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ATOMISTIC MODELING OF BORON ACTIVATION AND DIFFUSION IN STRAINED SiGe

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ABSTRACT

We used a combination of atomistic models, DFT and KLMC, to analyze the complex issues associated with B diffusion and activation in nanoscale Si devices. Using DFT, we developed general models which separate out global strain from local binding of B with Ge in $\text{Si}_{1-y}\text{Ge}_y$ alloys for both substitutional B as well as the B_i transition state which controls diffusion. The models were used to derive segregation/activation and diffusion of boron as a function of Ge content, plus any additional applied stress. We found that the increase of segregation and activation in strained $\text{Si}_{1-y}\text{Ge}_y$ alloys is mainly due to the effect of strain rather than binding, with model accurately predicting experimental observations. B diffusion in SiGe is a complex system due to multi-step diffusion process, anisotropic strain and multiplicity of local Ge arrangements. By using DFT calculations spanning a range of Ge configurations and strain conditions, we are able to identify the mechanisms leading to retarded B diffusion: a combination of local B_i -Ge repulsion and global strain interactions. KLMC using DFT parameters predicts experimental results accurately up to 50% Ge.

1. INTRODUCTION

There is great interest in utilizing SiGe for enhanced mobility, increased electrical activation, slower diffusion and reduced contact resistance of nanoscale MOSFETs [1-10]. In order to control device structures at the nanoscale, a fundamental understanding of the effects of alloy concentration and associated strain is critical. In this work, we investigated activation and diffusion of the dominant p-type dopant, B, in SiGe considering both global strain compensation as well as local Ge configuration. Based on density functional theory (DFT) calculations, we developed simple models that can be used to predict the formation energy of a given

Si/Ge/B configuration. These models were then used in kinetic lattice Monte Carlo (KLMC) simulations to extract nanoscale response of dopant redistribution and activation. The calculations were done using the VASP software [11] on systems with 64 atom supercells (plus interstitial atoms or vacancies), subject to periodic boundary conditions, using density functional theory with generalized gradient approximation (GGA) functional, plane wave basis and ultrasoft-pseudopotentials [12]. The diffusion paths were calculated using the nudged elastic band (NEB) method [13].

2. STRAIN ENERGY

We have done calculations of various $\text{Si}_{1-y}\text{Ge}_y$ compositions with Ge content ranging up to 50% and with different Ge configurations at each Ge concentration. The changes in strain energy upon bringing together B and Ge are shown in Fig. 1. The strain energies for a given system are calculated from the difference between the energies of $\text{B}_x\text{Si}_{63-y}\text{Ge}_y$ alloys with a lattice constant of pure Si and a relaxed lattice constant, $E_0 - E_{min}$. The strain energy of $\text{BSi}_{63-y}\text{Ge}_y$ is zero at 10% Ge concentration ($y = 6$, which gives minimum in ΔE_s). This result shows excellent agreement with experiment, in which the data for samples with 10^{20}cm^{-3} of boron concentration attain a value of zero strain for a Ge concentration of $6.5 \times 10^{20}\text{cm}^{-3}$ [14].

The strain model proposed in this study is derived from the strain dependence of the formation energy of a defect/impurity in a solid based on linear elasticity:

$$E(\vec{\epsilon}) = E_{min} + \frac{\Omega}{2} (\vec{\epsilon} - \Delta\vec{\epsilon}) \mathbf{C} (\vec{\epsilon} - \Delta\vec{\epsilon}), \quad (1)$$

where \mathbf{C} is the stiffness tensor of Si, $\vec{\epsilon}$ is defined relative to the equilibrium lattice vector of silicon, $\vec{\epsilon} = \vec{b}/b_{Si} - 1$, $\Delta\vec{\epsilon}$ is the induced strain relative to a reference lattice constant, and Ω is the volume of the system [15]. The proposed model of total strain energy with respect to the reference energies of BSi_{63} and Si_{63}Ge systems with a Si lattice constant ($\vec{\epsilon} = 0$) can be

	E_{1NN}^{ij}	E_{2NN}^{ij}	E_{3NN}^{ij}	E_{4NN}^{ij}	E_{5NN}^{ij}	E_{6NN}^{ij}
Ge-Ge	-0.0128	0.0022	-0.0048	-0.0028	0.0004	-0.0028
B-Ge	0.0170	-0.0164	0.0076	0.0019	-0.0074	

Table 1: Binding energies for Ge-Ge and B-Ge interaction in the n^{th} nearest neighbor model of the binding of B with multiple Ge-atoms in SiGe alloys. Note that Ge-Ge and B-Ge are nearly complementary.

represented by the induced strains. We have found isotropic induced strain for substitutional B and Ge in silicon, enabling the use of hydrostatic strain for calculations. The total strain energy (ΔE_s) is a function of the induced strains, $\Delta\vec{\epsilon}_B = (\Delta\epsilon_B, \Delta\epsilon_B, \Delta\epsilon_B)$ and $\Delta\vec{\epsilon}_{Ge} = (\Delta\epsilon_{Ge}, \Delta\epsilon_{Ge}, \Delta\epsilon_{Ge})$, due to dopant (boron) and alloy species (germanium) for system with a Si lattice constant.

$$\begin{aligned}
\Delta E_s &= E_s(\text{BSi}_{63-y}\text{Ge}_y) - yE_s(\text{Si}_{63}\text{Ge}) \\
&\quad - E_s(\text{BSi}_{63}) + yE_s(\text{Si}_{64}) \\
&= \frac{9\Omega K}{2} \left[(\Delta\epsilon_B + y\Delta\epsilon_{Ge})^2 \right. \\
&\quad \left. - y(\Delta\epsilon_{Ge})^2 - (\Delta\epsilon_B)^2 \right] \\
&= \frac{9\Omega K}{2} \left[(y^2 - y)(\Delta\epsilon_{Ge})^2 + 2y\Delta\epsilon_{Ge}\Delta\epsilon_B \right],
\end{aligned} \tag{2}$$

where $K = (C_{11} + 2C_{12})/3$ is the bulk modulus, and induced strains $\Delta\epsilon_B = -0.0047$ and $\Delta\epsilon_{Ge} = 0.00077$ are from BSi_{63} and Si_{63}Ge (note that induced strains normalized to atomic volume would be 64 times larger). The strain energy obtained from the above model can be compared with the calculated energy differences for Si lattice constant versus minimum energy lattice constant (relaxed). Fig. 1 shows the change in strain energy (ΔE_s) for $\text{Si}_{64-y}\text{Ge}_y$ and $\text{BSi}_{63-y}\text{Ge}_y$ versus Ge content over a variety of different configurations. The line is for the model represented by Eq. 3 and the symbols are the calculated total strain energies. The model for the strain energy in both $\text{Si}_{64-y}\text{Ge}_y$ and $\text{BSi}_{63-y}\text{Ge}_y$ closely matches the calculations, showing that the strain energies can be accurately predicted based on simple linear superposition of induced strains, $\Delta\epsilon_B$ and $\Delta\epsilon_{Ge}$, of isolated components.

3. BORON/GERMANIUM BINDING

The binding of B with multiple Ge-atoms in SiGe alloys is modeled as linear sum,

$$\begin{aligned}
E_b &= \sum_{ij} \left[n_1 E_{1NN}^{ij} + n_2 E_{2NN}^{ij} + n_3 E_{3NN}^{ij} \right. \\
&\quad \left. + n_4 E_{4NN}^{ij} + n_5 E_{5NN}^{ij} + n_6 E_{6NN}^{ij} \right]. \tag{3}
\end{aligned}$$

Here, binding energies due to B-Ge interaction in BSi_{62}Ge and Ge-Ge interaction in $\text{Si}_{62}\text{Ge}_2$ for the first

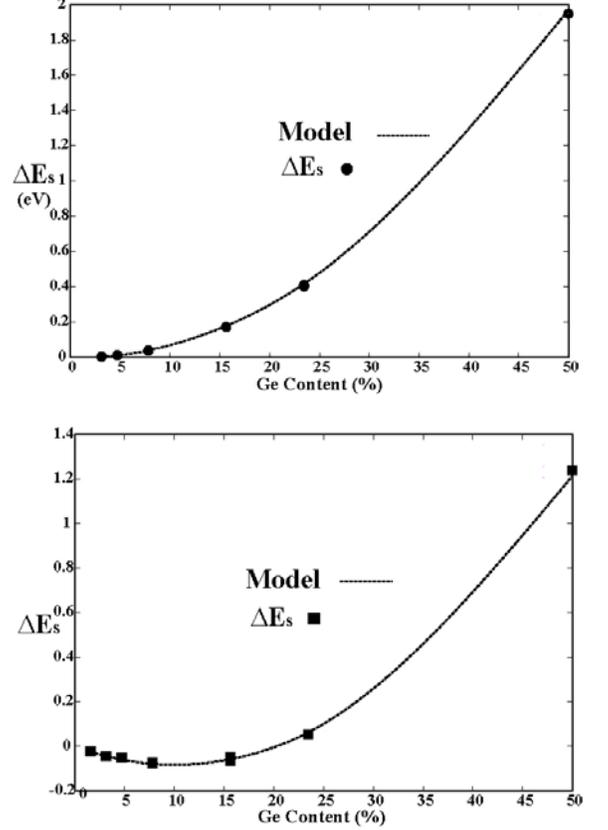


Figure 1: Strain energies (ΔE_s) versus Ge content for (a) $\text{Si}_{64-y}\text{Ge}_y$ and (b) $\text{BSi}_{63-y}\text{Ge}_y$ with a Si lattice constant with respect to the reference energies of BSi_{63} and Si_{63}Ge systems. Also shown is comparison to Eq. 3.

through 6^{th} nearest neighbor distances are summed, where n_m is the number of m^{th} nearest neighbors and E_{mNN}^{ij} is the binding energy of B-Ge or Ge-Ge interaction for the m^{th} nearest neighbor configuration. Binding energy terms used in the calculation of the total binding energy, E_{mNN}^{ij} , are given in Table 1. As seen in Table, Ge/Ge interactions are generally attractive, with the exception of displacement along 110 direction (2NN and 5NN) for which they repel. Conversely B and Ge generally repel except along 110 direction. This may be due to anisotropy in induced strain coupling. To predict the binding energy accu-

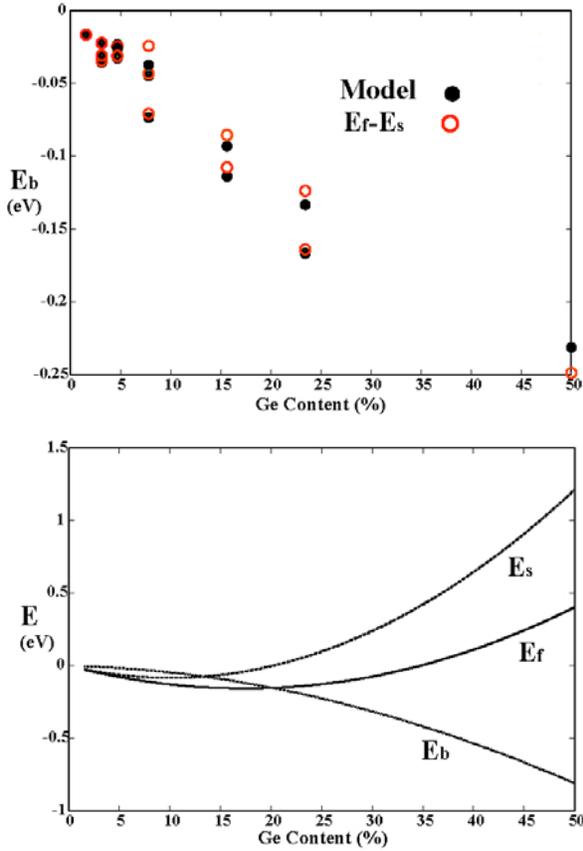


Figure 2: (a) The binding energy in $\text{BSi}_{63-y}\text{Ge}_y$, E_b . The model (closed symbols) and the subtraction between E_f and E_s (open symbols) are given for different Ge distributions (different configurations) as a function of Ge content. (b) The formation energy (E_f), the strain energy (ΔE_s), and the binding energy (E_b) for $\text{BSi}_{63-y}\text{Ge}_y$ averaged over possible configurations from the model.

rately, the long-range bonds as well as the short-range bonds should be included because there are many Ge-Ge and B-Ge bonds as the Ge content increases even though each binding energy is very small. The formation energy of substitutional boron-atom in $\text{Si}_{1-y}\text{Ge}_y$ alloys is represented by the sum of the total strain energy term (ΔE_s) and the total binding energy term (ΔE_b), $E_f = \Delta E_s + \Delta E_b$. Fig. 2(a) shows the binding energies for the model (closed symbols) compared to calculations (open symbols) for different Ge configurations as a function of Ge content. The binding energies obtained from the predictive model do a good job of accounting for changes in energy with local configurations. Figure 2(b) shows the contribution of the strain and binding terms to the formation energy averaged over possible configurations as a function of Ge con-

tent from the model.

4. SEGREGATION

The models of binding and strain energies over possible configurations can be used to derive activation (solubility/segregation) as a function of Ge content. One can write the segregation ratio which corresponds to increase in solubility with reference to an unstrained phase as product of strain factor (m_s) and binding factor (m_b) at a given Ge content, $m = m_s \times m_b$. The strain and binding terms in the segregation ratio are given by

$$m_s = \exp \left[\frac{\Delta \vec{\epsilon}_B \cdot \vec{\sigma}}{kT} \right]$$

$$m_b = \frac{\sum_{i=1}^N \exp \left[\frac{-E_b^i(\text{BSi}_{63-y}\text{Ge}_y)}{kT} \right]}{\sum_{i=1}^N \exp \left[\frac{-E_b^i(\text{Si}_{64-y}\text{Ge}_y)}{kT} \right]} \left(\frac{64-y}{64} \right), \quad (4)$$

where $\vec{\sigma}$ is stress, $\Delta \vec{\epsilon}_B$ is induced strain due to B, and N is number of possible configurations for a given Ge content. Fig. 3 shows the segregation of B to biaxially strained $\text{Si}_{63-y}\text{Ge}_y$ alloys on unstrained Si at 850°C as a function of Ge content. The contribution of global strain and local binding terms to the segregation is shown. The segregation of B is mainly due to global strain as previously shown [16]. The results show that boron preferentially segregates into SiGe alloys, as observed experimentally [1–3].

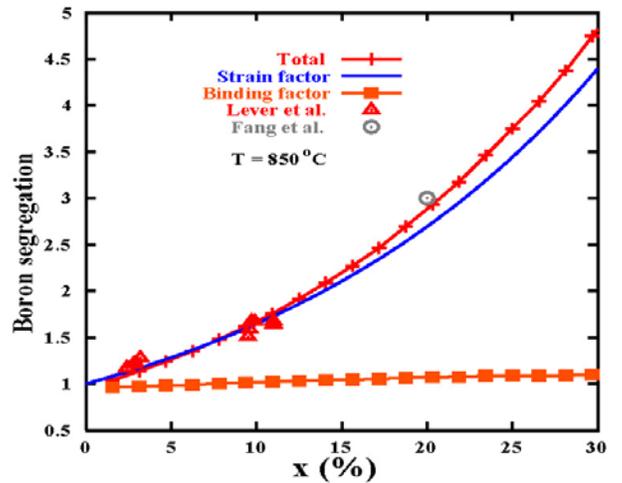


Figure 3: Segregation of B to biaxially strained $\text{Si}_{63-y}\text{Ge}_y$ alloys on unstrained Si at 850°C . The contribution of the strain and binding terms to the segregation is shown.

one Ge-atom	1NN	2NN	3NN	-1NN
ΔE_{ij}	0.0985	0.0474	0.0197	-0.0274

Table 2: The formation energy difference of the transition state for boron diffusion in $\text{Si}_{63}\text{Ge}_1$ versus pure silicon.

two Ge-atoms	1NN-1NN	1NN-2NN	1NN-2NN (Ge-Ge bond)	1NN-3NN	2NN-2NN	2NN-3NN
ΔE_{ij}	0.4840	0.2521	0.1552	0.1396	0.1192	-0.0030

Table 3: The formation energy difference of the transition state for boron diffusion in $\text{Si}_{62}\text{Ge}_2$ versus pure silicon.

5. DIFFUSION

B diffusion in Si is interstitial mediated, with the B_sSi_i^T complex (substitutional boron and interstitial Si) the lowest energy B/I structure. Diffusion occurs in a two-step process from B_sSi_i^T to a neighboring hexagonal site along a $[311]$ direction and then to another B_sSi_i^T structure in surrounding 6-membered ring. Using calculations over a wide range of Ge configurations, we are able to extract a discrete model for the energy of B transition state as function of local Ge arrangement. After we separate out the effect of global stress [17, 18], we find that the dominant effect is for Ge within the 6-membered ring surrounding target hexagonal site. The model is parameterized in terms of the number of Ge 1st, 2nd and 3rd NN from B_s site in ring (Tables 2 and 3). The presence of Ge in proximity to the transition state increases the migration energy. In the transition states, B tends to shift away from Ge sites due to a repulsive B_i -Ge interaction. The increase in activation energy is particularly large when Ge is present on both sides of ring, which makes it difficult for B_i to avoid both during transition.

Averaging over possible Ge configurations, we performed KLMC under anisotropic stress conditions. For a given Ge configuration, the diffusion coefficient is given as,

$$D_{pq}(\vec{\epsilon}) = \sum_i \sum_j \Gamma_0 \exp\left(-\frac{E_i^{m1}(\vec{\epsilon})}{k_b T}\right) \times \frac{\Gamma_0 \exp\left(-\frac{E_{ij}^{m2}(\vec{\epsilon})}{k_b T}\right)}{\sum_k \Gamma_0 \exp\left(-\frac{E_{ik}^{m2}(\vec{\epsilon})}{k_b T}\right)} \Delta X_{ij}^p \Delta X_{ij}^q \quad (5)$$

where Γ_0 is attempt frequency, E_{ij}^{m1} is migration barrier of the first hopping to hexagonal sites, E_{ijk}^{m2} is second migration barrier to lattice sites around a hex site, and ΔX_{ijk}^p is p th component of hopping vector. We find that the off-diagonal elements of D_{pq} are all zero. The diffusivity is statistically sampled by generating

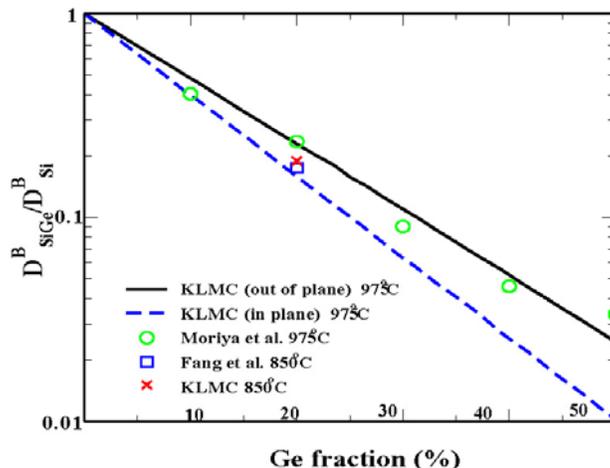


Figure 4: B diffusivity in strained SiGe. Moriya's data was matched with out-of-plane KLMC result at 20% since it was reported in arbitrary units.

random Ge distributions and averaging to obtain the ratio of diffusivity of B in SiGe to that in pure Si:

$$\frac{\overline{D}_{pq}^{\text{SiGe}}}{\overline{D}_{pq}^{\text{Si}}} = \frac{\sum_u^N \sum_v^{64} D_{uv,pq}^{\text{SiGe}}(\epsilon)}{N \times 64 \times \overline{D}_{pq}^{\text{Si}}(0)} \quad (6)$$

where N is number of samples for different Ge configurations and 64 accounts for possible occupation sites of B.

We calculated \overline{D}_{33} (out-of-plane) and \overline{D}_{11} (in-plane) since biaxial stress produces anisotropic diffusion. The KLMC results were compared to experimental data by Moriya *et al.* [19], shown in Fig. 4. The change in in-plane diffusivity is stronger than that in out-of-plane diffusivity, which is consistent with Diebel's prediction [15]. We matched out-of-plane diffusivity with Moriya's at 20% since data was given in arbitrary units. KLMC results give an excellent prediction of change in diffusivities with Ge contents for strained SiGe. Both strain effects and chemical effects are important. However, the chemical effects appears somewhat weaker

than suggested by data of Kuo *et al.* [10] who varied both composition and strain independently. This may be due to changes in dislocation structure of relaxed SiGe modifying the point defect concentrations in the experiments.

6. CONCLUSIONS

In conclusion, we used a combination of atomistic models, DFT and KLMC, to analyze the complex issues associated with B diffusion and activation in nanoscale Si devices. Using DFT, we developed general models which separate out global strain from local binding of B with Ge in $\text{Si}_{1-y}\text{Ge}_y$ alloys for both substitutional B as well as the B_i transition state which controls diffusion. The models were used to derive segregation/activation and diffusion of boron as a function of Ge content, plus any additional applied stress. We found that the increase of segregation and activation in strained $\text{Si}_{1-y}\text{Ge}_y$ alloys is mainly due to the effect of strain rather than binding, with model accurately predicting experimental observations. B diffusion in SiGe is a complex system due to multi-step diffusion process, anisotropic strain and multiplicity of local Ge arrangements. By using DFT calculations spanning a range of Ge configurations and strain conditions, we are able to identify the mechanisms leading to retarded B diffusion: a combination of local B_i -Ge repulsion and global strain interactions. Remarkably, KLMC using DFT parameters predicts experimental results accurately up to 50% Ge.

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