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The effect of a stacking fault on the electronic properties of dopants in gallium arsenide

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Abstract. We performed a theoretical investigation on the effects of extended defects on the structural and electronic properties of dopant atoms in gallium arsenide. We observed that silicon impurities segregate at GaAs stacking faults. A Si atom at a Ga site in a stacking fault in either a neutral or a negatively charged state is energetically favourable as compared to a Si atom at a Ga site in a crystalline environment by as much as 0.2 eV. Additionally, a substitutional Si impurity in the negative charge state in a stacking fault has a distinct structure as compared to the same impurity in a crystal. The results suggest that the stacking fault may prevent the formation of metastable defects, such as DX centres.

1. Introduction

The interaction of extended defects with impurities in semiconductors has been a subject of great interest recently [1]. Impurities have been observed to segregate at extended defects. This effect, called gettering, shows how extended defects may play an important role in controlling the detrimental effects of impurities on the electronic properties of semiconducting devices. On the other hand, extended defects, under certain conditions, may themselves be detrimental to the electronic properties of semiconductors. Therefore, understanding the properties of extended defects and their interactions with other defects is crucial to developing better semiconducting devices.

Studies on extended defects and their interactions with point defects have been focused on the properties of grain boundaries and dislocations [2, 3]. Although a stacking fault (SF) plays a central role in dislocation mobility, it has not received attention until very recently [4–7]. Geometrically, a SF is an irregularity in the stacking sequence of the material. In zinc-blende semiconductors, the normal sequence in the [111] close-packed direction is ... AaBbCcAaBbCc ..., each letter representing a stacking plane [8]. An intrinsic SF is equivalent to removing a double layer (Bb, for example) and gluing together the remaining pieces of material. An extrinsic SF, on the other hand, is equivalent to adding a double layer.

It has recently been suggested that the interaction of point defects with a SF may affect the electronic properties of semiconductors [6, 7]; for example, impurities have been found to segregate towards a silicon SF [7]. Here we studied the electronic and structural properties of dopants in GaAs in the presence of a SF, using *ab initio* total-energy calculations. Our calculations show that silicon segregates towards a GaAs SF. Additionally, we show that while a negatively charged Si impurity in the crystalline environment can occupy metastable positions,

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working as a trapping mechanism under certain conditions, in the SF the impurity presents a considerably different behaviour. As result, the SF prevents the formation of charge-trapping centres, possibly increasing the concentration of charge carriers in the semiconductor.

2. Method of calculation

The calculations are performed within the density functional theory and the local density approximation framework. The Kohn–Sham equations are solved using the Car–Parrinello scheme [9] with norm-conserving pseudopotentials [10, 11]. The valence electron wave-functions are expanded in a plane-wave basis set, with kinetic energy up to 12 Ryd, and the Brillouin zone is sampled by the Γ point. A reference orthorhombic supercell consisting of 160 atoms (80 Ga and 80 As) is used. This supercell comprised five double atomic layers stacked along the [111] direction (figure 1), simulating an infinite intrinsic SF in the (111) plane [6, 7]. The supercell has the dimensions 13.6 Å × 16.2 Å × 15.8 Å. This supercell may not be large enough to prevent interaction between the defects and their images. However, the same supercell is used in all calculations, which allowed direct comparison of total energies for the defects at different sites of the cell. We emphasize that this procedure has been used by several authors to compute segregation energies in grain boundaries [12] and dislocations [13].

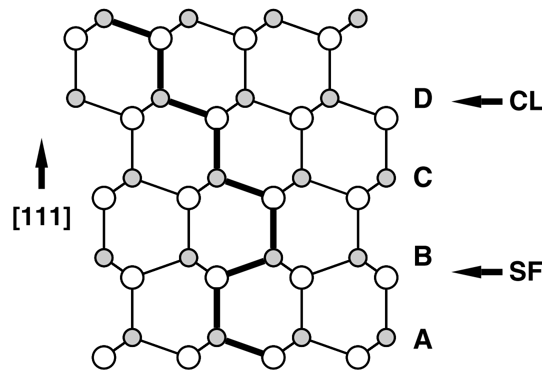

Figure 1. A side view of the orthorhombic supercell consisting of 160 atoms used as a reference cell. The figure shows the $(\bar{1}10)$ plane of a zinc-blende lattice having an intrinsic stacking fault in the (111) glide plane. SF and CL sites represent the stacking fault and the crystalline-like environments.

The optimization of the atomic structure is performed by allowing all atoms to move until the Hellmann–Feynman forces become smaller than 10^{-3} Ryd au^{-1}. The calculations are performed considering each defect in distinct layers in the cell (figure 1). Atoms in the CL layer, which is the layer furthest from the fault, are at distances of 8.1 Å from the fault or from its image. The surrounding environment of an atom at a CL site is that of an atom in a perfect crystal up to the fourth-nearest neighbour. Segregation energy is computed as the difference in total energy between SF and CL configurations.

3. Results and discussion

We have investigated the perturbations caused by a SF in Si-doped GaAs by comparing the microscopic and electronic structure of a Si impurity in a SF and in the crystal. Structurally, the bond lengths of a substitutional Si atom, at the Ga site, to the As first neighbours are practically

the same in the SF and in the perfect crystalline environment. On the other hand, some small changes can be observed in the bond lengths of the second neighbours of the impurity. Even with this apparently small structural change caused by the presence of the SF, our calculations give an energy reduction of 0.12 eV for the Si atom at the SF as compared to that for the CL site. In a crystalline environment, a Si atom at a Ga site introduces a shallow donor level, but at the SF, this level becomes 60 meV deeper in the gap. The results suggest that Si segregation to a SF, and the consequent localization of the respective donor level, could affect the carrier mobility of the semiconductor.

In order to understand the effects of a SF on the conductivity of an n-type doped system, we searched for some defect-trapping mechanism occurring as result of the SF. It is well known that a Si impurity in GaAs can capture electrons from the system, having a metastable behaviour, called DX centres, which can only trap electrons under certain conditions, such as under hydrostatic pressure or near an interface with another alloy [14–16].

The silicon impurity has been introduced at the Ga site in four different layers (A, B, C, and D) as shown in figure 1. Our results show that in the layer furthest from the fault (layer D), the negative charge state for the Si impurity presents a very weak metastability when the Si is moved from the substitutional Ga site in the [111] direction, as shown in figure 2. This trapping mechanism involves a large lattice relaxation and the Si atom can only stay out of the substitutional position, in this case, under large hydrostatic pressure. For the A layer, the metastability is even weaker, and for the C layer, no metastability is observed. For the Si atom at the SF (B layer), a completely different picture is observed. First, a segregation energy of

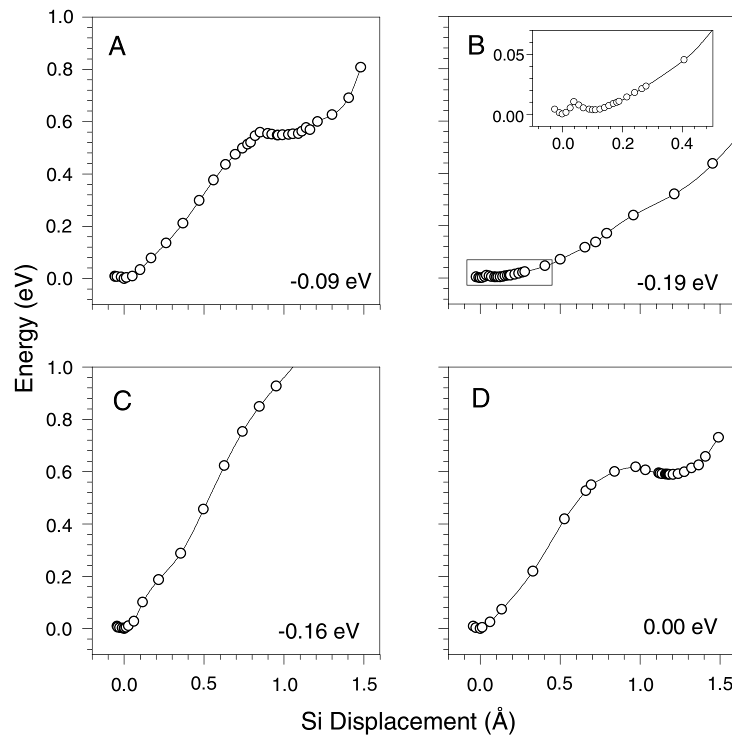

Figure 2. Total energy as a function of the Si_{Ga}^{-}-ion displacement in the [111] direction for the Si at four different layers (A, B, C, and D) as indicated in figure 1. The inset in B shows the energy in the metastable region. At the corner of each picture the segregation energy is shown.

0.19 eV is verified favouring the Si^- ion at the fault. A metastable position for the Si atom is also found, but with a small lattice relaxation. The metastable position is reached with the Si^- ion displaced by only 0.10 Å in the [111] direction from the most stable Ga position (figure 2(b)). This displacement is accompanied by small relaxations of all neighbouring atoms. The Si bond lengths are still practically the same as for the substitutional position (the changes are less than 0.01 Å). Again, for the second-nearest neighbours the relaxations are more pronounced. The Si^- ion, due to the excess electron, has a weak bond with a second-neighbour As atom, as shown in figure 3. In this figure we also observe a localization of the impurity level in the metastable position for the Si^- ion, which can affect the electronic mobility of this n-type material. The donor impurity level of the Si^- ion (in the Ga substitutional position) at the SF is 79 meV deeper than the impurity level of the Si^- ion far from the fault. And for the Si^- ion in the metastable position near the SF, the donor level becomes 93 meV deeper than the level at a crystal-like substitutional position.

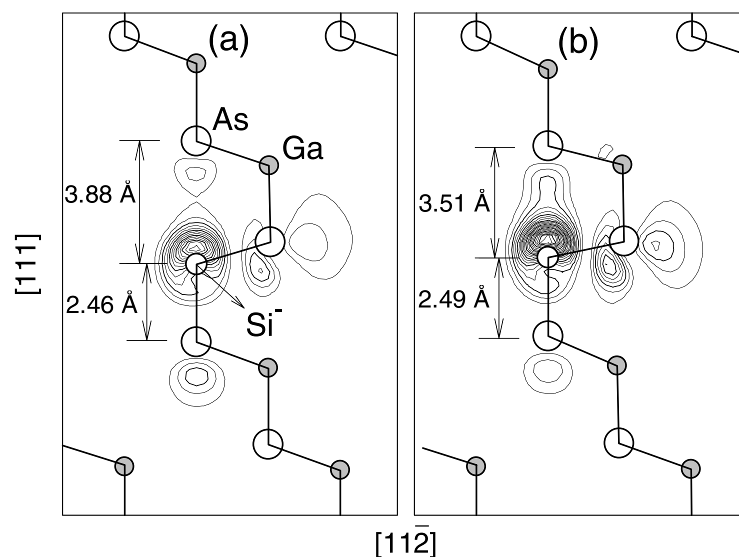

Figure 3. A side view of the electronic charge density of the impurity level of the Si^- ion in (a) the Ga substitutional position and (b) the metastable position.

The results show very distinct behaviours for the Si^- ion in the SF and in the crystalline environment. The most important difference is that in the SF, the ion does not present a metastable configuration as a result of a large lattice relaxation. Therefore, under hydrostatic pressure, the SF may prevent the formation of a DX centre. However, the Si^- ion in the SF could still work as a charge-trapping centre similar to a DX centre. For a certain donor defect to become a charge-trapping centre, it should have a negative Mott–Hubbard potential (U), i.e., it should be energetically favourable for a defect centre to receive an additional electron. The impurity level is a shallow donor for the neutral Si atom in a crystalline substitutional position, having a small but positive value for the Mott–Hubbard potential (as expected due to the presence of many empty states in the conduction band, close to the highest occupied level). For the Si at the SF our calculated value for U, obtained from different charge-state total energies, is very small (0.004 eV). With this vanishing value of U, we could not rule out the possibility that this defect is a charge-trapping centre, although considerably different to the known DX centre.

In summary, we have investigated the interaction of an n-type impurity with a SF in GaAs. The n-type impurity, a Si atom at a Ga site, segregates towards the SF. Therefore, in conditions of thermodynamic equilibrium, the concentration of these extrinsic defects should be larger at the SF than in the crystalline environment. We also observed that the Si impurity in the SF core has a structure considerably different from that of the same defect in the crystalline environment. Since the impurity does not present a metastability (with a large lattice relaxation) near the fault, the stacking fault may serve as a mechanism which prevents the formation of charge-trapping centres.

Acknowledgments

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