Tensile Stress Effect on Indium Diffusion in Silicon Substrate: *Ab-initio* Study

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ABSTRACT

In this paper, we present our *ab-initio* study on energy configurations, minimum energy path (MEP), and migration energy for neutral indium diffusion in a uniaxial and biaxial tensile strained {100} silicon layer. Our *ab-initio* calculation of the electronic structure allowed us to figure out transient atomistic configurations during the indium diffusion in strained silicon. We found that the lowest-energy structure (In_S - Si_i^{Td}) consists of indium sitting on a substitutional site while stabilizing a silicon self-interstitial in a nearby tetrahedral position. Our *ab-initio* calculation also revealed that the next lowest energy structure is In_i^{Td}, the interstitial indium at the tetrahedral position. We employed the nudged elastic band (NEB) method for estimating the MEP between the two structural states. The NEB method implies that the diffusion pathway of neutral indium is kept unchanged while the migration energy of indium fluctuates in strained silicon.

Keywords: *Ab-initio* calculation, strained silicon, indium, diffusion pathway.

1 INTRODUCTION

Recently, a heavy ion implantation has attracted a great of attention as a promising method for achieving a very shallow junction in silicon microelectronic devices. Due to its heavier mass, indium is considered to be one of the alternatives to boron atom as a p-dopant [1,2]. Now, strain engineering has also received a lot of attention due to the enhanced mobility of carriers [3].

Consequently, studies on the properties of indium diffusion in strained silicon would help us to develop successful process integration. That is because modeling of diffusion profiles of the dopant impurities is imperative for design of the devices due to dopant diffusion in silicon crystal plays a central role[4]. In this work, we investigated the diffusion pathway as well as the energy barrier of indium in an effort to obtain the physical parameters of indium in silicon through *ab-initio* calculations.

2 COMPUTATIONAL DETAILS

2.1 Diffusion Pathway of Indium

The *ab-initio* calculations were implemented within density functional theory (DFT) with Vienna *Ab-initio* Simulation Package (VASP) which combines ultrasoft pseudopotentials[5] and generalized gradient approximation (GGA) in the Purdew and Wang formulation. The simulation condition was set as the followings: a cutoff energy E_c = 150.62 eV, $2 \times 2 \times 2$ grid for the *k*-points mesh of Monkhorst-Pack[6], and a $3 \times 3 \times 3$ simple cubic super-cell (216 atoms). The optimized silicon lattice constant for GGA in our system is 5.461Å. An energy landscape for In-Si complex can be provided by employing VASP. The lowest-energy structure was found to be In_s - Si_i^{Td}, as shown in Fig. 1. The second lowest-energy structure is found to be In_i^{Td}, as shown in Fig. 2.

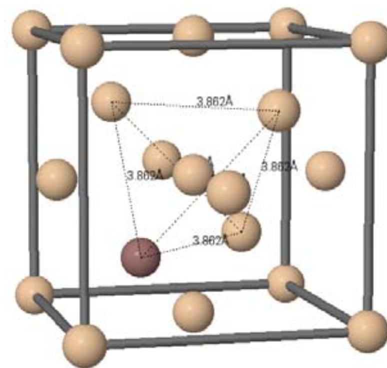


Fig. 1 A plot illustrating In_s-Si_i^{Td} configuration wherein the indium atom (red-colored) sits on a substitutional site and stabilizes self-interstitial silicon (yellow-colored) in a tetrahedral position.

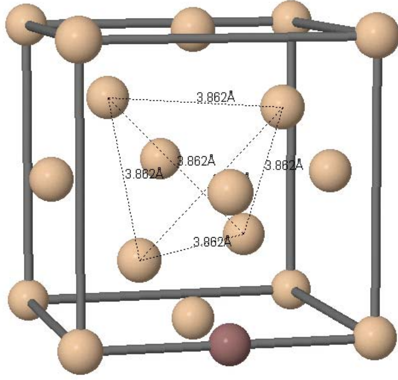
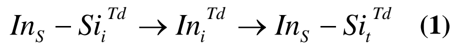


Fig. 2 In_i^{Td} structure wherein the interstitial indium atom(red-colored) is in the tetrahedral position.

The energy difference between the first and the second lowest energy configuration has been calculated to be 0.492 eV. The energy landscape allows us to figure out the diffusion pathway of neutral indium as the following:



$$In_S - Si_i^{Td} \rightarrow In_i^{Td} \rightarrow In_S - Si_t^{Td} \quad \mathbf{(1)}$$

2.2 Correlation between Stress and Strain

Fig. 3 is a schematic diagram illustrating a Metal-Oxide Semiconductor Field Effect Transistor (MOSFET) structure with a strained silicon layer on silicon-germanium buffer. To introduce uniaxial and biaxial strain in silicon, we applied the lattice constant of relaxed $Si_{1-x}Ge_x$ to the two crystallographic directions on the (100) plane since the strained silicon grown on relaxed SiGe buffer layer has the same lattice constant as SiGe.

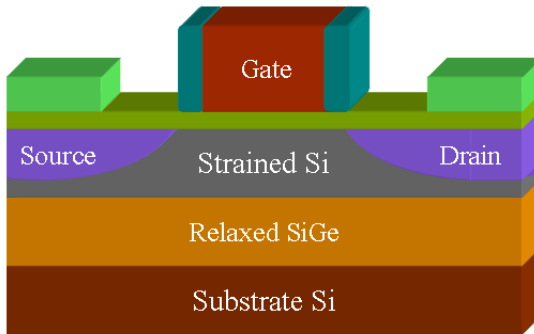


Fig. 3 Schematic diagram showing the strained silicon MOSFET structure employed in this work.

We investigated the change of $Si_{1-x}Ge_x$ lattice constant with respect to x (Ge mole fraction) wherein the lattice constant of $Si_{1-x}Ge_x$ can be expressed as:

$$a_{SiGe} = (1-x)a_{Si} + xa_{Ge} \quad (2)$$

where a_{Si} and a_{Ge} are lattice constants of Si and Ge, respectively. The lattice constant in the perpendicular direction was calculated from the elastic theory while "In-plane" and "Out-of-plane" strain can be calculated from the following three equations:

$$\varepsilon_{\parallel} = (a_{SiGe} - a_{Si}) / a_{Si} \quad (3)$$

$$\varepsilon_{\perp} = (a_{\perp} - a_{Si}) / a_{Si} \quad (4)$$

$$\varepsilon_{\perp} / \varepsilon_{\parallel} = -2(C_{12} / C_{11}) \quad (5)$$

where C_{11} and C_{12} are elastic constants of Si.

For our *ab-initio* calculations, we assumed C_{11} = 156Gpa and C_{12} = 56Gpa with basis on density functional theory results[7]. The results of elastic constant of silicon allow us to derive stresses in strained Si from Hooke's laws[8] with the following equations (6):

$$\begin{bmatrix} \sigma_X \\ \sigma_y \\ \sigma_z \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{bmatrix} \quad (6)$$

where C is the elastic compliance, ε is the strain, and σ is the stress. We formulated a correlation between the stress and strain as a function of germanium mole fraction, as shown in Tables I and II, with energy parameters of In-Si complex in uniaxial and biaxial strained silicon.

2.3 Minimum Energy Path

In order to search for the minimum energy path (MEP), we performed the nudged elastic band (NEB) calculation[9] which stems from a transition state theory (TST)[10]. The calculation approach in our work is based on the optimization of a number of intermediate images along the reaction path. Each initial image finds the possible lowest energy while maintaining equal spacing to the neighboring images.

The NEB is an efficient method for finding saddle points and minimum energy paths between the given initial and final states of diffusion. In our previous section, we searched the initial and final states of indium diffusion. The initial state is the lowest energy configuration (In_s - Si_i^{Td}) and the final state the second lowest energy configuration (In_i^{Td}). Repeating the transitions between the two states, neutral indium diffuses in silicon. Therefore, if we investigate the MEP from the initial state to the final state, we can now obtain the energy barrier for indium migration.

Fig. 4 shows the minimum energy path of indium in uniaxial strained silicon calculated by the NEB method wherein stress induced from 0, 1 and 2 GPa, respectively. Column-axis is the migration energy along the MEP of Si: In from In_s - Si_i^{Td} to In_i^{Td}.

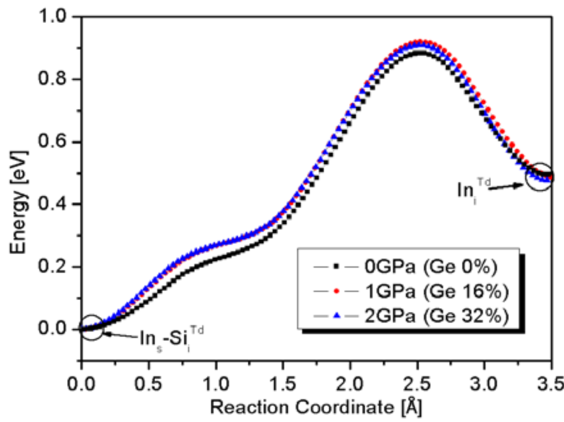


Fig. 4 The relative energy along the minimum energy path from In_s-Si_i^{Td} to In_i^{Td} in uniaxial strained silicon.

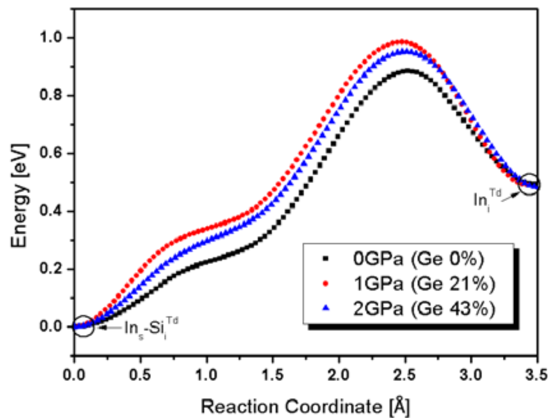


Fig. 5 The relative energy along the minimum energy path from In_s-Si_i^{Td} to In_i^{Td} in biaxial strained silicon.

Fig. 5 also shows the minimum energy path and migration energy of indium in biaxial strained silicon wherein 0, 1 and 2 GPa stresses are induced to silicon layer. Finally, we listed the migration energy in Table I and II with total energies for the initial (In_s - Si_i^{Td}) and final (In_i^{Td}) configurations in 216 atom super cell.

Stress (GPa)	*Strain(ratio)*	*Total energy (eV)*		*Migration energy (eV)*
		In_s-Si_i^{Td}	*In_i^{Td}*	
0	0	-1167.628	-1167.136	0.884
1	0.006	-1167.643	-1167.162	0.920
2	0.013	-1167.483	-1167.009	0.910

Table I. Correlation among the strain ratio, Ge concentration (%), total energy (eV) of initial and final configurations and migration energy (eV) as a function of stress in uniaxial strained silicon.

Stress (GPa)	*Strain(ratio)*		*Total energy (eV)*		*Migration energy (eV)*
	X axis	*-Y axis*	*In_s-Si_i^{Td}*	*In_i^{Td}*	
0	0	0	-1167.628	-1167.136	0.884
1	0.009	0.006	-1167.552	-1167.065	0.984
2	0.017	0.012	-1167.111	-1166.631	0.952

Table II. Correlation among the strain ratio, Ge concentration (%), total energy (eV) of initial and final configurations, and migration energy (eV) as a function of stress in biaxial strained silicon.

Referring to Table I, the migration energy from the initial (In_s - Si_i^{Td}) to final (In_i^{Td}) configuration is 0.884, 0920, and 0.910 eV for stress-free, 1Gpa stress, and 2Gpa stress, respectively. We can observe that the migration energy for uniaxial strain increases by 4 % with the 1 GPa stress while the migration energy then decreases with further increase of stress. Table II reveals that the migration energy under biaxial strain increases by 11% with the 1 GPa stress while the migration energy then returns to decrease with further increase of stress. If we consider the simulation region (217 atoms: 216 Si atoms + 1 In atom), the change in the total and migration energy are significantly noticeable which will retard the diffusion. We can see that the strain does not affect the migration pathway, however, it changes the diffusivity of indium based on changing total and migration energies.

3 RESULTS AND DISCUSSION

We investigated the effect of strain on indium diffusion for differently stressed In-Si complexes. In uniaxial tensile strained silicon, total energies for initial (In_s - Si_i^{Td}) and final (In_i^{Td}) configurations (Si: 216 atoms + In: 1 atom) were found to be decreasing until the threshold of 0.5GPa stress. In other words, the super cell which composed 216 Silicon atoms plus an indium atom becomes a more stable state than unstrained structure for super cell. This is the reason why In-Si complex has the highest barrier energy when 0.5GPa stress is induced for super cell. In the meanwhile, our *ab-initio* calculation revealed that the lowest total energy in biaxial tensile strained silicon occurs when 0.25GPa stress is induced. We also found that the barrier energy of In-Si complex is highest when we introduce a stress of 1GPa. That is because the lattice constant along the Y-axis decreases continuously while the lattice distance along the X-axis increases.

4 CONCLUSION

Atomic diffusion is an important phenomenon in condensed matters. Dopant diffusion plays a central role in fabricating the electronic devices in Si crystal. On this account, modeling of diffusion profiles of the dopant impurities is imperative for design of the devices. In this paper, we reported our *ab-initio* calculation on the tensile uniaxial and biaxial strain effects on indium atom migration for the research on ULSI devices. Our theoretical study enlightens us how the stress imposed on silicon substrate affect the total and migration energy of In-Si complex, while migration pathway of In-Si complex does not affect strain on silicon layer.

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