First-Principles Study on Indium Diffusion in Silicon Substrate under Hydrostatic Strain

Kwan-Sun Yoon, Young-Kyu Kim, and Taeyoung Won

Computational Electronics Center and Department of Electrical Engineering, Inha University
253 Yonghyun-dong, Nam-gu, Incheon 402-751, Korea
Phone: +82-32-875-7436 Fax:+82-32-862-1350 E-mail: yks@hsel.inha.ac.kr

Abstract

In this paper, we investigate indium diffusion in strained Si by using *ab-initio* calculation. We report the minimum energy path and the migration energy of indium in the hydrostatic strained silicon on SiGe substrate with 20% Ge. Stable configurations during indium diffusion were obtained from the calculation of the total energy, and we estimated the minimum energy path (MEP) with the nudged elastic band (NEB) method. After finding the MEP, we found the energy barrier for the diffusion of indium to be 1.1 eV from the calculation of the energy values at the minimum and the transition state. The energy barrier is about 0.3 eV higher than the case of unstrained Si.

1. Introduction

As complementary metal-oxide semiconductor (CMOS) devices are scaled down to the nanometer region, it is even more stringent to control the impurity profiles at the front-end process. Especially, the necessity for ultra-shallow junctions in nano-CMOS technology pushes the emergence of a novel alternative technology and material with a low diffusivity coefficient and lower activation energy for the impurity-doping process. Recently, stress effects on dopant diffusion also have become more important to achieve an excellent performance goal. And indium also has been attracting a great deal of interest as a candidate for a p-type dopant, especially for the fabrications of retrograde p-tubs and halo regions for n-channel FETs. Nevertheless, we do not understand the exact diffusion mechanism for indium, including diffusion parameters when we compared to the case of boron.

Recently, the kinetic Monte Carlo (KMC) method has been widely employed to model the thermal annealing process in nano-CMOS devices [1]. The KMC method is needed to simulate the diffusion of indium atoms on an atomistic scale. However, we do not have enough parametric values to perform the KMC calculation. Therefore, we performed *ab-initio* calculations in an effort to obtain parameters such as the input parameters of a migration event, one of the main events in thermal annealing. In this work, we investigated the MEP and the migration energy of indium diffusion in strained silicon by *ab-initio* calculations and transition state theory tools.

2. Numerical Calculations

We performed defect structure calculations in a cubic super- cell, comprising 216 silicon atoms with a single indium atom. The super-cell consists of 217 atoms including the indium atom with periodic boundary conditions [Fig. 1]. The calculations are implemented within density functional theory (DFT) by using Vienna *ab-initio* simulation package (VASP) which combines ultrasoft pseudopotentials and generalized gradient approximation (GGA) in the Perdew and Wang formulation [2-5].

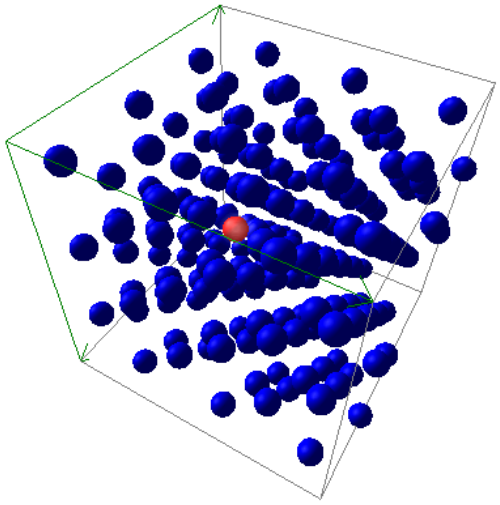


Fig. 1. A plot, drawn by VASP viewer, illustrating a super-cell with 256 silicon atoms (dark spheres) and one indium atom (light sphere).

NSTI-Nanotech 2007, www.nsti.org, ISBN 1420061828 Vol. 1, 2007

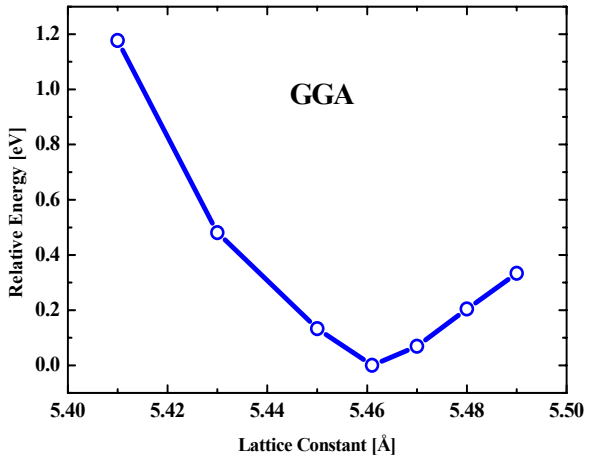
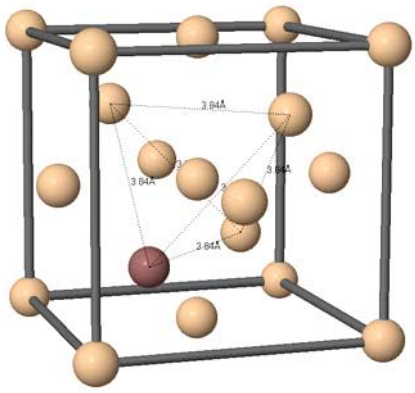


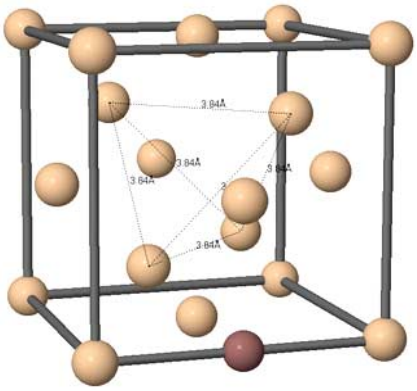
Fig. 2. Energy vs. Lattice constant for Si under hydrostatic strain. All energies are reported with respect to their minimum energy strain condition (unstrained Si) under GGA.

We used a cutoff energy E_c = 150.62 eV, 2 × 2 × 2 grid for the *k*-points mesh of Monkhorst-Pack [6], and a 3 × 3 × 3 simple cubic super-cell (216 atoms). Our optimized Si lattice constant for GGA in our system is 5.461 Å [Fig. 2]. To introduce hydrostatic strain in Si, we applied the lattice constant of relaxed SiGe since the strained Si grown on relaxed SiGe layer has same lattice constant as SiGe. The lattice constant of SiGe can be calculated as $a_{SiGe} = (1-x)a_{Si} + xa_{Ge}$, where a_{Si} and a_{Ge} are the lattice constants of Si and Ge, respectively.

Firstly, our *ab-initio* calculation revealed that the lowest-energy configuration of indium in strained Si is $In_s + Si_i^{Td}$, which means that the indium atom sits on a substitutional site and stabilizes a self-interstitial silicon in a nearby tetrahedral position [Fig. 3(a)], while the second lowest-energy structure is found to be In_i^{Td} [Fig. 3(b)]



(a) $In_s + Si_i^{Td}$



(b) In_i^{Td}

Fig. 3. Defect configurations: In atoms (dark-colored), Si self-interstitial (light-colored) are shown over the underlying diamond lattice. The $In_s + Si_i^{Td}$ (a) and the interstitial In at the tetrahedral position, In_i^{Td} (b) are also shown.

. Finally, the configuration of first and second lowest energy level has the same configuration with the case of unstrained Si, but the total energy of configuration has a gap as shown in Fig. 4.

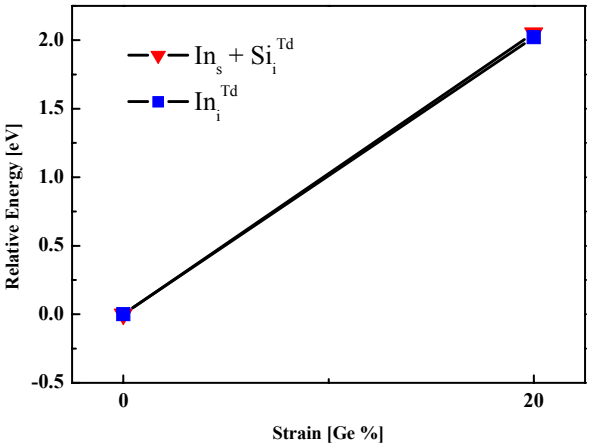
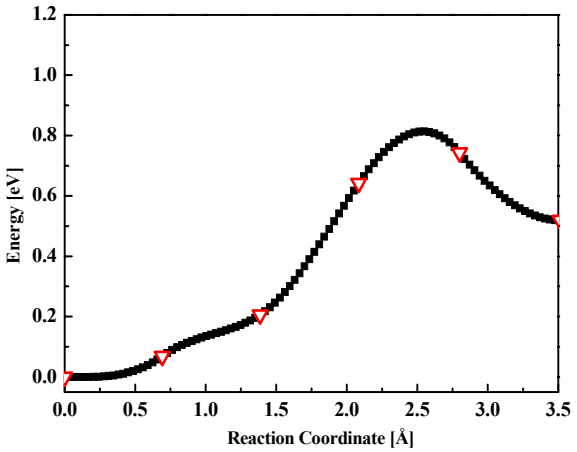


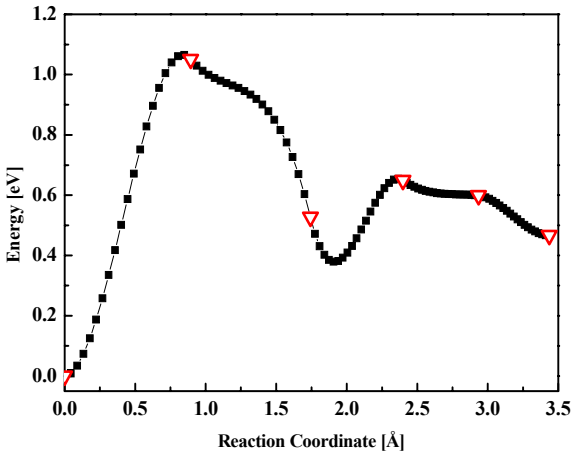
Fig. 4. The effect of strain on the total energy of the first and second lowest energy level: The triangles are the lowest energy configuration ($In_s + Si_i^{Td}$), and the squares are the second lowest energy configuration (In_i^{Td}). The energy of defect configuration in unstrained Si (Ge 0%) is used as the reference.

We can now obtain the energy barrier for indium migration if we investigate the minimum energy path (MEP) from the initial state to the final state. In order to search for the MEP, we performed the nudged elastic band (NEB) [7] calculation which is a kind of TST. The method

works by optimizing a number of intermediate images along the reaction path. Each initial image finds the lowest energy possible while maintaining equal spacing to neighboring images.



(a)



(b)

Fig. 5. The relative energy along the MEP of Si:In from $In_s + Si_i^{Td}$ to In_i^{Td} by the NEB method: (a) The squares line is the MEP in unstrained Si, (b) The circles line is the MEP in strained Si on SiGe substrate with 20% Ge.

Figure 5 is a diagram illustrating the MEP for indium, which was calculated by using the NEB method with four intermediate images. Figure 5 shows the minimum energy path of indium in unstrained and strained silicon. The initial and final states are fixed at the lowest-energy structure ($In_s + Si_i^{Td}$) and second lowest-energy structure (In_i^{Td}). The squares line is the MEP in unstrained Si, and the circles line is the MEP in strained Si on SiGe substrate with 20% Ge. The initial intermediate images, denoted with triangles, are linearly interpolated between the initial and the final images. Along the y-axis is shown the relative energy along the MEP of Si: In from the initial state ($In_s + Si_i^{Td}$) to the final state (In_i^{Td}). In Fig. 5, the interval between the initial intermediate images is interpolated with reference to the force being calculated during the simulation. In order to obtain an estimate of the saddle point and to sketch the MEP, it is important to interpolate between the images of the converged elastic band [8]. From the results, we can know that the MEP for indium migration in silicon has a higher energy barrier under strain.

3. Conclusion

In this paper, we studied the effect of strain on indium diffusion. In order to investigate the stress effect, it is essential to find out the migration path of indium. *Ab-initio* study in this work enabled us to quantum-mechanically perform electronic structure relaxation and get its total energy. We could figure out the atomistic configurations and migration energy during indium diffusion in strained silicon on SiGe substrate with 20% Ge. A After we found the minimum energy path, we tried to get the energy barrier for diffusing the particle through the calculation of the exact total energy at the transition state. We could also realize that the parameter extraction for In-related defects can be essential for exact modeling of the experimental diffusion profiles in the manufacture of the next-generation CMOS devices.

Acknowledgment

This research was supported by the MIC (Ministry of Information and Communication), Korea, under the ITRC (Information Technology Research Center) support program supervised by the IITA (Institute of Information Technology Advancement). (IITA-2006-C109006030030)

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