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Arsenic segregation, pairing and mobility on the cores of partial dislocations in silicon

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Abstract

We studied the effects of arsenic on properties of dislocations in silicon. The theoretical investigation was carried out using *ab initio* total energy methods, based on the density functional theory. We find that the interaction of an arsenic impurity in the crystal with a dislocation results in a charge exchange, driving the dislocation core to a negative charge state. This interaction is essentially electrostatic and attractive, and leads to arsenic segregation. Although arsenic segregation to the core is energetically favourable, formation of arsenic pairs inside the core is energetically unfavourable. We also investigated the role of vacancies in arsenic diffusion inside the dislocation core.

1. Introduction

The interactions of extended defects, such as dislocations and grain boundaries, with dopants in semiconductors have important effects on the transport properties of carriers [1]. Dislocations, for example, can be very detrimental to the operation of electronic devices; their presence in a device’s active region gives rise to leakage currents, as a result of dopant diffusion along the dislocation cores. On the other hand, dislocations can be intentionally introduced far from those active regions—such as in the substrate—to work as sinks for undesirable impurities. Dislocations move by thermally assisted kink mechanisms [2], with activation energy of about 2.2 eV in undoped Si. However, even low concentrations of dopants can change this activation energy, reducing it by as much as 0.5 eV in n-type doped Si [3, 4]. In that sense, dopant impurities affect the electronic and the mechanical properties of dislocations.

The interaction between dislocations and dopants can be understood in terms of competing non-local and local effects. The non-local effect arises from the displacement of the Fermi level resulting from doping. According to that model, the increase in the dislocation mobility is a direct consequence of the negatively charged dislocation cores, which facilitates the formation

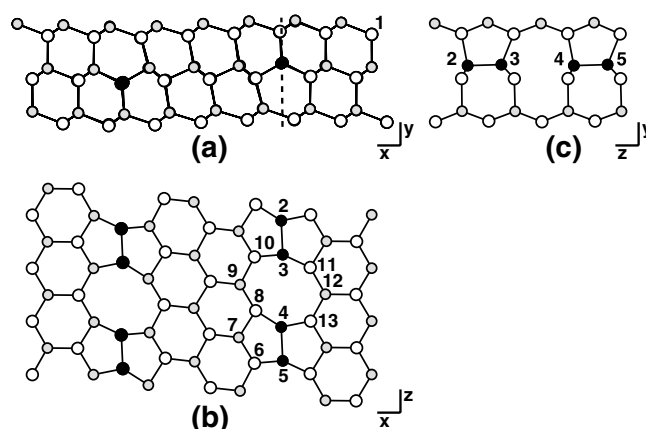


Figure 1. An atomic configuration containing a 30° dislocation dipole. The x -, y - and z -axes are respectively parallel to the $[11\bar{2}]$, $[111]$ and $[\bar{1}10]$ directions of the zinc-blende lattice. The figure shows the configuration on three different planes: (a) a plane normal to the dislocation line (xy -plane); (b) the glide plane where the dislocation belongs (xz -plane); and (c) the plane along the dashed line from (a) (the zy -plane).

and propagation of kinks [5]. The local effect arises from a segregation of impurities in the dislocation cores. In that case, dislocations must break away from the impurity clouds, which form around the cores, in order to move. In addition to these effects, as impurities segregate to dislocations, their diffusion inside the dislocation core, called pipe diffusion, is generally higher than in a crystalline environment.

Here we have used *ab initio* total energy calculations to investigate the interactions of arsenic with the cores of partial dislocations in Si. We find that arsenic segregates to the dislocation core, but arsenic pairing inside the core is energetically unfavourable. We also investigated the vacancy-assisted mechanisms of arsenic mobility inside the dislocation core as compared to the same mechanisms in a crystalline environment.

2. Theoretical model

In silicon, as well as in other zinc-blende semiconductors, dislocations generally belong to the $\{111\}$ glide planes [6], lying along the $\langle 110 \rangle$ directions. Perfect (screw and 60°) dislocations in that glide system dissociate into (30° and 90°) partial dislocations, forming a stacking fault between the partials. We focused this investigation on the properties of 30° dislocation because of its controlling role in the mobility of perfect dislocations in semiconductors [7]. Still, we expect that all the conclusions could be extrapolated to the 90° partial dislocation.

We used *ab initio* total energy calculations [8] to investigate the arsenic properties in the core of a 30° partial dislocation in Si. The calculations considered a 192-atom reference orthorhombic supercell with a dislocation dipole, as shown in figure 1. The cell geometry is such that dislocations of the dipole are four lattice parameters apart from each other along a $\langle 112 \rangle$ direction (~ 13.5 Å) in the glide plane, which prevents core–core interactions. The length of the cell along the dislocation is 15.3 Å, which provided enough space for analysing the properties of arsenic inside the core, without having the influence of the periodic images. We focused on three properties: the electronic properties of dislocations as results of arsenic interaction; the arsenic segregation and pairing inside the dislocation core; and finally the vacancy-assisted mechanism of arsenic mobility inside the core.

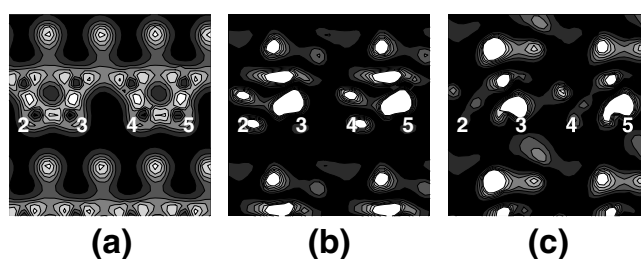


Figure 2. Electronic charge density on the zy -plane (as shown in figure 1(c)): (a) total charge density for the pure silicon system showing the reconstructed core bond (as represented by bonds between atoms 2 and 3 and between 4 and 5); (b) probability density of the lowest unoccupied level (with an antibonding character) of the pure Si system; and (c) charge density of the highest occupied level for the system containing one arsenic atom away from the dislocation. Atoms are numbered according to figure 1.

We devised a two-step configurational relaxation procedure, using first an interatomic potential and only later an *ab initio* method. This procedure saves considerable computational effort in the investigation of dislocation properties [9, 10]. For a certain configuration, the atomic positions were initially relaxed using a reliable interatomic potential for Si [11, 12], combined with a conjugate gradient minimization method. The output atomic positions were then used as input to the *ab initio* calculations, then with relaxation based on the Hellmann–Feynman forces. The *ab initio* calculations were performed using the density functional theory in the local density approximation. The Kohn–Sham equations were solved self-consistently using a plane-wave basis set, with a cut-off in the kinetic energy of 326 eV, and norm-conserving pseudopotentials [13, 14]. The sampling in the Brillouin zone was performed using the Γ point. Geometric optimization of the atomic structure was carried until forces were smaller than 0.02 eV \AA^{-1} in all atoms.

3. Results and discussion

We first considered a configuration in which an arsenic impurity sits in a crystalline-like position, which is the position furthest away from the dislocation core inside the simulation cell. This atomic position is indicated by the number 1 in figure 1(a). With the inclusion of arsenic in the system, we investigated the interaction between the arsenic donor level and the dislocation-related energy levels. First of all, a recent investigation [10] has shown that 30° dislocations in Si give rise to (occupied and unoccupied) mid-gap levels. These levels comprise bonding (occupied) levels that move up out of the valence band and antibonding (unoccupied) levels that move down out of the conduction band. Figure 2(a) shows the total charge density on a plane containing atoms of the dislocation core for a pure Si system, where bonds can be observed between Si dimers. Figure 2(b) presents the probability density of the lowest unoccupied level on the same plane as in figure 2(a) for pure Si. This level has an antibonding character, being delocalized along the dislocation. An isolated substitutional arsenic atom in bulk Si gives rise to a shallow defect level about 0.1 eV below the conduction band edge. As a result of the interaction between arsenic and the dislocation, the impurity gives away one electron, from that shallow defect level, becoming positively charged. This charge is captured by the dislocation core, occupying the dislocation-related antibonding level which sits in the mid-gap region. Figure 2(c) displays the charge density of the highest occupied level for the case where an arsenic atom is in a crystalline-like position. It is clear that the charge density

of this level, which is now occupied by a single electron, is distributed along the dislocation; the density plot is similar to that displayed in figure 2(b). Therefore, the dislocation core is now negatively charged and should attract the positively charged As impurity by the Coulomb interaction [15].

Arsenic segregates to the dislocation core. We computed the segregation energy by comparing the total energies between configurations with those for the arsenic in the crystalline environment (position 1) and in the dislocation core (position 2). We should stress that this energy is in fact a lower bound of the real segregation energy. Since the Coulomb interaction is long ranged, a considerably larger simulation cell would be necessary to provide a converged value for the segregation energy. The resulting segregation energy from our calculations is 0.18 eV. In addition, the presence of arsenic in either a crystalline site or inside the dislocation core distorts the lattice only slightly, as compared to the respective atomic configurations of a system without arsenic. In position 1 (figure 1), As does not break the local symmetry, only relaxing the first neighbours to 2.40 Å, compared to 2.35 Å for the crystalline Si distance. Arsenic in position 2 also keeps the symmetries of the core. The distance in the dimer (2, 3) changes from 2.45 Å in pure Si to 2.50 Å with the As impurity in position 2. Therefore, the change in the total energy coming from elastic interactions, as arsenic goes from a crystalline environment to the core region, is negligible. This suggests that the segregation energy results primarily from electronic processes, which would give rise to an electrostatic interaction between the impurity and the dislocation core [16].

We then investigated the possibility of arsenic pairing inside the dislocation core. We started with a configuration where there is an As pair (as nearest neighbours) in the crystalline region. If one of these atoms is placed inside the core, the total energy is lowered by 0.67 eV. If now the other arsenic atom in the crystalline region is also brought to the dislocation core, forming a pair in the positions 2 and 3 (according to figure 1), there is a gain in energy of 0.05 eV. Therefore, the total segregation energy of an As pair is 0.72 eV. We have checked the possibility of a metastability of this As dimer configuration. In fact, there is an additional gain of 0.37 eV if the pair is dissociated by placing the two As atoms at positions 2 and 4, thus increasing the segregation energy of the pair to 1.09 eV. The results indicate that As impurities remain fourfold coordinated inside the core of 30° dislocations and As pairing is not energetically favourable.

Recent theoretical investigations [9, 17] have found that the formation energy of vacancies in silicon can be as much as 1.3 eV lower in extended defects, such as dislocation cores and stacking faults, as compared to that energy in the crystalline environment. Therefore, the dislocation cores will be full of impurities and vacancies. It is well known that arsenic diffusion in crystalline silicon is vacancy assisted [18, 19]. This raises the question of whether the higher concentration of vacancies inside the dislocation cores could facilitate arsenic mobility. To investigate this possibility, we first considered the stability of the arsenic–vacancy pair (as nearest neighbours) inside the dislocation. This was done by comparing the total energy between a configuration with the pair in a crystalline environment and a configuration with the pair inside the dislocation core (arsenic in position 4 and removing the atom labelled by number 5 in figure 1(b)). The total energy is lowered by 0.83 eV as the pair is brought from the crystalline environment to the dislocation core. However, the stable configuration for the pair inside the core is when the arsenic impurity sits in position 4 and the vacancy is formed by removing atom number 8 (as shown in figure 1(b)). For this configuration, there is an additional gain in energy of 1.14 eV. Taking this last configuration as the reference for the arsenic–vacancy pair, the total energy increases by 0.42 and 0.71 eV as the vacancy is formed by removing atoms numbered 9 and 10, respectively. It should be pointed out these configurations are formed by a vacancy on the side of the stacking fault. Formation energies of the pairs for the

vacancy on the crystalline side (atomic positions 11, 12 or 13) are more than 2 eV higher than the respective configurations next to the stacking fault (atomic positions 8, 9 or 10).

4. Summary

In summary, we have investigated the properties of arsenic interactions with the core of a 30° partial dislocation in silicon. Our results show that arsenic doping drives the dislocation cores to a negative charge state, consistently with recent experimental data [20]. Segregation of arsenic to the dislocation core is controlled by the Coulomb interaction between the positively charged arsenic impurity and the negatively charged dislocation core. The vacancy–arsenic pair is also energetically favourable inside the dislocation core. In that sense, vacancy-assisted diffusion of arsenic should be highly facilitated inside the dislocation core.

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