of the interaction of point defects with dislocations is an important issue for the doping control and to elucidate how defects affect the dislocation velocity [1]. Recently, point-defects migration along dislocation lines have been shown to be responsible for the nanostructural stability of dislocation-mediated surface [2].

Ab initio calculations [3–5] as well as experimental results [1] show that, in general, point defects in group-IV semiconductors as well as in zinc-blende semiconductors segregate to the extended defect region. An exception is verified for Mg doped GaN wurtzite in the presence of a stacking fault, where a first principles calculation showed that the impurity prefers to stay far from the stacking fault plane [6]. The interaction of point defects with dislocations usually have been described either by a local or nonlocal effect [5]. The local effect comes from the segregation of impurities in the dislocation core, and the nonlocal effect comes from the displacement of the Fermi level due to defects [7].

Among the two most important dislocations in Si, 30° and 90° partials, we focus on the latter one. It has been verified that the 90° partial can reconstruct in different periods [8]. In this work, using a first principles calculation we investigate the interaction of substitutional As impurities with a 90° partial dislocation in silicon. We will show that the As impurity at the dislocation core is energetically favorable compared to the As far from the dislocation. This segregation is mainly due to structural effects.

II. THEORETICAL PROCEDURES

Ab initio total energy calculations based on the Density Functional Theory [9] have been used here. For the exchange-correlation potential we used the local density approximation (LDA) with norm-conserving pseudopotential in the Kleinman Bylander form [10, 11]. We used plane wave basis set with energy cutoff up to 150 eV, and the Brillouin zone was sampled using the Γ point. All atoms are allowed to move until all force components are smaller than 0.025 eV/Å.

The total energy has been computed with 384 and 192 atoms in orthorhombic periodic cells, in which a 90° partial dislocation dipole is introduced. This dislocation comes from a dissociated 60° dislocation belonging to $\{111\}$ glide planes, which is present in group-IV and zinc-blende semiconductors. Each supercell contains two dislocations having opposite Burgers vector, with two or four reconstructions along the dislocation lines, depending on the supercell size.

III. RESULTS AND DISCUSSIONS

First, using a 192-atom supercell we compute the total energy of the unreconstructed 90° partial dislocation, then we permit a single period (SP) reconstruction. There are two possibilities for the SP reconstruction because the Burgers vector in the supercell needs to be zero to avoid an infinite elastic strain energy. In Fig. 1-a is showed the atomic arrangement of the SP reconstruction with parallel dislocation dipole (SP_p), while in the Fig. 1-b is the SP with non parallel dislocation dipole (SP_{np}). The energy required to form an unreconstructed 90° partial dislocation is 0.57 eV/Å, and to reconstruct in the SP the formation energy drops to 0.43 eV/Å (this is the average formation energy of the two SP reconstructions). The energy difference between the two SP reconstructions is just 0.05 eV/Å.

Our results show that the dislocation reconstructions shown in Fig. 1 affect the electronic structure, mainly around the

band gap, differently for each reconstruction. The SP_p presents, besides the double occupied state just above the top of the valence band, two empty energy levels at the Middle of the band gap, while in the SP_{np} these two empty states go up, staying in the upper part of the band gap.

We compute the total energy for several positions of an As impurity substitutional at Si sites, as showed in Fig. 2. The most stable position for the As atom is at the dislocation core in the stacking fault side (site 3 in Fig. 2). The energy difference with the As atom at this most stable position compared with the As atom far from the core is -0.26 eV, which is in agreement with previous calculation, -0.33 eV [12]. There is a segregation energy gradient with the approximation of the As to the dislocation core (see Table I).

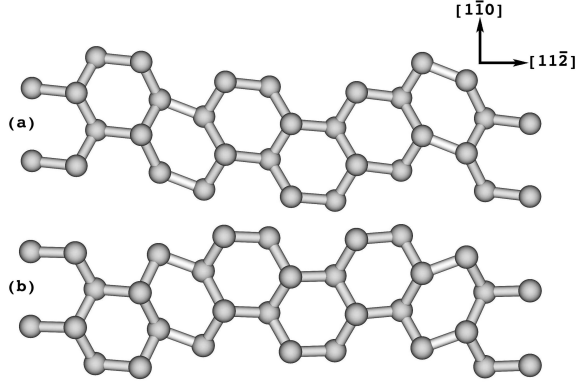


FIG. 1. Top view of the 90° partial dislocation in a ball-and-stick representation. (a) the parallel SP_p reconstruction, and (b) the non parallel SP_{np} reconstruction.

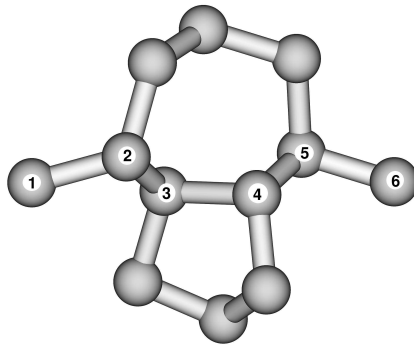


FIG. 2. Atomic positions at the core of the SP dislocation. The labels indicate the sites where an As atom has been substituted.

TABLE I: Segregation energy (eV) for an As substitutional around the SP reconstruction. The labels refers to the atomic sites showed in Fig. 2.

Site	Energy
Out of core	0.00
1	-0.14
2	-0.13
3	-0.26
4	-0.17
5	-0.12
6	-0.02

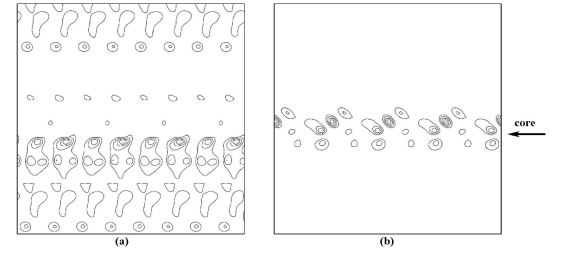


FIG. 3. Charge density of the As defect level: a) with the As atom far from the dislocation core, and b) with the As atom at the core of the dislocation.

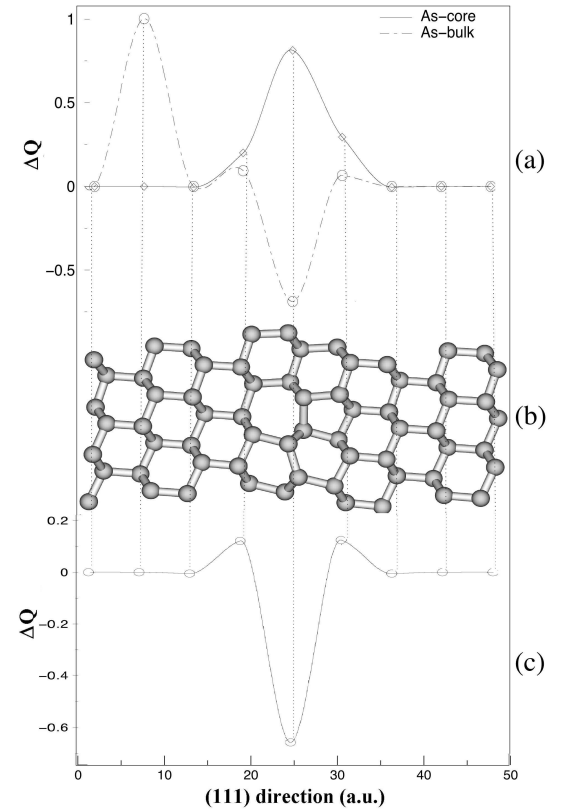


FIG. 4. Total electronic charge density by atomic bilayer along the (111) direction with a) an As impurity in the presence of an b) SP dislocation, and c) is the charge for a pure SP dislocation. Zero charge is for a reference bilayer far from the dislocation core.

The presence of the As impurity at a Si site in a position far from the dislocation core breaks slightly the tetrahedral symmetry. The average bond lengths of the Si first neighbors of the impurity suffer an inward relaxation around 3%. This symmetry breaking is due to the presence of the dislocation dipole in the cell. The average bond lengths of the As impurity in the dislocation core is 2.37 Å, which is at the same order of the bond lengths among the Si atoms located at the dislocation core free of impurity (2.36 Å), and is a little bigger than the crystalline interatomic distances, 2.35 Å. That makes the As atom at the dislocation core more stable than the As far from the dislocation. This results are different compared to that of As impurity in the presence of a 30° partial dislocation in Si [5], where the structural changes does not play an important role on the stability of the impurity.

The substitutional As at a Si site introduces a single occupied donor level in the gap region at 0.06 eV from the bottom of the conduction band. When the As atom is at the most stable position of the dislocation core (position 3 from Fig. 2), the donor level goes down pinning at 0.16 eV inside the band gap. This deeper state present a very localized charge density along the dislocation line, as we can see in Fig. 3-b. However the As atom at a crystalline environment presents typically a shallow donor level charge distribution (Fig. 3-a).

In order to clarify the origin of the stability of the As impurity, if is a result of structural or electronic processes, we investigate the charge transfer mechanism between the impurity and the dislocation core. We sum the total electronic charge density by atomic bilayer along the (111) direction (Fig. 4). First, we observe that the bilayer located between the seven- and four-fold coordinated rings (at the dislocation core), presents a lack of charge density compared to a bilayer far from the dislocation. This is observed for a cell with an As atom far from the dislocation (Fig. 4-a), as well in a cell free

of As atom (Fig. 4-c). Also from this figure we can see that, when the As atom is located three bilayer away from the dislocation core, a net charge around 1.0 of the unit electron charge stay around this bilayer, and the lack of charge at the core of the dislocation still allmost the same as compared to the As free cell (Fig. 4-c). In this way, although there is a lack of charge at the core of the dislocation, there is not charge transfer from the impurity to the dislocation. The charge transferring occurs only when the As impurity is at the first neighbor bilayer (not shown in Fig. 4) or at the core of the dislocation as showed in Fig. 4-a. Therefore when the dislocation is negatively charged, as found in highly doped materials [13], the charge is due to the impurities located at the core of the dislocation and not charge transfer of impurities away from the dislocation.

IV. CONCLUSIONS

In summary our *ab initio* calculations show that As impurities segregate to the 90° partial dislocation in Si. The most stable site for the As atom is at the stacking fault side, which is favorable by 0.26 eV as compared to an As atom in a bulk site position. Differently for that has been observed from As in a 30° partial dislocation in Si [5], our results showed that there is not charge transfer from the As impurity to the dislocation core, and the segregation of the impurity can be understood mainly as structural effects.

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