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Kinetic Monte Carlo (KMC) Modeling for Boron Diffusion in Strained Silicon

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1. Introduction

Since strained silicon is widely used in the current nano-CMOS technology, it is essential to understand the diffusion mechanism of impurities in strained Si/SiGe. We undertook an investigation on boron diffusion in biaxial tensile strained {001} Si and SiGe layers by using KMC (kinetic Monte Carlo) method. As a scheme for generating a strain on the silicon layer system, we created a virtual SiGe layer on the silicon substrate. The strain energy of the charged defects was calculated from *ab-initio* calculations while the diffusivity of boron was extracted from the Arrhenius form [1, 2]. In the case of strained SiGe layer simulation, we considered wide range of implant energy from the electronic stopping model of Lindhard theory [3] as well as the charged defects and diffusivity. Finally, we also calculated the distribution of stresses around the Si/SiGe interface with basis on the elastic theory.

2. Experiment

The penetration depth of ion implanted dopants in SiGe is reduced when compared with the case of pure silicon. This is because the electronic stopping power in SiGe is higher than that in silicon from the Lindhard theory [3]. Consequently, we had to adjust the range of implant energy in accordance with each Ge concentration for making virtual SiGe layer on the silicon substrate. We performed numerical simulations with varying the implant energy between 0 ~ 50keV, a dosage of 10^{15}cm^{-2} for this adjustment. After simulation, we compared SIMS profiles for 50keV boron implantations in $Si_{1-x}Ge_x$ with a thickness of 330nm on a silicon substrate. From this study, we could find that the calibrated implant energy which takes into the effect of strain should be approximately 8 ~ 9% lower than the case of normal silicon. Figure 1 is a simulated ion profile illustrating the effect of strain on the projected range of ion implantation for the strained silicon due to virtual SiGe layer.

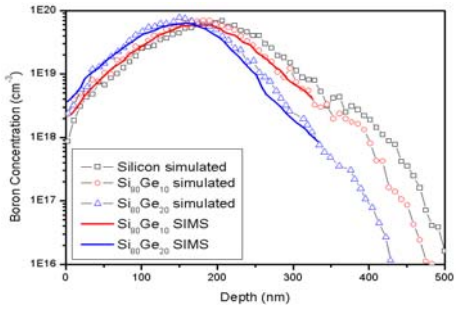

Fig. 1. 50keV boron implantation simulations (symbol + line) and SIMS profiles (line) in the $Si_{1-x}Ge_x$ with x=0%, 10% and 20%.

In order to calculate the corresponding implant energy in the SiGe layer, we took into account the charged defects of boron via density functional theory (DFT). After introducing the defects of super cell, all the atoms in the cell were relaxed to get the minimum energy. The NEBM (nudged elastic band method) determines the minimum energy from starting point (the lowest formation energy) to the saddle point. We referred to the charged defect values of boron from the prior art [1, 2] and then approximated the formation and migration energies of boron in strained structure. We assumed the migration pathway as Bs-Si^{T} → Bi^{S} → Bi^{H} (neutral), Bs^{-} → Bi^{B+} → Bs-Si^{T+} (positive) and Bi^{X-} → Bi^{S-} (negative) path [4]. In Tables 1 and 2 are shown the energy of B-Si complex with respect to Ge mole fraction.

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 1. Formation energy of charged defects as a function of the 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

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

It should be noted that more Ge concentration in the layer causes the reduction in energy when compared with unstrained case. This phenomenon seems to be due to the combination of elastic stress and band gap narrowing.

Finally, boron diffusivity should be adjusted in accordance with the data shown in Tables 1 and 2 when strain is generated due to the virtual SiGe layer. The boron diffusivity can be written by Arrhenius form as the following:

$$D^{BI} = D_0^{BI} \exp(-E_a / kT) = D_0^{BI} \exp[-(H^f{}_{BI} + H^m{}_{BI}) / kT] \quad (1)$$

where D_0^{BI} is pre-factor, and the activation energy E_a includes the formation enthalpy of stable B-Si complex H^f_{BI} and migration enthalpy H^m_{BI}. After preparatory work for numerical simulation, we performed simulations on boron diffusion in strained SiGe and Si above the virtual SiGe layer. In the case of strained SiGe layer, boron was implanted into the SiGe layer with energy of 5keV, a dosage of $10^{15}cm^{-2}$ and a tilt angle of 7°, followed by the spike RTA annealing process at 970℃. We investigated three cases wherein Ge concentration was varied from 20%, 40% and 60%, respectively. The profiles were compared with the experimental SIMS (secondary ion mass spectrometry) data.

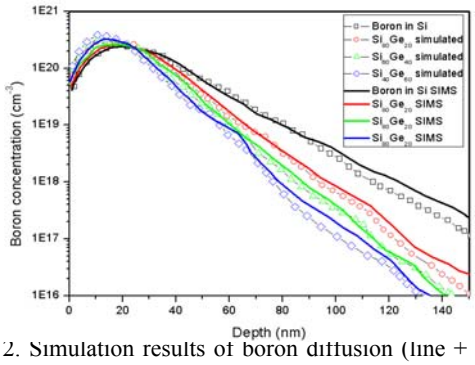

Fig. 2. Simulation results of boron diffusion (line + symbol) and SIMS profiles (line) in strained SiGe.

In the meanwhile, the adjustment of implant energy is not needed for the diffusion modeling in strained Si. However, it is needed to take the charged defects energies and diffusivity of boron into account. This is because germanium atoms are not present in strained Si layer. Therefore, we came to a conclusion that it is not necessary to adopt Lindhard theory. We assumed that boron was implanted into the silicon layer above the silicon-germanium layer with 400eV for ultra shallow junction, with same dose and 20% Ge concentration. Finally, the strained silicon layer was annealed at 940℃ under the spike RTA condition, which was compared with SIMS data.

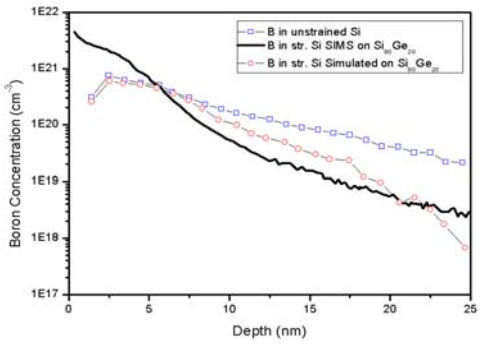

Fig. 3. Simulation results of boron diffusion (line + symbol) and SIMS profile (line) in strained Si.

The simulation results shown in Figures 2 and 3 imply that the diffusion of boron is drastically retarded in a strained structure when compared to a case with unstrained silicon. Furthermore, we calculated the distribution of stress at the Si/SiGe interface with basis on the elastic theory [1]. The lattice constant of $Si_{1-x}Ge_x$ can be expressed by $a_{SiGe}=(1-x)a_{Si}+xa_{Ge}$, where a_{Si} and a_{Ge} lattice constant of Si and Ge, respectively. "In-plane strain" and "out-of-plane strain" can also be calculated from the elastic theory when C_{11}=167 Gpa and C_{12}=65 Gpa are the elastic constant of Si. Finally, we formulated a correlation between the in-plane and our-of-plane strain as a function of germanium mole fraction as shown in Table 3.

Ge concentration	In-plane Strain	Out-of-plane strain	Physical 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

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

3. Conclusions

We investigated the effect of strain on boron diffusion in a strained silicon and silicon-germanium layer by creating a virtual SiGe layer on silicon substrate. We adjusted the implant energy in accordance with the Ge concentration, and we calculated the charged defect energy as well as diffusivity in terms of annealing temperature. During the investigation on the correlation of the implant energy between the strained silicon and the unstrained silicon, we found that Ge can affect the penetration depth of boron implant, which makes the strained Si to be one of the key technologies for shallow junction. Our simulation study enabled us to observe the boron retardation in a strained structure. Moreover, we derived the distribution of physical stresses along the Si/SiGe interface direction. Finally, a physical stress in silicon could be calculated from the knowledge of the amount of germanium mole fraction in silicon for atomistic simulation.

Acknowledgements

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