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AB INITIO CALCULATIONS OF AS-VACANCY INTERACTIONS IN SILICON

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ABSTRACT

Atomistic simulation of a vacancy-assisted dopant diffusion in silicon needs details of the dopant-vacancy interaction, i.e., the potential as a functional of dopant-vacancy separations. In this paper, we present a detailed study on the energetics of As-vacancy reaction in silicon and the lattice distortions surrounding the As-vacancy defect by using an *ab initio* plane wave pseudopotential method and the density functional theory (DFT). A potential-energy diagram as a function of As-vacancy separation is provided, which can be used in the atomistic diffusion simulations. We also calculate the binding energy and the formation energy of different complexes such as AsV, As₂V and AsV₂ (V represents vacancy). We find that the stable configuration of As₂V is As-V-As, while the stable configuration of AsV₂ is As-V-V. The nature of the binding between As and vacancy is explained from the lattice distortions and the change of chemical bond configuration introduced by the As-vacancy complex.

INTRODUCTION

Arsenic has been regarded as an important *n*-type dopant in silicon-based integrated circuits. The implanted As atoms dissolve in the silicon lattice almost exclusively on substitutional lattice sites [1]. The diffusion of these dopant atoms takes place via interactions with the host atoms and the native defects (such as vacancies and interstitials) in silicon. As the minimum size of the Si-base semiconductor devices decreases and approaches the dopant diffusion length under processing conditions, it is highly desired to understand the details of interaction between the dopant and the native defects in order to predict and control the dopant diffusion.

It is widely accepted [1] that the diffusion of the substitutional dopant in silicon is mainly mediated by vacancies and interstitials. The vacancy mechanism [2, 3] requires that a dopant atom forms a pair with an adjacent vacancy. The vacancy moves away from the dopant atom around a six-fold ring to at least a third-neighbor position. It can then return by a different path, placing itself next to the dopant. The vacancy and the dopant exchange positions and the process repeats itself. The interstitial-mediated diffusion [4] may occur through the "kick out" or "coordinated push" mechanism via interaction of dopant atom with an interstitial silicon atom. Although above pictures are well developed, there is still a great deal of controversy about the relative importance of vacancies and interstitials in dopant diffusion in silicon, i.e., which mechanism is dominant for a given dopant. There is in fact no direct experimental evidence demonstrating an implanted dopant is mediated by a specific mechanism because the obtained diffusion profile includes all the possible mechanism. The contributions from each mechanism are actually determined by fitting the experimental profile of the dopant through solving the macroscopic diffusion

equations.

Atomistic simulations provide more details of the microscopic diffusion mechanism. The prerequisite for this kind of simulation is the dopant-defect interaction potentials. Recently, Dunham and Wu [5] performed atomistic simulations of a vacancy-assisted diffusion in silicon. They assumed that the dopant-vacancy interaction decrease linearly and vanishes at the fourth nearest neighbors. The second and the third nearest neighbor binding energies were taken as $2/3$ and $1/3$ of the binding energy on the first nearest neighbor site. More recently, List and Ryssel [6] carried out an atomistic analysis of the vacancy mechanism of dopant diffusion in silicon using Monte Carlo method. Since there were no accurate data available for the interaction potential between dopants and vacancies, they also assumed that the dopant-vacancy interaction vanishes at the fourth nearest neighbor site. They tested several very simple potentials: rectangular shape, linear shape and Coulomb shape ($1/r_{ij}$). It was found that the simulation results were dependent on the shape of potentials. They concluded that an assessment of the relative importance of the vacancy mechanism compared to interstitial related mechanisms for the different dopant atoms required accurate quantitative data on the atomistic potentials. In this paper, we report a thorough investigation of the structure and energetics of the As-vacancy complex in silicon, using the first-principles total energy calculations. A detailed quantitative potential diagram for As-vacancy interactions has been provided. We find that The binding range of the As-vacancy is beyond the third-nearest neighbor distance. The shape of the potential is quite different from the simple assumptions in Refs. [5, 6]. By checking the lattice distortions around the defect, we find that the As displaces its neighboring Si atoms outward and the vacancy attracts its neighboring atoms inward. The existence of As lowers the migration barrier of a vacancy moving toward As and increases the barrier of a vacancy moving away from As. Considering the complexity of a real diffusion process, we also studied the formation energy and the binding properties of As_2V and AsV_2 complexes. It was found that the AsV pair can attract another As atom forming an As-V-As complex due to the binding between As and vacancy. The AsV pair can also attract another nearby vacancy. However, the binding force is not from the interaction between As and vacancy, but mainly from the interaction between vacancy and vacancy.

COMPUTATIONAL DETAILS

The ground state total energy was obtained within density functional theory (DFT) [7] in the local-density approximation (LDA) to the exchange-correlation energy functional [8, 9]. Electronic wave-functions were expanded in a plane wave basis [10], with a 12 Ry cutoff. Nonlocal and norm-conserving pseudopotentials constructed by the scheme of Hamann [11] were used to describe the valence electron interactions with the atomic core. Periodic supercell with 64 atomic sites was employed to model the considered system. The integration of $\mathbf{k}$ points over Brillouin zone (BZ) was performed by summing a $2 \times 2 \times 2$ mesh in the first BZ. The iterative damped Joannopoulos algorithm [12] was used to obtain the self-consistent one-electron Kohn-Sham equation. The Hellmann-Feynman theorem was used to evaluate the forces on all atoms which were allowed to move. Atomic relaxations were considered to the point where the magnitude of the calculated Hellmann-Feynman forces on each atom

was smaller than 0.4 mRy/Bohr. The convergence of the k point summation and the kinetic energy cut-off were checked by using a $4 \times 4 \times 4$ mesh in the first BZ and a 16 Ry energy cut-off. The results of the binding energy and the formation energy of the As-vacancy pair differed by less than 0.1 eV, which gives an estimate of the accuracy of the calculation.

RESULTS AND DISCUSSIONS

We first calculated the static equilibrium lattice constant of bulk silicon. The obtained lattice constant was $a_0 = 5.40 \text{ \AA}$, which is 0.5% smaller than the experimental value of $5.43 \text{ \AA}$ due to the LDA approximation. Using this theoretical lattice constant, we calculated the lattice distortions around an isolated substitutional As dopant before considering the As-vacancy interactions. The first-nearest-neighbor and the second-nearest neighbor atoms around As are relaxed as shown in Figure 1. Before introducing the As impurity, pure silicon has the T_d symmetry. The existence of As will result in a lattice distortion and may reduce the symmetry. We therefore relaxed the system starting from initial configurations which have different symmetries, i.e., T_d , D_{2d} , and C_{3v} . It is found that there are two stable distorted geometries: one has a T_d symmetry, another has a D_{2d} symmetry. The C_{3v} geometry is not stable and eventually evolves to T_d geometry. These two final configurations have nearly the same total energy; the T_d geometry is 0.02 eV lower than D_{2d} . This is somewhat similar to the relaxations around a vacancy [13], where two final configurations have also been found with nearly the same total energy. The obtained results for lattice relaxations around As in the two configurations are listed in Table 1. It is found that the first-nearest-neighbor silicon atoms of As are displaced outwards about 2.5-2.6% by As. The relaxations of the second-nearest-neighbors of As are rather small. For the D_{2d} geometry, there is a slight pairing effect for the first-nearest-neighbor atoms around As. The distances between atoms 15-14 and 13-16 are a little smaller than that of 15-13 and 14-16 (see Fig.1 for the position labels).

Figure 1: The first and second nearest-neighbors around a substitutional As impurity in silicon.

Table 1: Relaxation properties of the atoms neighboring an isolated As dopant. Atoms are labeled as illustrated in Fig. 1. All distances are in Å. The distances between atoms are denoted as d for the relaxed crystal, and d_0 for a perfect crystal. $\Delta d/d_0 = (d - d_0)/d_0$.

Symmetry	pair	d	d_0	$\Delta d/d_0$
D_{2d}	As- i ($i=13 \rightarrow 16$)	2.398	2.337	2.6%
	15-14, 13-16	3.904	3.816	2.3%
	15- i , 14- i ($i=13, 16$)	3.922	3.816	2.8%
	As- i ($i=5 \rightarrow 12$)	3.827	3.816	0.3%
	As-2, As-3	3.820	3.816	0.1%
	As-1, As-4	3.820	3.816	1.1%
T_d	As- i ($i=13 \rightarrow 16$)	2.395	2.337	2.5%
	15-14, 13-16	3.911	3.816	2.5%
	15- i , 14- i ($i=13, 16$)	3.911	3.816	2.5%
	As- i ($i=1 \rightarrow 12$)	3.823	3.816	0.2%

Next, we consider a vacancy moving near the As dopant. One Si atom is replaced by an As impurity and another atomic site is left empty representing a vacancy. The potential energy of the As-vacancy pair is calculated as a function of the As-vacancy separation. The vacancy is placed on different sites in the six-fold ring as shown in Figure 2(a). For each As-vacancy configuration, the first-nearest-neighbor and the second-nearest-neighbor atoms around the defects are fully relaxed. We also calculated the diffusion of the vacancy along the six-fold ring. Note that the diffusion of vacancy is equivalent to the diffusion of silicon atoms in the opposite direction. The diffusion barriers are obtained by moving the hopping atom along the diffusion path and relaxing its position in a plane perpendicular to the diffusion direction. Other atoms up to the second-nearest-neighbors of the defects as well as the hopping atom are relaxed simultaneously. The obtained potential-energy diagram of As-vacancy interaction is shown in Figure 2(b). The vacancy coordinates labeled as 1, 2, 3 etc. refer to the atomic sites shown in Figure 2 (a). However, after the lattice relaxation, they are not at the ideal lattice site. Details of the relaxation will be discussed below. It can be seen in Figure 2 (b) that the energy barrier for the vacancy moving from site 3 (third-nearest-neighbor of As) to site 2 (second-nearest-neighbor of As) is 0.23 eV. Once the vacancy is located at site 2, it will move quickly to site 1 (first-nearest-neighbor of As) which experiences a very small energy barrier of only 0.08 eV. The position of this small energy barrier is very close to site 2. The barrier between sites 1 and As is 0.55 eV high, which describes the $\text{As} \leftrightarrow \text{vacancy}$ exchange. After exchanging position with As, the vacancy may move away along a different ring which connected with As (see Figure 2(a)). The vacancy first overcomes an energy barrier of 0.92 eV arriving at a second-nearest-neighbor site of As. Then it moves to the third-nearest-neighbor site by passing over another barrier with height 0.35 eV. Once the vacancy overcomes the third-nearest-neighbor site, it can return to the As via a different path. By repeating such a process, diffusion of the As-vacancy complex occurs. The migration barrier $E_m(\text{AsV})$ for the whole As-vacancy complex is 1.19 eV

as shown in figure 2(b), which is close to the experimental result of 1.07 eV [3]. We also calculated the first-neighbor binding energy of an As-vacancy pair (the vacancy is located next to As) relative to the As-vacancy separation at 9.35 Å (vacancy is located at the 12th-nearest-neighbor of As), where the As-vacancy interaction is negligible. The obtained result is $E_b(\text{AsV}) = 1.21$ eV, which is in a good agreement with other *ab initio* calculations of 1.20 eV [4] and the experimental measurements of 1.23 eV [14]. It is found that the attractive potential of As-vacancy is beyond the third-nearest-neighbors since the binding energy of the As-vacancy pair is still 0.25 eV (1.21 minus 0.96) when the vacancy is located at the third-nearest-neighbor site of As, which is different from the assumptions in Refs [5, 6]. For comparison, we calculated the formation energy and the migration barrier of a vacancy in pure silicon. The obtained formation energy is 3.57 eV which is in good agreement with the experimental measurement of 3.6 eV and other *ab initio* calculations [15]. The calculated migration barrier is 0.31 eV. Comparing with the migration barriers of the vacancy moving near an As, it is found that the As lowers (increases) the migration barrier of the vacancy hopping toward (away from) it.

Figure 2: (a) Different As-vacancy separations along the six-fold ring. The atomic sites are projected onto the (111) surface. The filled and the empty circles represent the atomic sites from different layers. 1, 2 and 3 denote the first-nearest-neighbor, second-nearest-neighbor and third-nearest-neighbor sites of As, respectively. (b) Potential-energy for As-vacancy complex as a function of vacancy coordinate.

We calculated the activation energy Q for As diffusion via the vacancy mechanism by summing the formation and migration energies for the As-vacancy complex. The formation energy of an As-vacancy pair is calculated as [4]

$$E_f(\text{AsV}) = E(\text{AsV}) - E_s(\text{As}) + \frac{1}{64}E(\text{Si}_{64}), \quad (1)$$

where $E(\text{AsV})$ is the calculated total energy of the 64-atomic sites supercell containing an As-vacancy pair, $E_s(\text{As})$ is the total energy of the supercell containing a substitutional As impurity, and $E(\text{Si}_{64})$ is the total energy of the 64-atomic sites supercell of pure silicon. The calculated result for $E_f(\text{AsV})$ is 2.37 eV. The corresponding activation energy $Q = E_f(\text{AsV}) + E_m(\text{AsV}) = 3.56$ eV. This value is in good agreement with the experimental result of 3.44 eV [16] for the diffusion of neutral As in silicon and is smaller than that of 4.05 eV [16] for the charged As. Masters and Fairfield [17] observed an activation energy of 4.2 eV for As diffusion in silicon, but the authors pointed out at the same time that the effective activation barrier would be 3.4 eV in the high doping level and the lower temperature range.

Table 2 lists the detailed relaxation properties around the As-vacancy complex in the process of a vacancy moving along the six-fold ring. The corresponding atom sites around the As-vacancy complex are shown in Figure 3. The arrows indicate the relaxation direction and the length of the arrow is proportional to the displacement of the corresponding atom. It can be seen from Table 2 and Figure 3 that when a vacancy is located next to an As (Fig. 3(a)), As atom moves significantly towards the vacancy site. The distance between As and its nearest-neighbor silicon atoms (6,7,8 in Fig.3 (a)) is 3.4% larger than the bond length of pure silicon reflecting the repulsion between As and silicon. On the other hand, the vacancy attracts the surrounding atoms (including As) inward. This geometry possess a C_{3v} symmetry, which is different from that of an isolated As dopant discussed above. When the vacancy moves away from As (Fig. 3(b)), atoms neighboring the vacancy relax inward and those neighboring the As relax outward. There is then no symmetry maintained. The displacement of atom 2 is most significant due to the repulsion of As and the attraction of vacancy. When the vacancy is located at the third-nearest-neighbor site of As (Fig. 3(c)), the lattice relaxation around vacancy is still affected by the As. Two silicon atoms, 3 and 5, which are the second-nearest-neighbors of As, move more significantly than atoms 13 and 14.

Figure 3: Lattice relaxation of an As-vacancy complex for different As-vacancy separations. The circles denote the atomic sites corresponding to the perfect silicon. The arrows point in the relaxation direction and the length of the arrow is proportional to the displacement of the atom in 3-dimensions. The dashed line shows the six-fold ring: (a) vacancy is next to As, (b) vacancy is the second-nearest-neighbor of As, (c) vacancy is the third-nearest-neighbor of As.

Up to now, we have had a detailed diagram of As-V potential. The dopant As can then migrate in the silicon crystal assisted by vacancy. In real cases, there exist a lot of other implanted As atoms and other vacancies. One can easily ask that how this AsV pair interacts with other As and vacancy. We therefore calculated the formation energy and the binding energy for As_2V and AsV_2 complexes. The results are listed in Table 3. The corresponding values for As_2 , V_2 (divacancy) and AsV pairs are also listed for comparison. We can see that the formation energy of a single vacancy (3.57

Table 2: Relaxation properties of the atoms neighboring the As-vacancy complex. Atoms are labeled as illustrated in Fig. 3. All distances are in Å. $\Delta d/d_0 = (d - d_0)/d_0$, where d_0 denotes the distance in the perfect silicon crystal. The symbols + and - denote expansion and shrinkage, respectively.

system	pair	d	d_0	$\Delta d/d_0$ (%)
Fig. 3 (a)	As- i ($i=6,7,8$)	2.415	2.337	+3.4
	As- i ($i=3,9,10$)	3.498	3.816	-8.3
	6-8, 7-8, 6-7	3.749	3.816	-1.8
	3-9,9-10,10-3	3.631	3.816	-4.9
Fig. 3 (b)	As-8	2.392	2.337	2.4
	As-7	2.406	2.337	+2.9
	As-6	2.392	2.337	+2.4
	As-2	2.440	2.337	+4.4
	2-4	3.463	3.816	-9.3
	2-11	3.463	3.816	-9.3
	2-12	3.418	3.816	-10.4
	4-11	3.620	3.816	-5.1
	4-12	3.623	3.816	-5.1
	11-12	3.620	3.816	-5.1
Fig. 3(c)	As-6	2.411	2.337	+3.2
	As-7	2.394	2.337	+2.4
	As-8	2.397	2.337	+2.6
	As-2	2.411	2.337	+3.2
	13-14	3.615	3.816	-5.3
	13-3	3.571	3.816	-6.4
	13-5	3.571	3.816	-6.4
	14-3	3.512	3.816	-8.0
	14-5	3.512	3.816	-8.0
	3-5	3.514	3.816	-7.9

eV) is lowered by 1.20 eV when an As atom binds with it forming an As-V pair (2.37 eV). The formation energy of As-V pair is further reduced by 1.16 eV when another As atom binds together creating an AsV-As complex (the formation energy is 1.21 eV). The formation energy of a divacancy (V-V) (5.30 eV) is reduced by 1.18 eV when forms a As-V₂ complex (4.12 eV). Therefore, the formation energy of As_nV_m complex is monotonically reduced with the increase of As atoms, which means that the As_nV_m complex will be dominant when the doping level is high. If we check the binding energies, we can see that an AsV pair can attract another vacancy, the binding energy of AsV-V complex (1.82 eV) is very close to that of a divacancy (1.84 eV). The AsV pair can also attract another As atom, the binding energy between AsV and As is nearly the same as that of an AsV pair. Since the two As atoms do not bind with each other (the binding energy is negative), the binding between AsV and As is thus resulted from the interaction between As and vacancy. On the other hand, the binding between AsV pair and another vacancy is resulted from the V-V

interactions. In order to make this clear, we compared the total energies of AsV_2 and As_2V with different configurations (see Fig. 4). It is found that the total energy of As-V-V (Fig. 4(a)) is 1.22 eV lower than that of V-As-V (Fig. 4(b)), which clearly shows that the binding between AsV and V comes from the binding between two vacancies. Meanwhile, the total energy of As-V-As (Fig. 4(c)) is 1.01 eV lower than that of As-As-V (Fig. 4(d)). This indicates that the binding between AsV and As mainly comes from the binding of As-V pair.

Table 3: Formation energies and binding energies of the complexes of As atoms with vacancies.

Defect complex	Formation energy (eV)	Binding energy (eV)
As-As	0.19	-0.13
V(vacancy)	3.57	
As-V	2.37	1.21
AsV-As	1.21	2.55
V-V	5.30	1.84
AsV-V	4.12	1.82
As- V_2	4.12	1.22

Figure 4: Several As-vacancy complex configurations: (a) two vacancies are nearest neighbors, (b) two vacancies are separated by one As atom, (c) two As atoms are separated by one vacancy, (d) two As atoms are nearest neighbors. Other atomic sites are occupied by silicon atoms.

The above discussions reveal that there are two binding mechanisms when AsV pair interacts with other As atoms and vacancies, i.e., interaction between V and As and interaction between V and V. The binding of two vacancies can be understood from the reduction of the number of silicon dangling bonds. The formation of a single vacancy (3.57 eV) is divided by 4, each bond gains a amount of about 0.9 eV energy. When two vacancies binds together, the number of silicon dangling bonds reduces

from 8 to 6. There will be 1.8 eV (2 times 0.9) energy released. This is almost same with the binding energy (1.84 eV) of two vacancies (the relaxation effect is already included in the calculation of the formation energy of a single vacancy). Here we quantitatively confirmed the empirical analysis of Chadi and Chang [18] about the aggregation of vacancy clusters in silicon. The binding between As and vacancy comes from the following facts. When an As impurity is implanted into silicon, it pushes the surrounding atoms outward and increases the elastic energy of the lattice. The existence of a neighboring vacancy provides the space for As and releases the elastic energy by inward relaxation. On the other hand, As has 5 valence electrons. When As and vacancy binds together, As reverts to its three-fold coordinated *neutral* state from a four-fold coordinated state. The number of silicon dangling bond reduces from 4 to 3. Therefore, the binding energy of As-vacancy arises mainly from the release of the elastic energy and the reduction of one silicon dangling bond.

SUMMARY

In summary, we have provided a detailed potential-energy diagram for As-vacancy interactions in silicon based on the *ab initio* total energy calculations. The energy barriers for a vacancy moving away from As along the six-fold ring are 0.92 eV and 0.35 eV. While for a vacancy moving toward As, the barriers are 0.23 eV and 0.08 eV. The exchange barrier of As-vacancy pair is 0.55 eV. The migration barrier for the whole As-vacancy complex is 1.19 eV. The calculated activation energy for the vacancy mediated diffusion of the neutral As impurities in silicon is 3.56 eV. We also calculate the formation energies and binding energies of different As-vacancy complexes such as AsV, As₂V and AsV₂. Complexes like V₂, AsV, As₂V and AsV₂ were found to form naturally with binding energies that are larger than 1 eV. By comparing the binding properties of different As-vacancy complexes, we concluded that the origin of the binding for the As-vacancy pair can be understood as the release of the elastic energy accumulated around As and vacancy and the reduction of the silicon dangling bond.

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