

**Modeling of Germanium and Antimony
Diffusion in Si_{1-x}Ge_x**

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Since electron and hole mobility can be enhanced in strained Si, the material of strained Si/Si_{1-x}Ge_x is a potential candidate for strained Si CMOS devices [1]. Therefore, it is important to understand and model impurity/dopant diffusion in Si_{1-x}Ge_x. In their recent paper, Laren *et al* [2] studied the Ge composition effect on the activation energy of antimony (Sb) diffusion in Si_{1-x}Ge_x. Ramanarayanan *et al* [3] modeled stress and Ge composition effect on the activation energy of Ge diffusion in terms of their *ab initio* calculations. However, as we point out later, it is crucial to consider the changes of both the diffusivity pre-factor and the activation energy in order to accurately model the diffusion of Ge and dopants in Si_{1-x}Ge_x.

If impurity diffusion in a diamond lattice is dominated by the vacancy mechanism and the binding energy between the impurity and vacancy is much larger than vacancy migration energy (which is the case for Ge in Si and Si_{1-x}Ge_x [3]), the diffusivity of the impurity can be expressed by [4]:

$$D = D_0 \exp\left(-\frac{(E_v^f - E_{b3} + E_{32}^m)}{kT}\right), \quad (1)$$

where D_0 , E_v^f , E_{b3} , and E_{32}^m are respectively the pre-factor of the diffusivity, vacancy formation energy, the binding energy between the impurity and a vacancy at the 3rd nearest neighbor (NN), and vacancy migration energy from the 3rd NN to the 2nd NN. The value of $E_a (= E_v^f - E_{b3} + E_{32}^m)$ is actually vacancy-formation-energy with the vacancy sitting on the saddle-point between the impurity's 2nd and 3rd NNs. For Si_{1-x}Ge_x we need to average over all possible jumping paths and corresponding atomic configurations shown in Fig. 1 to determine the impurity diffusivity

$$D_{\text{imp}} = \sum_{i=1}^6 \binom{6}{i} x^i (1-x)^{6-i} [xD_0(i, \text{Ge}) \exp\left(-\frac{E_a(i, \text{Ge}, x)}{kT}\right) + (1-x)D_0(i, \text{Si}) \exp\left(-\frac{E_a(i, \text{Si}, x)}{kT}\right)], \quad (2)$$

where $E_a(i, \text{Ge}, x)$ or $E_a(i, \text{Si}, x)$ is the formation energy of the vacancy sitting on the saddle-point (note: when a vacancy sits on the saddle-point, the saddle-point can be occupied either by a Si or Ge atom, see Fig. 1) with the vacancy's first atomic shell containing i Ge atoms and $(6-i)$ Si atoms. We should point out that our method is different from traditional methods [2, 3] that model the Ge composition effect by averaging all possible activation energies. Instead, we average all possible jumping paths to obtain diffusivity. The reasons for that are: 1) it is consistent with diffusivity definition (second Kramers-Moyal coefficient [5]) based on statistical physics and 2) our model takes into account the changing of the diffusivity pre-factor in Si_{1-x}Ge_x. This is particularly important for the Si_{1-x}Ge_x system since a very large change (three orders of magnitude) of the diffusivity pre-factor was observed in Si_{1-x}Ge_x [6].

We showed that $E_a(i, \text{Ge}, x) = E_a(i, \text{Ge}, 0) + \alpha x + \Delta_h x^2$ and $E_a(i, \text{Si}, x) = E_a(i, \text{Si}, 0) + \alpha x + \Delta_h x^2$, where α is a constant and Δ_h is the heat of mixing. Since $\Delta_h = 0$ for stoichiometrically miscible alloy of Si_{1-x}Ge_x, we obtained a linear function of Ge fraction for $E_a(i, \text{Ge}, x)$

and $E_a(i, \text{Si}, x)$. For the first time, we show that the linear expressions are universal for miscible alloys and valid for large values of x validating the assumptions from early work [3, 7], which asserted similar linear expressions. Figure 2 shows the excellent agreement between experimental data and Eq. (2) in a large range of Ge fractions and annealing temperatures. We also modeled Sb diffusivity using Eq. (2) and excellent agreement with the measured data in Ref. [2] was achieved. To the best of our knowledge, it is the first time Ge and Sb diffusivities can be accurately modeled.

The author thanks Dr. P. Oldiges, Dr. K.L. Lee, Dr. C. Murthy, and Dr. R.J. Miller for interesting discussions.

- [1] Ken Rim *et al*, Symp. of VLSI Tech, p.98-99, 2002.
- [2] A. N. Laren *et al*, Appl. Phys. Lett. 68, 2684 (1996)
- [3] P. Ramanarayanan *et al*, J. Apl. Phys. 94 (2003) 174-185
- [4] H. Bakker and H.V.M. Mirani, Z. Naturforschung. 27a, 1467 (1972); H. Zhu, to be submitted
- [5] H. Risken, The Fokker-Planck Equation, Springer Verlag, Berlin, (1988)
- [6] N.R. Zangenberg *et al*, Phys. Rev. Lett. 87, 125901 (2001)
- [7] N. Moriya *et al*, Phys. Rev. Lett., 71, p.883 (1993); N.E.B. Cowern *et al*, Phys. Rev. Lett., 72, p.2585 (1994).

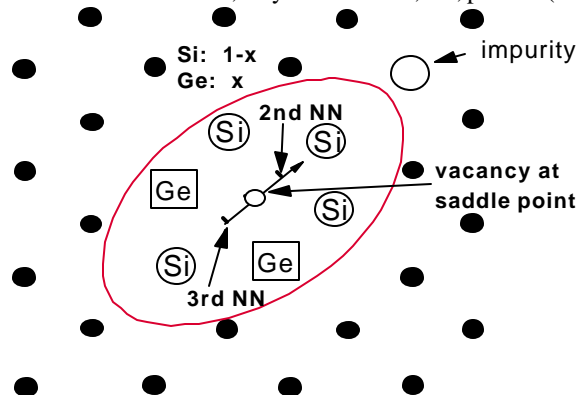


Fig. 1 Schematic of a vacancy at activation state in Si_{1-x}Ge_x. The open circle is a Si or Ge atom at the saddle-point between the second and third nearest neighbors. Solid circles are the lattice sites which have probability $(1-x)$ being occupied by Si or x by Ge. The atoms in the first atomic shell are those in the oval, except the one at the saddle-point. In this particular case, there are four Si atoms and two Ge atoms in the first atomic shell.

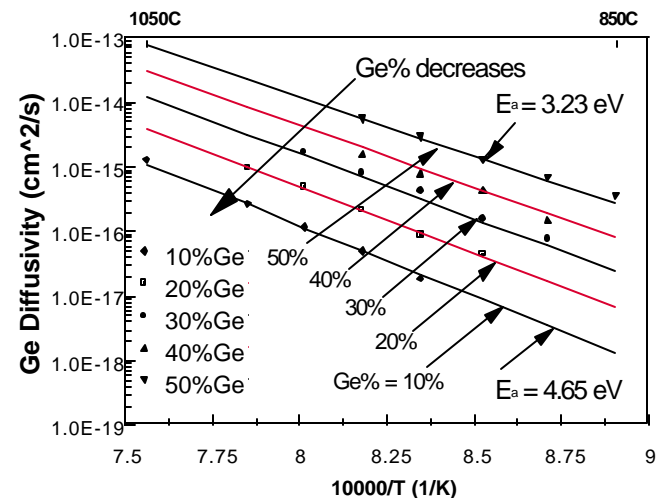


Fig. 2 Comparison of present work to experimental data of Ge diffusion in relaxed Si_{1-x}Ge_x [6]. The solid symbols are the experimental measurements and the lines from present model. It can be seen that our model can accurately describe the experimental data.