Extended Abstracts of the 2006 International Conference on Solid State Devices and Materials, Yokohama, 2006, pp. 700-701

P-8-14

Ab-initio Study on Energy Barrier for Neutral Indium Migration in a Silicon Substrate

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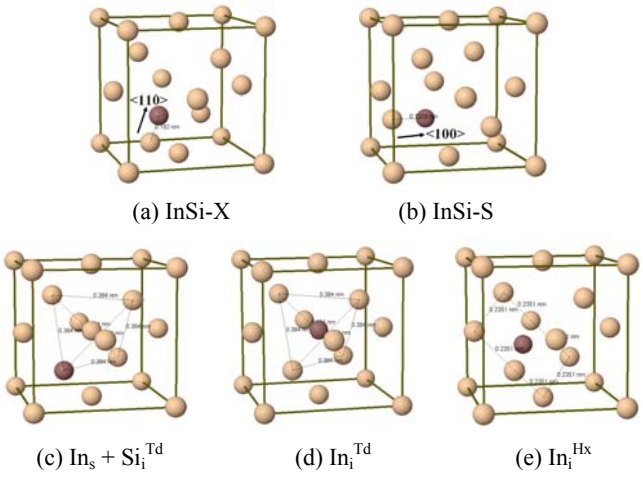
1. Introduction

Recently, indium attracts a great of attention due to possible exploitation for the fabrication of retrograde p-tub and halo region for n-channel in CMOS. Due to its heavier mass, indium is utilized as an alternative to boron in the silicon process in order to achieve shallow and steep profiles required for ultra-large-scale integration technology. It is known that indium diffuses mainly through the interstitial-mediated mechanism during the thermal annealing process. Recently, Kinetic Monte Carlo (KMC) method has been extensively investigated for the modeling of thermal annealing process for nano-CMOS devices [1]. The input parameters of a migration event, one of the main events in thermal annealing, should be provided either from experiments or from *ab-initio* calculations.

In this work, we investigated the atom-scale characterizations and MEP of indium diffusion in silicon by *ab-initio* calculations and transition state theory tools for estimating the migration energy for KMC.



(a) InSi-X (b) InSi-S

(c) $In_s + Si_i^{Td}$ (d) In_i^{Td} (e) In_i^{Hx}

Fig. 1. Indium atom is depicted as dark-colored and silicon atoms are depicted as light colored for each configuration. The InSi-X consists of silicon self-interstitial with an indium atom sharing the same lattice site, with the Si-indium dimer lying in the <110> direction. If the direction is <100> with the same configuration, the structure is referred to as InSi-S. The $In_s + Si_i^{Td}$ configuration means the case when indium atom sits on a substitutional site and stabilizes a silicon self-interstitial in a nearby tetrahedral position. The In_i^{Td} and In_i^{Hx} structures are the interstitial indium atom respectively in the tetrahedral position and in the hexagonal position.

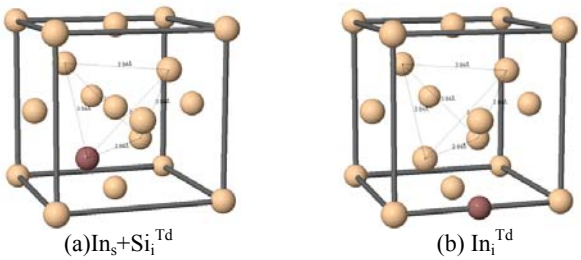
2. Numerical Calculations

First of all, we performed a defect structure calculation in a cubic super-cell, comprising 216 silicon atoms with a single neutral indium atom. In Fig. 1 is shown a schematic diagram illustrating the atomic structures comprising an indium atom in the silicon lattice. The *ab-initio* calculations were implemented within density functional theory (DFT) with VASP (Vienna *Ab-initio* Simulation Package) [2] which combines ultrasoft pseudopotentials and generalized gradient approximation (GGA) in the Perdew and Wang formulation.

Table 1. A table showing the calculated energies of the Si:In defect configuration: the listed energies are relative energies with reference to the ground-state configuration.

Configuration (In)	Relative energy [eV]
InSi-X	46.11
InSi-S	58.09
In_i^{Td}	0.43
$In_s + Si_i^{Td}$	0.00
In_i^{Hx}	1.63

Relative energy values of each defect configuration are shown in Table 1. The energy landscape, calculated by VASP for Si: In, indicates that the lowest-energy structure ($In_s + Si_i^{Td}$) consists of indium sitting on a substitutional site stabilizing a silicon self-interstitial in a nearby tetrahedral position [Fig. 2(a)]. The second lowest-energy structure is In_i^{Td}, the interstitial indium in the tetrahedral position [Fig. 2(b)]. The energy difference between the two defect configurations is 0.43 eV.



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

Fig. 2. Plots illustrating defect configurations: In atom (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.

Figure 3 shows another nearby tetrahedral position of indium. Both the middle of edge and the body center are tetrahedral sites in the cubic unit cell, while they have a little different total energy because of the finite size limitation of the super cell. The energy gap between them is about 0.02 eV, but we assume that the error is negligible. If the indium atom moves to the body center in the same unit cell, the indium atom must be switched by the silicon self-interstitial in the tetrahedral site (Si_i^{Td} of In_s + Si_i^{Td}) because the silicon atom is located at the body center. Because the energy barrier of diffusion path for the switching mechanism is too high, we believe that the indium atom diffuses to the tetrahedral site at the middle of edge.

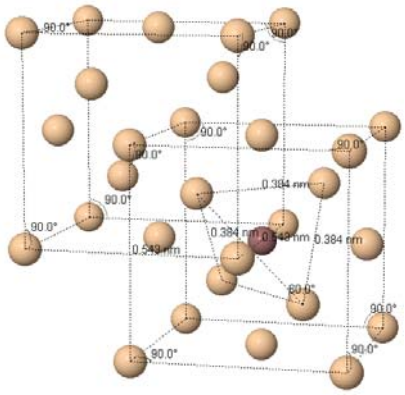


Fig. 3. Another nearby tetrahedral site is shown in the cubic unit cell. In atom (dark colored) in the middle of edge is located at the body center of other unit cell.

In the prior investigation, we found that the initial state is In_s + Si_i^{Td} while the final state is In_i^{Td}. Repeating the transitions between those two states, the neutral indium diffuses in silicon. Consequently, we can now obtain the energy barrier for indium migration if we investigate the MEP from the initial state to the final state.

In order to search for the MEP, we performed the climbing image nudged elastic band (CINEB) [3] calculation which is a kind of TST. Figure 4 is a diagram illustrating the calculated minimum energy path for indium via the CINEB method with four intermediate images. The initial intermediate images, denoted with triangles, are linearly interpolated between the initial and final images. The Migration energy is estimated as an energy difference to move from a local energy minimum state to another local minimum along the diffusion path. We find that the migration energy of In-interstitial defect is 0.79 eV in Fig. 4, which is in agreement with previous estimation [4].

3. Conclusion

In order to decide the migration energy for the diffusion of indium, it is essential to find out the migration path of

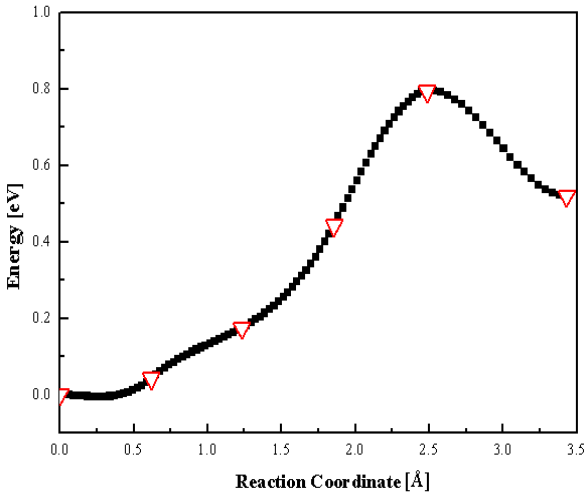


Fig. 4. The relative energy along the MEP of Si:In from In_s + Si_i^{Td} to In_i^{Td} by the climbing image nudged elastic band method. The triangles indicate the simulation images and the squares are the interpolation by using the force parallel to the band.

the interstitial-mediated mechanism. *Ab-initio* study in this work comprises steps of performing the electronic structure relaxation and obtaining its total energy at the local minimum. We could come up with the atomistic configurations and migration energy during indium diffusion in silicon, wherein we tried to find out saddle points from a minimum and reaction pathway between those two stable states by using TST. After we found the transition state, we tried to get the energy barrier for diffusing the particle through the calculation of the exact total energy at the transition state. These *ab-initio* results of indium diffusion in silicon are essential in obtaining an exact modeling of the experimental profiles.

Acknowledgements

This work was supported partly by the Korean Ministry of Information & Communication (MIC) through the Information Technology Research Center (ITRC) Program supervised by the Institute of Information Technology Assessment (IITA) and partly by the Korea Institute of Science and Technology Information (KISTI) through the Seventh Strategic Supercomputing Applications Support Program. The authors would like to express special thanks to the Supercomputing Center at the KISTI for providing us the computing resources.

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