Stacking fault effects in pure and *n*-type doped GaAs

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Using *ab initio* total-energy calculations, we investigate the effects of stacking faults on the properties of dopants in pure and *n*-type doped GaAs. We find that the Si impurity segregates towards a GaAs stacking fault. A Si atom at a Ga site in the stacking fault, in either a neutral or a negative charge state, is energetically favorable as compared to a Si atom at a Ga site in a crystalline environment by as much as 0.2 eV. We also find that a Si impurity in the stacking fault cannot occupy metastable positions, as occurs in the formation of *DX* centers. Thus, stacking faults can prevent the formation of *DX*-like centers in GaAs. © *2001 American Institute of Physics.*
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Extended defects are known to affect both the mechanical and electronic properties of semiconducting materials.[1] While dislocations and grain boundaries in semiconductors have been intensively investigated over the last decade, stacking faults have received some attention only more recently.[2–5] This recent interest in stacking faults has been justified by their role in the mechanisms of dislocation motion, being present between {111} dissociated glide dislocations.[6] Geometrically, a stacking fault (SF) is an irregularity in the stacking sequence of the material. In zinc-blende materials, the normal stacking sequence along a $\langle 111 \rangle$ close-packed direction is $\ldots AaBbCcAaBbCc \ldots$, where each letter represents a stacking plane.[7] An intrinsic SF is equivalent to removing a double layer (*Bb*, for example) and gluing together the remaining material. An extrinsic SF, on the other hand, is equivalent to adding a double layer.

Theoretical work on extended defects has focused on the interaction of defects with dislocations.[6,8,9] What is not clear so far is how or whether the interaction of point defects with a SF may affect the mechanical or electronic properties of semiconductors. Impurities have been found to segregate towards a SF in silicon,[5] suggesting that a SF may play an active role in the properties of the material. Here, we used *ab initio* calculations to investigate the electronic and structural properties of pure and Si-doped GaAs in the presence of a SF. 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, working as a trapping center under certain conditions, in the SF the impurity presents a considerably different behavior. As a result, the SF may prevent the formation of *DX*-like trapping centers.

Our calculations were performed within the density functional theory and local density approximation framework. The Kohn–Sham equations were solved using the Car–Parrinello scheme[10] with norm-conserving pseudopotentials.[11,12] The valence electron wave functions were expanded in a plane-wave basis set, with the kinetic energy up to 12 Ry. The Brillouin zone was sampled by the Γ point. An orthorhombic supercell consisting of 160 atoms (80 Ga and 80 As) was used as a reference. This supercell comprised five double atomic layers stacked along the [111] direction, simulating an infinite intrinsic SF in the (111) plane,[4,5] and has the dimensions: $13.6\,\text{Å} \times 16.2\,\text{Å} \times 15.8\,\text{Å}$. This cell may not be large enough to prevent interaction between the defects and their images, especially in the case of shallow-level dopants. However, the same supercell was used in all calculations, which allowed a direct comparison between defects in different cell sites. We emphasize that this procedure has been used by several authors to compute segregation energies in dislocations[13] and grain boundaries.[14] The optimization of the atomic structure was performed by allowing all the atoms to move until the Hellmann–Feynman forces were smaller than 10^{-3} Ry/a.u. The calculations were performed considering each defect in two distinct sites in the cell: a crystal-like (CL) site and a SF site. Atoms at the CL layer are at distances of 8.1 Å from the fault or from its image. The surrounding environment of an atom in a CL site is that of an atom in a perfect crystal up to the fourth nearest neighbor. Segregation energy was computed by the total-energy difference between configurations with the impurity in the SF and CL layers.

A SF introduces perturbations in the electronic energy levels of GaAs, which are more pronounced at the valence-band maximum (VBM) states. These perturbations split the VBM in two levels, a doubly degenerated *e* level at the top of the valence band and an a_1 level 75 meV below. Since our calculations do not include spin-orbit interactions, these energy levels should be degenerated in the absence of the SF. Figure 1(a) shows a contour plot of the charge density in the $(1\bar{1}0)$ plane of the last occupied *e* state, where a charge localization is observed in the fault region. The a_1 level is not perturbed by the presence of the SF, as can be seen in Fig. 1(b) The energy levels at the conduction-band minimum (CBM) suffer small changes due to the SF. Although the

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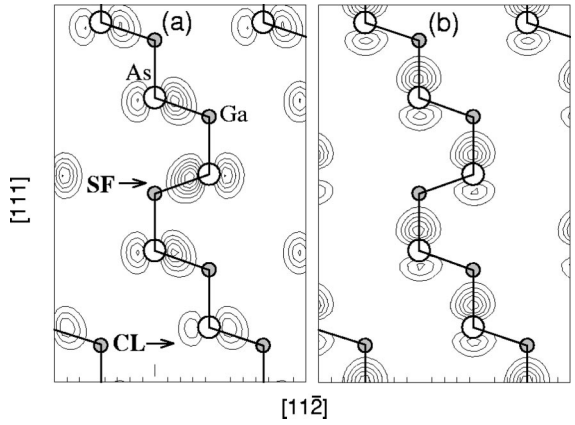

FIG. 1. Contour plot of the electronic charge density along the $(1\bar{1}0)$ plane for the (a) e level at VBM, and (b) the penultimate occupied level a_1, in the presence of a SF.

conduction-band states present a delocalized character, the electronic transport properties could still be affected. Figure 2 shows a weak localization around the fault for the first unoccupied conduction-band level.

The perturbations caused by the SF in n-type GaAs (here, Si doped) deserve special attention because the electronic properties of the semiconductor may be affected. Structurally, the bond lengths between the Si atom (in the Ga site) and the As first neighbors are practically the same in the SF as compared to the substitutional Si atom in the perfect crystalline environment. On the other hand, small changes can be observed in the bond lengths of the second neighbors of the impurity. Even with these apparently small structural changes caused by the SF presence, our calculations give an energy reduction of 0.12 eV/impurity for the Si atom at the SF as compared to that in the CL site. In a crystalline environment, a Si atom in the Ga site introduces a donor shallow level, but at the SF, this level becomes 60 meV deeper in the gap. The electronic charge localization of the donor level could have important effects on the carrier mobility.

In order to understand the effects of a SF on the conductivity of an n-type GaAs, we searched for some trapping

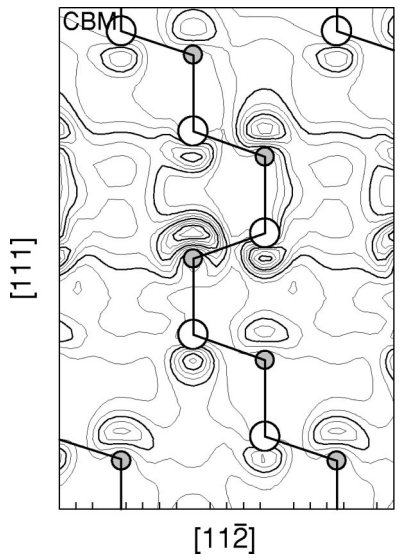

FIG. 2. Contour plot of the electronic charge density along the $(1\bar{1}0)$ plane for the first unoccupied level, in the presence of a SF.

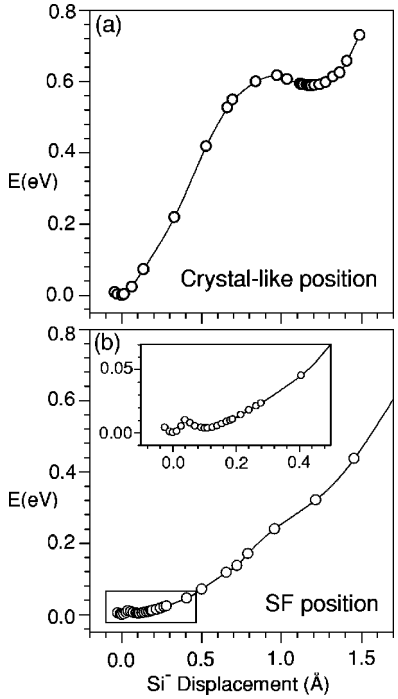

FIG. 3. Total energy (in eV) as a function of the Si^-_{Ga} ion displacement along the [111] direction in (a) the crystal-like environment, and (b) in the SF core. The inset in (b) shows the energy in the metastable region.

mechanism as a result of the SF. It is known that a Si impurity in GaAs can capture electrons from the system, having a metastable behavior, called DX centers, which can only trap electrons under certain conditions, such as hydrostatic pressure or near an interface with another alloy.[15–17] Our results show that far from the fault (at the CL site), the negative charge state for the Si impurity presents a metastability when the Si is moved from the substitutional Ga site in the [111] direction, as shown in Fig. 3(a). This trapping mechanism involves a large lattice relaxation and the Si atom can only stay out of the substitutional position, in this case, under hydrostatic pressure. For the Si atom at the SF, a completely different picture is observed. First, a segregation energy of 0.19 eV is verified favoring the Si^- ion at the fault. A metastable position for the Si atom is also found, but with small lattice relaxation. The metastable position is reached with the Si^- ion displaced by only 0.10 Å, in the [111] direction, from the equilibrium Ga site [Fig. 3(b)]. This displacement is accompanied by small relaxations of all neighboring atoms. The Si bond lengths are still practically the same as in the substitutional position (changes are less than 0.01 Å). The Si^- ion, due to the exceeding electron, has a weak bond with a second neighboring As atom, as shown in Fig. 4. For the Si^- ion in the metastable position, a localization of the impurity level can be observed. 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. 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.

Our results show a distinct behavior for the Si^- ion in the SF as compared to that in the crystalline environment. The most important aspect is that, in the SF, the ion does not present a metastable configuration as a result of large lattice

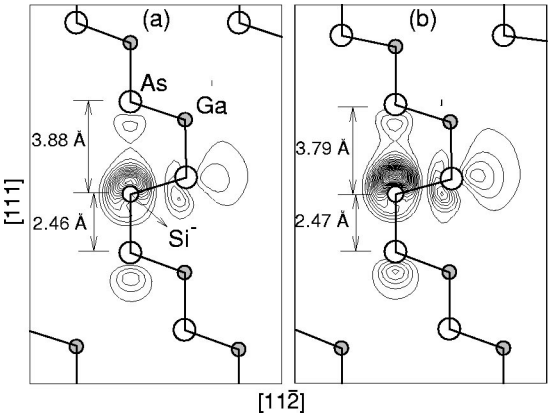

FIG. 4. Contour plot of the electronic charge density along the $(1\bar{1}0)$ plane for the impurity level of the Si^- ion in (a) the Ga substitutional position and (b) the metastable position.

relaxation. The results suggest that, under hydrostatic pressure, the SF may prevent the formation of *DX* centers. However, the Si^- ion in the SF could still work as a charge trapping center, similar to a *DX* center, with small lattice relaxation [Fig. 3(b)]. For a certain donor defect to become an electron trapping center, it should have a negative Mott–Hubbard potential (U),[18] i.e., it should be energetically favorable for a defect center to receive an additional electron. Our results show that 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. For the Si at the SF, our calculated value for U, obtained from different charge-state total energies, is also positive (0.004 eV). With this vanishing value of U, we could not rule out the possibility that this defect is a charge trapping center, although considerably different from the known *DX* center.

In summary, we have investigated the effects of a SF in pure GaAs and the interaction of an *n*-type impurity with a SF in GaAs. The *n*-type impurity, a Si atom in the Ga site, segregates towards the SF. Therefore, in thermodynamic equilibrium conditions, the concentration of extrinsic defects should be larger at the SF than in the crystalline environment. We also observe that the Si impurity at the SF core cannot occupy metastable interstitial positions with large lattice relaxations, as opposed to what happens to the Si in the crystalline environment.[15–17] This may prevent the formation of charge trapping centers, like *DX* centers.

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