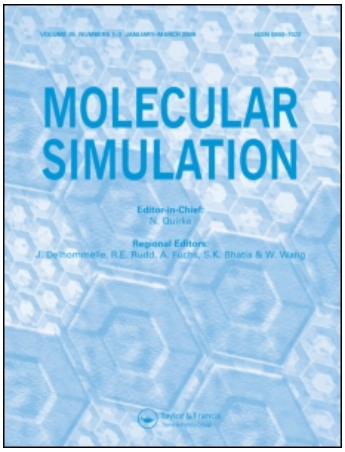

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Ab-initio study on indium diffusion in silicon substrate under hydrostatic stress

K. -S. Yoon[a]; Y. -K. Kim[a]; T. Won[a]
[a] ITRC for Computational Electronics, Department of Electrical Engineering, Inha University, Incheon, Korea

To cite this Article Yoon, K. -S. , Kim, Y. -K. and Won, T.(2008) '*Ab-initio* study on indium diffusion in silicon substrate under hydrostatic stress', Molecular Simulation, 34: 1, 47 — 50
To link to this Article: DOI: 10.1080/08927020801895377
URL: http://dx.doi.org/10.1080/08927020801895377

Molecular Simulation
Vol. 34, No. 1, January 2008, 47–50

Taylor & Francis
Taylor & Francis Group

Ab-initio study on indium diffusion in silicon substrate under hydrostatic stress

K.-S. Yoon, Y.-K. Kim and T. Won*

ITRC for Computational Electronics, Department of Electrical Engineering, Inha University, 253 Yonghyun-dong, Nam-gu, Incheon 402-751, Korea

(Received 14 August 2007; final version received 3 December 2007)

In this paper, we report our *ab-initio* study on indium diffusion in strained Si. We investigated the minimum energy path as well as the migration energy for indium atoms in the hydrostatic strained silicon wherein the strain was incorporated by constructing a silicon layer on SiGe substrate with 20% germanium mole fraction. The *ab-initio* calculation allowed us to figure out the lowest-energy structure ($In_S + Si_i^{Td}$) and the next lowest energy structure (In_i^{Td}) during indium diffusion. The energy of migration barrier was also predicted from the nudged elastic band and climbing nudged elastic band method. Consequently, we found that the energy barrier was a little higher than the case of unstrained Si.

Keywords: *ab-initio*; indium; hydrostatic stress

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 (Field Effect Transistors). 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 minimum energy path (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. The calculations are implemented within density functional theory by using Vienna *ab-initio* simulation package which combines ultrasoft pseudopotentials and generalized gradient approximation (GGA) in the Perdew and Wang formulation [2–5].

We used a cutoff energy $E_c = 150.62\,\text{eV}$, $2 \times 2 \times 2$ grid for the *k*-points mesh of Monkhorst–Pack [6], and a $3 \times 3 \times 3$ simple cubic super-cell (216 atoms). Our optimized Si lattice constant for GGA in our system is 5.461 Å (Figure 1). Furthermore, we also calculated the lattice constant of Ge for our system, which was supposed 216 atoms of Ge. We derived Ge lattice constant of 5.677 Å using similar method like Figure 1.

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. We investigated the alteration of SiGe lattice constant by x (Ge mole fraction). The lattice constant of SiGe can be calculated as

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

where a_{Si} and a_{Ge} are the lattice constant of Si and Ge, respectively. Through the equation of number one, we derived 5.504 Å as the lattice constant of $Si_{0.8}Ge_{0.2}$ for our GGA calculations. Indium has similar coordinate-bond like boron in silicon substrate basis on a periodic

*Corresponding author. Email: twon@hsel.inha.ac.kr

ISSN 0892-7022 print/ISSN 1029-0435 online

DOI: 10.1080/08927020801895377
http://www.informaworld.com

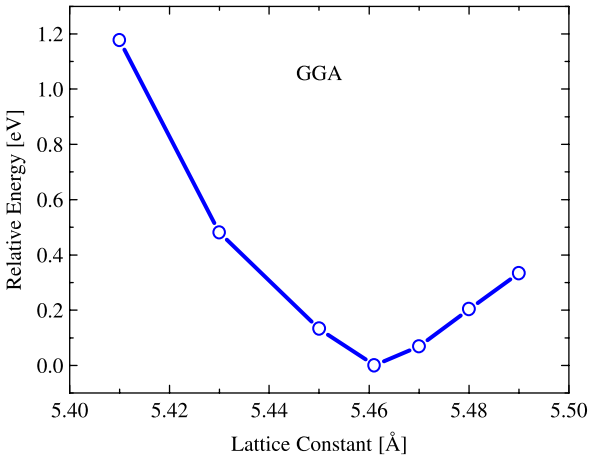

Figure 1. A plot illustrating energy dependence on lattice constant for Si under hydrostatic strain. All energies are expressed with respect to their minimum energy strain condition (unstrained Si) under GGA.

table of elements. Having an eye on this character, we calculated energies of five possible configurations like boron. We expressed relative energy of configuration basis on the lowest potential energy configuration in Table 1. $In_s + Si_i^{Td}$ consists of indium atom sitting on a substitutional site stabilizing a silicon self-interstitial in a nearby tetrahedral position. In_i^S is the configuration that In atom and silicon interstitial share one lattice site along the ⟨100⟩ direction, and In_i^X is indium atom and silicon interstitial joint along the ⟨110⟩ direction. In_i^{Td} is the interstitial indium in the tetrahedral position and In_i^{Hx} is the interstitial indium in the hexagonal position.

Our *ab-initio* calculation revealed that the lowest-energy configuration of indium in hydrostatic strained Si is $In_s + Si_i^{Td}$ (Figure 2(a)), while the second lowest-energy structure is found to be In_i^{Td} (Figure 2(b)). 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 approximately increased 2 eV contrast with unstrained Si.

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 nudged elastic band (NEB) [7] calculation. After performing the NEB calculations, we also performed climbing image nudged elastic band (CINEB) for the maximum energy point. The method works

Table 1. Relative energy for various configurations.

Configuration	Relative energy [eV]
$In_i + Si_i^{Td}$	0.00
In_i^S	58.09
In_i^X	46.11
In_i^{Td}	0.43
In_i^{Hx}	1.65

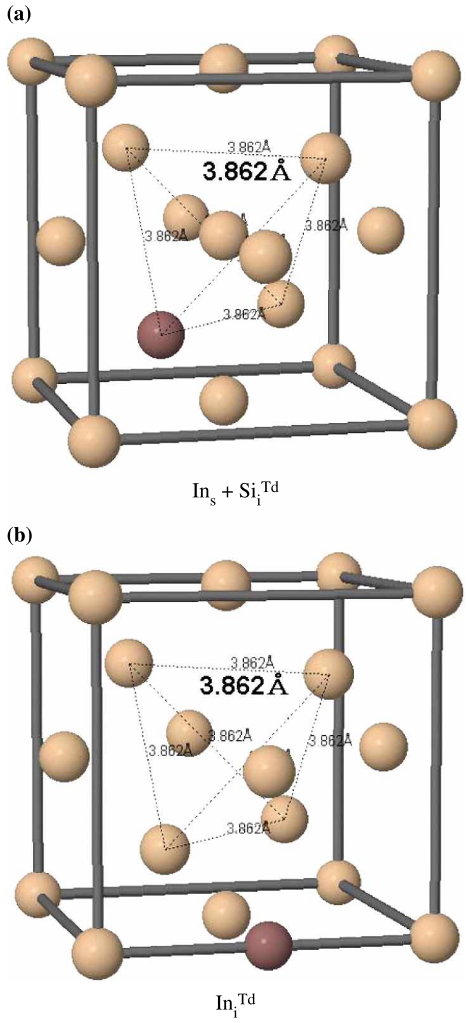

Figure 2. Defect configurations: Indium atoms (dark-colored), silicon self-interstitial (light-colored) are shown over the underlying diamond lattice. The $In_s + Si_i^{Td}$ (a) and the interstitial In at the tetrahedral position, In_i^{Td} (b) are also shown.

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. Figure 3 is a diagram illustrating the MEP for indium, which was calculated by using the NEB and CINEB method with four intermediate images.

The average rate of movement of defects in solids by thermal activation can be calculated on the classical rate theory. A migration event is specified by the following two parameters:

$$d = d_0 \exp[-E_m/kT] \tag{2}$$

where d_0 is the prefactor and E_m is the migration energy, the free energy needed to carry the defect from an initial equilibrium position to a saddle point. T denotes the absolute temperature, and k is the Boltzmann's constant.

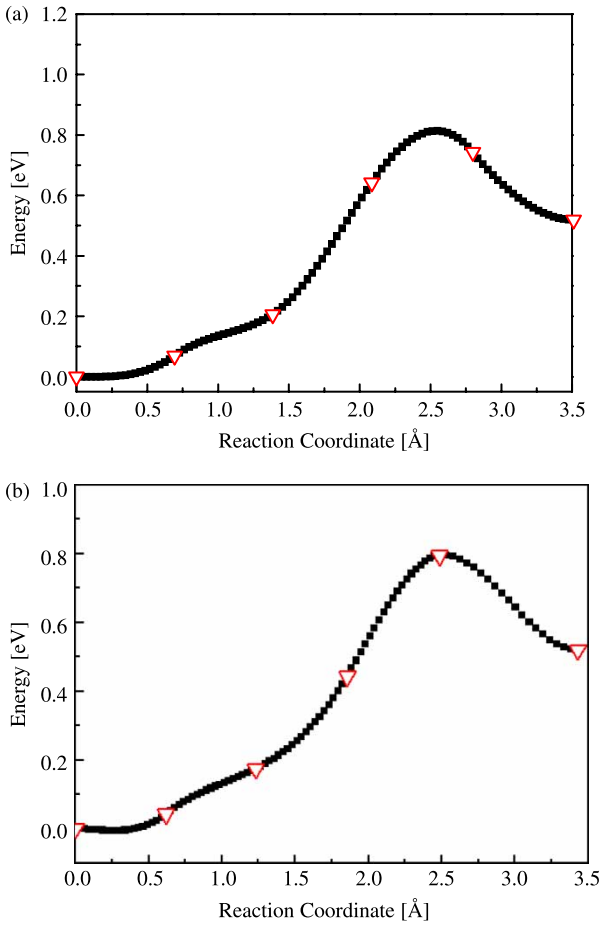

Figure 3. The relative energy along the MEP of Si:In from $In_s + Si_i^{Td}$ to In_i^{Td} by the (a) NEB and (b) CINEB method in unstrained Si.

Under the assumption that the diffusion process though discrete jumps of equal length, the prefactor can be written as

$$d_0 = \frac{z}{6}\nu^* r^2. \tag{3}$$

Here, z is the number of possible neighboring jump sites, ν^* the jump, or attempt, effective frequency of the point defect from one equilibrium site to another and r the jump distance.

If we know the effective frequency, we can calculate the prefactor because the values of z and r are constants. In order to obtain the effective frequency, we use the dynamical matrix method. The dynamical matrix method is used for the calculation of harmonic frequencies and the prefactor of a reaction. The basic idea is that the potential is assumed to be harmonic for both the local minimum state and the transition state. With this assumption, one can formulate the migration prefactor as the ratio of the products of the frequencies of the normal modes of the initial state over the transition state. Therefore, one needs to know before hand both the initial state and the transition state in order to perform a dynamical matrix calculation. In our previous section, the transition state configuration is obtained by the CINEB.

According to the dynamical matrix theory, the transition rate ν^* in the harmonic approximation is given by

$$\nu^* = \frac{\prod_{j=1}^{N} \nu_j}{\prod_{j=1}^{N-1} \nu_j'} \tag{4}$$

where ν_j and ν_j' are the normal mode frequencies at the minimum energy state and the transition state respectively. The product in the denominator does not include the imaginary frequency at the saddle point. As a result, the attempt frequency of the indium migration is calculated to be $2.35 \times 10^{12}\,s^{-1}$ by the dynamical matrix method. For the normal modes, we displace 8 atoms with displacement 0.05 Å in x, y and z directions (24×24 dynamical matrix). The corresponding migration prefactor of neutral indium is $0.87 \times 10^{-3}\,cm^2\,s^{-1}$.

Figure 4 shows the minimum energy path of indium in 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 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}). 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.

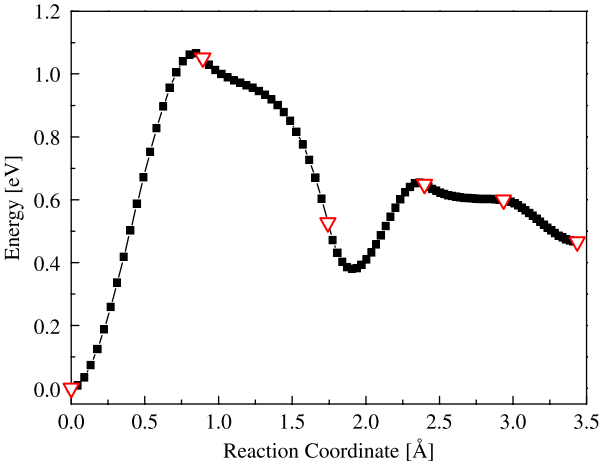

Figure 4. The relative energy along the MEP of Si:In from $In_s + Si_i^{Td}$ to In_i^{Td} in strained Si on SiGe substrate with 20% Ge.

3. Conclusion

In this work, 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 obtain the total energy. After we calculated total energy of five possible configurations, we could figure out the minimum energy path of indium in strained silicon on SiGe substrate. We obtained the energy barrier for diffusing the particle through the calculation of the exact total energy at the transition state basis on the minimum energy path. Hereby, 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. 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.

Acknowledgements

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-2007-C109007010030) and partly by the Korea Institute of Science and Technology Information (KISTI) through the Tenth Strategic Super- computing Applications Support Program (KSC-2007-S00-1013).

References

[1] K.A. Fichthorn and W.H. Weinberg, *Theoretical foundations of dynamical Monte Carlo simulations*, J. Chem. Phys. 95 (1991), p. 1090.
[2] G. Kresse and J. Hafner, *Ab initio molecular dynamics for liquid metals*, Phys. Rev. B 47 (1993), p. 558, ibid. 49 (1994), p. 14251.
[3] G. Kresse and J. Furthmüller, *Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set*, Comput. Mat. Sci. 6 (1996), p. 15.
[4] G. Kresse and J. Furthmüller, *Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set*, Phys. Rev. B 54 (1996), p. 11169.
[5] G. Kresse and J. Hafner, *Norm-conserving and ultrasoft pseudopotentials for first-row and transition elements*, J. Phys. Condens. Matter 6 (1994), p. 8245.
[6] H.J. Monkhorst and J.D. Pack, *Special points for Brillouin-zone integrations*, Phys. Rev. B 13 (1976), p. 5188.
[7] G. Henkelman and H. Jónsson, *Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points*, J. Chem. Phys. 113 (2000), p. 22.
[8] H. Jónsson, G. Mills, and K.W. Jacobsen, *Nudged Elastic Band Method for Finding Minimum Energy Paths of Transitions*, B.J. Berne, G. Ciccotti, and D.F. Coker, eds., World Scientific, Singapore, 1998.