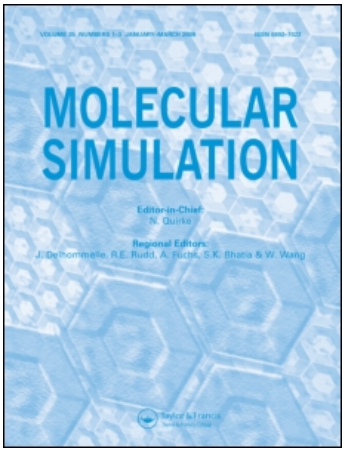

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Atomistic modelling for boron diffusion in strained silicon substrate

Young-Kyu Kim[a]; Kwan-Sun Yoon[a]; Joong-Sik Kim[a]; Han-Geon Kim[a]; Taeyoung Won[a]
[a] Department of Electrical Engineering, School of Engineering, Inha University and National IT Research Center for Computational Electronics, Incheon, Korea

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Atomistic modelling for boron diffusion in strained silicon substrate

Young-Kyu Kim*, Kwan-Sun Yoon, Joong-Sik Kim, Han-Geon Kim and Taeyoung Won

Department of Electrical Engineering, School of Engineering, Inha University and National IT Research Center for Computational Electronics, 253 Yonghyun-dong, Nam-gu, Incheon 402-751, Korea

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We discuss the issue of boron diffusion in biaxial tensile strained {001} Si and SiGe layer with kinetic Monte Carlo (KMC) method. We created strain in silicon by artificially adding a germanium mole fraction to the silicon in order to perform a theoretical analysis. The strain energy of the charged defects was calculated from *ab initio* calculation whereas the diffusivity of boron was extracted from the Arrhenius formula. Hereby, the influence of the germanium content on the diffusivity of the impurity atom was estimated. Our KMC study revealed that the diffusion of the boron atoms was retarded with increasing germanium mole fraction in the strained silicon layer. Furthermore, we derived the functional dependence of the in-plane strain as well as the out-of-plane strain as a function of the germanium mole fraction, which is based on the distribution of equivalent stress along the Si/SiGe interface.

Keywords: boron; diffusion; kinetic Monte Carlo

1. Introduction

Recently, the incorporation of a biaxial tensile strain in the channel region has attracted a great deal of attention due to enhance carrier mobility and make shallow junction for nano-scale metal oxide semiconductor field effect transistor (CMOS) [1–4]. Despite semiconductor industry adopts the strained silicon technology for the channel, the understanding of the dopant diffusion in the strained silicon is premature [5–7]. We investigated energies of boron charged defects and minimum migration path by performing *ab initio* calculation. We undertook the atomistic investigation on the boron diffusion in biaxial tensile strained {001} silicon as well as the relaxed Si_xGe_{1-x} layer with kinetic Monte Carlo (KMC) method with basis on *ab-initio* results.

2. Simulation and results

Figure 1 is a schematic diagram illustrating a metal-oxide semiconductor field effect transistor (MOSFET) structure with a biaxial strained silicon layer on silicon–germanium buffer. We assumed that the silicon–germanium buffer layer is thick enough for the wide range of germanium mole fraction (10 ~ 60%) to be considered as being relaxed. In this work, we investigated the impurity profile from the surface vertically down to the 500 nm during the implant process as well as the diffusion process.

We investigated the alteration of $Si_{1-x}Ge_x$ lattice constant by x (Ge mole fraction). The lattice constant of $Si_{1-x}Ge_x$ can be expressed by

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

where a_{Si} and a_{Ge} lattice constant of Si and Ge, respectively. The perpendicular elements were calculated by elastic theory. According to the elastic theory, 'In-plane' and 'Out-of-plane' strain can be calculated by

$$\varepsilon_{\parallel} = \frac{(a_{SiGe} - a_{Si})}{a_{Si}} \tag{2}$$

$$\varepsilon_{\perp} = \frac{(a_{\perp} - a_{Si})}{a_{Si}} \tag{3}$$

and the each strain ingredient was able to be changed other strain it according to Equation

$$\varepsilon_{\perp}/\varepsilon_{\parallel} = -2(C_{12}/C_{11}) \tag{4}$$

where C_{11} and C_{12} are the elastic constants of Si. We used experimental consequence of $C_{11} = 167$ Gpa and $C_{12} = 65$ Gpa [5,6]. Through the Equation (3), we completed the $Si_{1-x}Ge_x$ lattice constant on Ge concentration. The lattice constants of parallel direction had increasing trend on the Ge concentration. And those of perpendicular direction had decreasing drift by Ge concentration. But, the altering trend of parallel component was small bigger than other. Such an each of lattice constant had a thread of connection with the lattice constant of strained Si.

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

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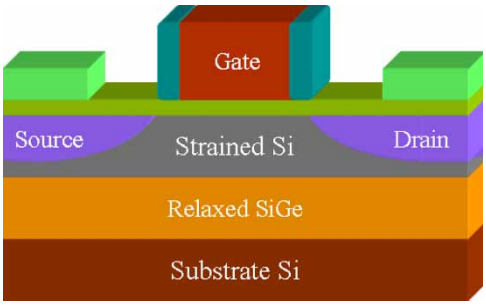

Figure 1. Schematic figure of the strained silicon MOSFET structure employed in this work. The strained silicon layer is thin enough to be less than critical thickness on the relaxed silicon–germanium buffer layer wherein the silicon–germanium buffer layer is a source for providing the stress on the silicon channel layer.

Table 1 shows the list of magnitude of the formation energy for charged defects, i.e. Bi^{+}, Bi, and Bi^{-}, respectively, with varying the germanium mole fraction from 10 to 60%. The formation energy is needed for the next-step KMC calculation for boron. Table 2 shows the list of magnitude of the migration energy for charged defects, i.e. Bi^{+}, Bi, and Bi^{-}, respectively, with varying the germanium mole fraction from 10 to 60%. Both chemical and mechanical effects due to the presence of strain in silicon layer are merged into the numerical numbers such as the migration and formation energy in Tables 1 and 2.

In order to calculate the corresponding energy of boron in the SiGe and strained Si layer, we took into account the charged defects of boron via Vienna *Ab initio* Simulation Package. The *ab initio* calculations were implemented with density functional theory which combines ultra-soft pseudo-potentials and generalised gradient approximation (GGA) in the Perdew and Wang formulation. We employed a cutoff energy of $E_c = 150.62$ eV, $2 \times 2 \times 2$ grid for the k-points mesh of Monkhorst–Pack, and a $3 \times 3 \times 3$ simple cubic super-cell (216 atoms). Our optimised silicon lattice constant for GGA in our system is 5.461 Å.

Table 1. Formation energy of charged defects as a function of Ge concentration.

Ge concentration (%)	Positive (eV)	Neutral (eV)	Negative (eV)
10	2.36	2.6	3.54
20	2.31	2.6	3.59
40	2.23	2.6	3.67
60	2.16	2.6	3.74

Table 2. Migration energy of charged defects as a function of Ge concentration.

Ge concentration (%)	Positive (eV)	Neutral (eV)	Negative (eV)
10	0.71	0.41	0.80
20	0.67	0.37	0.74
40	0.59	0.28	0.63
60	0.50	0.20	0.52

After introducing the defects to a super cell, all the atoms in the cell were relaxed to get the minimum energy. The nudged elastic band method determines the minimum energy from starting point (the lowest formation energy) to the saddle point [7]. We referred to the charged defect values of boron from the previous experiment articles and then extracted the formation and migration energies of boron following each charged defect by Ge concentration. We assumed the migration pathway as:

$$B_s - Si_i^{T} \rightarrow B_i^{S} \rightarrow B_i^{H} \quad \text{(neutral)} \tag{5}$$

$$B_s - Si_i^{T+} \rightarrow B_i^{B+} \quad \text{(positive)} \tag{6}$$

$$B_i^{X-} \rightarrow B_i^{S-} \quad \text{(negative)} \tag{7}$$

For neutrally charged B–Si complex, B_s–Si^{T} is the most stable state which is composed by a substitutional B and tetrahedral Si interstitial. B_i^{S} is the second stable state where B and Si interstitial share one lattice site along the ⟨100⟩ direction. B_i^{H} is the third stable configuration where B is in hexagonal interstitial site. For a positively charged B–Si complex, B_s–Si^{T+} is the most stable configuration which comprises one electron less than B_s–Si^{T}. B_i^{B+} is the next stable state in a positive pathway where interstitial B is located at a bond-centered site. For negatively charged B–Si complex, B_i^{X-} is the most stable site where B and Si interstitial share one lattice site along the ⟨110⟩ direction. B_i^{S-} is the next stable configuration where one extra electron is present than B_i^{S}. We expressed the each boron site on Figure 2.

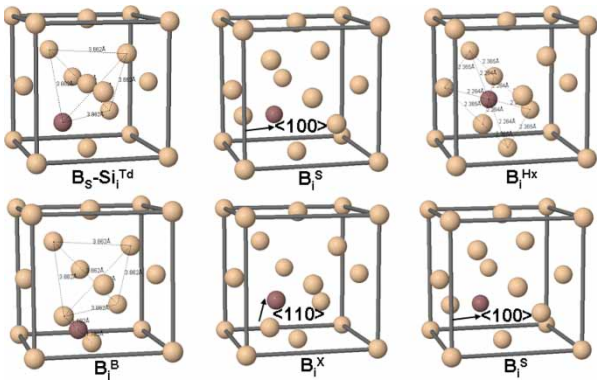

Figure 2. The B atom (red-coloured) and the self interstitial Si (yellow-coloured) complexes concerned in boron diffusion.

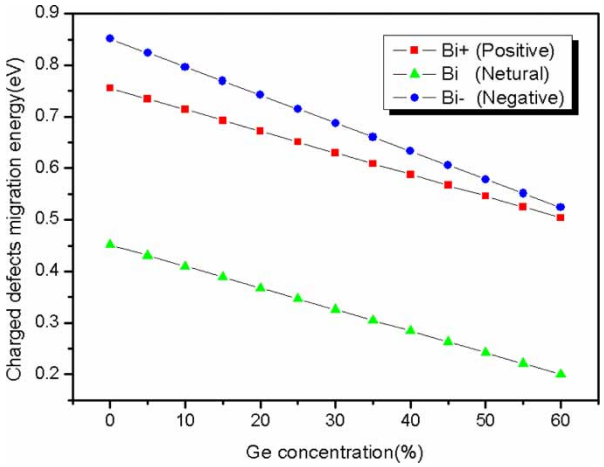

Figure 3. Migration energies of charged boron interstitials by Ge concentration.

This calculation allowed us to notice that E_F (formation energy) of positive B_s–Si^T increases a little bit and that E_F of negative Bi^X decreases a little. We also found that all of charged defects decrease more energy with Ge concentration than E_F. Figure 3 is shown the E_M (migration energy) trend. These investigations enabled us to discover B diffusivity trend in strained silicon by Ge concentration. The boron diffusivity should be modified by taking the strain effect into account with the data shown in Tables 1 and 2. The boron diffusivity can be written by Arrhenius form [8]. We displayed B diffusivity by Ge concentration in Figure 4 on 970°C temperature. It showed that B diffusivity was a sharp decline by increasing Ge concentration. This figure gave a hint that diffusion of B will be retard to us. Consequently, it should be noted that more Ge concentration in the layer causes the reduction in energy

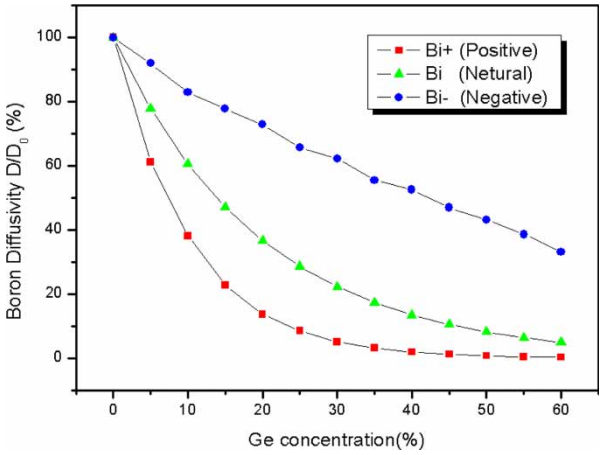

Figure 4. In case of 970°C, B diffusivity in biaxial strained Si/SiGe layer by Ge concentration.

when compared with unstrained case. This phenomenon seems to be due to the combination of elastic stress and band gap narrowing.

It was calculated from Arrhenius form by using results of *ab initio* calculations (formation and migration energies of charged defect).

We performed numerical simulations on boron diffusion in silicon–germanium and strained Si above the silicon–germanium layer with basis on the preparatory work for numerical simulation. We applied solid phase epitaxial regrowth velocity, Faulted frank Dislocation Loops are considered for the geometry and binding energy for {311} defects in our KMC method. KMC methods consists of many possible events which evolve as a series of independent event occurring. All events have their own event rates. Event rates are calculated by Equation (8). E_b is a migration energy barrier for jump event of the mobile species or a binding energy for clusters evaporation. v_0 is the attempt frequency, which is simply the vibration frequency of the atoms. Typically, it is of the order of 1/100 fs. These parameters come from *ab initio* calculation or experimental data.

$$v = v_0 \exp\left(\frac{-E_b}{K_B T}\right). \tag{8}$$

We consider thermally activated events in a thermal-annealing simulation after ion implantation. If the probability for the next event to occur is independent of the previous history, and the same at all times, the transition probability is a constant. Then, the process is a so-called Poisson process. To derive the time dependence, consider a single event with a uniform transition probability r. Let f be the transition probability density, which gives the probability rate at which the transition occurs at time t. The change of $f(t)$ over some short time interval dt is proportional to r, dt and f, because f gives the probability density that the physical system still remains at time t.

$$df(t) = -rf(t)dt. \tag{9}$$

Further, the solution is given by with boundary conditions.

$$f(t) = re^{-rt}, \quad f(0) = r \tag{10}$$

Therefore, the simulation time is updated for $(t = t + \Delta t)$ according to event rates as follows, because an ensemble of independent Poisson processes will behave as one large Poisson process:

$$\Delta t = -\frac{\ln u}{R}. \tag{11}$$

Here, u is a random number and R is the total sum of all possible event rates. We select an event according to the event rates, and KMC is suitable to simulate non-uniform time evolution processes. We simply expressed KMC flow chart in Figure 5 above detailed explanations.

In the case of the SiGe layer, boron was implanted with energy of 5 keV, a dosage of $10^{15}\,cm^{-2}$ and a tilt angle of 7°, followed by the spike rapid thermal anneal (RTA) process at 970°C. We investigated three cases wherein Ge concentration was varied from 20, 40 and 60%, respectively. The profiles were compared with the experimental SIMS data in Figure 6.

In the simulation of strained Si layer, the adjustment of implant energy is not needed for the diffusion modelling in strained Si. However, it is needed to take the energies of the charged defects and the diffusivity of boron into account. This is due to the fact that there does not present a germanium atom in the strained Si layer. We assumed that boron was implanted into the silicon layer above the silicon–germanium layer with 400 eV for ultra shallow junction with a dosage of $10^{15}\,cm^{-2}$, which is identical with the implantation condition for the silicon–germanium layer when the germanium mole fraction is 20%. The strained silicon layer was annealed at 940°C under the spike RTA condition, which was compared with SIMS data in Figure 7.

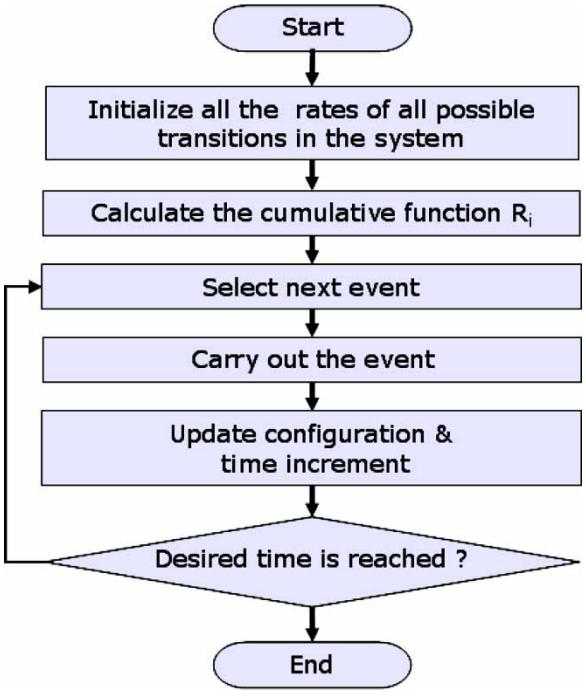

Figure 5. The flow chart of kinetic Mote Carlo (KMC) method: KMC in based on Monte Carlo approach combined with Poisson process, which is found to be more accurate than the continuum models.

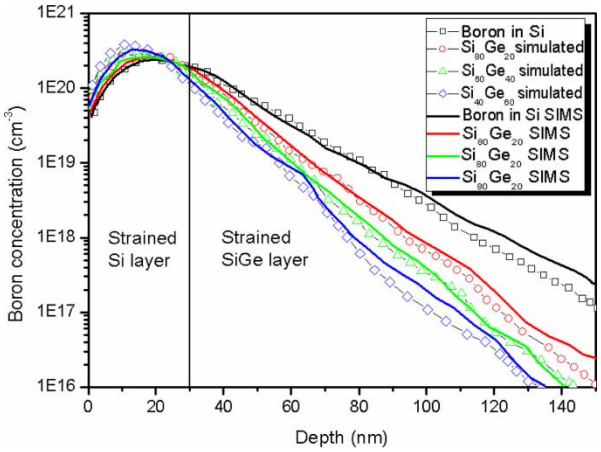

Figure 6. Simulation results of boron diffusion (line + symbol) and SIMS profiles (line) in relaxed SiGe. The energy of 5 keV, a dosage of $10^{15}\,cm^{-2}$ and a tilt angle of 7°, followed by the spike RTA process at 970°C.

The energy of 400 eV, a dosage of $10^{15}\,cm^{-2}$, which is identical with the implantation condition for the silicon–germanium layer when the germanium mole fraction is 20%. Finally, the strained silicon layer was annealed at 940°C under the spike RTA condition.

Furthermore, we formulated a correlation between the equivalent stresses, the in-plane strain and the out-of-plane strain as a function of germanium mole fraction as shown in Table 3.

Referring to Table 3, we can see that the silicon germanium layer with 10% mole fraction exhibits the in-plane strain of 0.004 and out-of-plane strain of -0.003 which corresponds to 0.47 GPa of stress.

Finally, the relationship correlating the magnitude of equivalent stress and the Ge mole fraction in the silicon–germanium layer makes it possible for us to figure out the

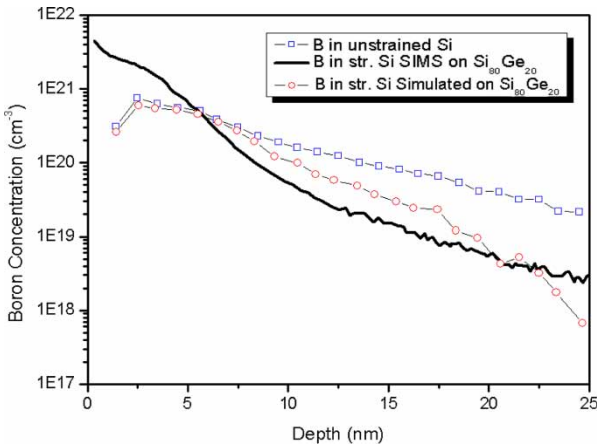

Figure 7. Simulation results of boron diffusion (line + symbol) and SIMS profile (line) in strained Si.

Table 3. In-plane strain, out-of-plane strain, and equivalent stress of Si/SiGe interface direction in terms of Ge concentration.

Ge concentration (%)	In-plane Strain	Out-of-plane strain	Equivalent stress (GPa)
10	0.004	−0.003	0.47
20	0.008	−0.006	0.93
40	0.016	−0.012	1.87
60	0.024	−0.018	2.80

influence of strain in the silicon layer even if the strain is applied to the silicon layer by mean of any arbitrary method.

3. Conclusion

We report our KMC study on the effect of strain on B diffusion in silicon and relaxed SiGe layer by using charged defect energy and diffusivity. The simulation results imply that boron diffusion is drastically retarded in a strained Si and relaxed SiGe when compared to a case with unstrained silicon. We also derived the distribution of equivalent stress along the heterojunction interface with varying the Ge implant for giving rise to a strain to the pure silicon.

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