

Modeling of Germanium/Silicon Interdiffusion in Silicon/Silicon Germanium/Silicon Single Quantum Well Structures

M. Hasanuzzaman and Yaser M. Haddara

Department of Electrical and Computer Engineering
McMaster University, Hamilton, ON, Canada L8S 4K1

ABSTRACT

Purely substitutional diffusion equations were applied to model the interdiffusion of Si and Ge in Si/Si_{1-x}Ge_x/Si single quantum well structures grown by molecular beam epitaxy and annealed at 900°C, 1000°C and 1100°C for different times in inert and oxidizing ambients. Intrinsic diffusivities of Si and Ge as a function of Ge fraction in the structure used as the fitting parameters match values reported in the literature. Once these parameters were fixed for the inert ambient, the diffusion behavior under oxidizing conditions was completely accounted for by the model with no additional fitting parameters. Excellent fits were obtained in all the cases.

Keywords: SiGe, interdiffusion, modeling

1 INTRODUCTION

Interest in silicon/silicon germanium (Si/SiGe) structures has been evident since mid-1980's [1]-[3]. One of the most important applications of Si_{1-x}Ge_x is in the fabrication of HBT's with Si_{1-x}Ge_x forming the base and silicon (Si) forming the emitter and collector regions. This type of transistor can run at much higher speeds compared to conventional Si based bipolar transistors [4]-[5]. For integration with conventional CMOS technology, the device structure undergoes several high temperature process steps. Intermixing of Si and Ge during such high temperature steps can cause broadening of the Si/SiGe interface and can cause a shift in the physical location of interfaces: both these effects may be detrimental to device characteristics. Si-Ge interdiffusion may be *beneficial* in the case of SiGe quantum dots, where controlled interdiffusion may be utilized in tuning optical properties [6]. Thus it is important to accurately model Si-Ge interdiffusion both for applications where it is desirable and cases where it may degrade device performance. Several studies have reported an effective interdiffusivity for Si and Ge in Si/SiGe heterostructures using Rutherford Backscattering (RBS) [7]-[8], photoluminescence (PL) [9]-[10] and x-ray diffraction (XRD) [11]-[14]. Some studies have explicitly reported the effect of Ge concentration and/or strain on the interdiffusivity [8]-[9], [13], but most have simply reported an effective interdiffusivity of Ge for the specific structures studied. In this work we have used the purely substitutional diffusion to model the interdiffusion of Si and Ge in Si/Si_{1-x}Ge_x/Si single quantum well (SQW) structures grown

by molecular beam epitaxy (MBE) and annealed at 900°C, 1000°C and 1100°C for different times in inert and oxidizing ambients [15]-[16]. We begin by discussing the model, then our simulation approach. This is followed by a description of the sample structure considered and a discussion of the simulation results.

2 MODELING SUBSTITUTIONAL DIFFUSION

Kirkendall *et al.* [17] described interdiffusion in metallic alloys via a vacancy exchange mechanism. Later, Smigelskas *et al.* [18] and Darken [19] reported results demonstrating the vacancy diffusion mechanism and provided further mathematical modeling. By contrast, dopant diffusion in semiconductors is usually described by substitutional-interstitial mechanisms, and numerically solved under assumptions of quasi-equilibrium, and dilute dopants [20]-[21]. The dilute dopant approximation is inappropriate in the case of interdiffusion of host atoms, and it is necessary to go back to the vacancy flux model to describe the phenomenon, explicitly taking into account conservation of lattice site density.

The governing equations for interdiffusion via a vacancy mechanism are given by [22],

$$\frac{\partial C_{Si}}{\partial t} = -\frac{\partial}{\partial x} \left[D_{Si}^{int} \frac{C_{Si}}{C_V^{eq,int}} \frac{\partial C_V}{\partial x} - D_{Si}^{int} \frac{C_V}{C_V^{eq,int}} \frac{\partial C_{Si}}{\partial x} \right] \quad (1)$$

$$\frac{\partial C_{Ge}}{\partial t} = -\frac{\partial}{\partial x} \left[D_{Ge}^{int} \frac{C_{Ge}}{C_V^{eq,int}} \frac{\partial C_V}{\partial x} - D_{Ge}^{int} \frac{C_V}{C_V^{eq,int}} \frac{\partial C_{Ge}}{\partial x} \right] \quad (2)$$

$$\frac{\partial C_V}{\partial x} = \frac{\partial}{\partial x} \left[D_{Si}^{int} \frac{C_{Si}}{C_V^{eq,int}} \frac{\partial C_V}{\partial x} - D_{Si}^{int} \frac{C_V}{C_V^{eq,int}} \frac{\partial C_{Si}}{\partial x} + D_{Ge}^{int} \frac{C_{Ge}}{C_V^{eq,int}} \frac{\partial C_V}{\partial x} - D_{Ge}^{int} \frac{C_V}{C_V^{eq,int}} \frac{\partial C_{Ge}}{\partial x} \right] \quad (3)$$

where, D_{Si}^{int} and D_{Ge}^{int} are respectively the silicon and germanium self-diffusivities under inert intrinsic conditions, C_{Si} and C_{Ge} are respectively the silicon and germanium concentrations and $C_V^{eq,int}$ is the inert intrinsic concentration of vacancies which may vary as a function of Ge concentration. The first two equations take into account the diffusion of each atom under its own concentration gradient and the lattice motion to compensate for the difference in the diffusivities. The third equation arises from the constraint of lattice site conservation.

3 SIMULATION APPROACH

Griglione *et al.* [16] used the Florida Object Oriented Process Simulator (FLOOPS) [21] to extract effective diffusivities from the diffused Ge profiles in SQW structures at different temperatures for different anneal times both in inert and oxidizing ambients. The reported effective diffusivities were extracted from reasonable fits to the experimental profiles and were used as reference for this work since we do not have the actual experimental profiles. These diffusivities give rise to the “experimental” profiles labeled in our figures as ‘Extracted Profile’. The samples studied in this work were underwent anneals in inert and oxidizing ambients. The inert anneals were conducted at 900°C for 330 min, 980 min, 1532 min, and 2206 min, at 1000°C for 43 min, 55 min, 87 min, and 125 min, and at 1100°C for 1min, 2 min, 3 min, 4 min. The oxidizing anneals were conducted at 900°C for 330 min, at 1000°C for 43 min, 55 min, 87 min, and 125 min, and at 1100°C for 1min, 2 min, 3 min, 4 min. We implemented the substitutional diffusion model described by equations (1)-(3) using ISE-FLOOPS [23]. We imposed the condition,

$$C_{Ge} + C_{Si} + C_{Vac} = C_{total_lattice_sites} \quad (4)$$

in setting the initial state. The total lattice site density, $C_{total_lattice_sites}$ used in the simulations was $5 \times 10^{22} \text{ cm}^{-3}$. The initial Ge profile was set to the as-grown Ge profile in the SQW structures as reported by Griglione [16]. The initial vacancy profiles were set equal to the intrinsic equilibrium vacancy concentration, $C_V^{eq,int}$, at the anneal temperature. This was initially taken to be constant and equal to the ISE-FLOOPS default for pure Si. We comment later on the variation of $C_V^{eq,int}$ with the Ge concentration.

4 SAMPLE STRUCTURE

A single quantum well Si/Si_{1-x}Ge_x/Si structure grown by Molecular Beam Epitaxy (MBE) at a temperature of 520°C fabricated and studied by Griglione [15]-[16] was taken as a reference work in this study. The studied structure consists of an undoped 50 nm Si cap, followed by an undoped 50 nm Si_{0.85}Ge_{0.15} layer, followed by an undoped 100 nm Si buffer and a lightly p-doped (100) Si substrate. The samples were thoroughly characterized for layer depth, Ge concentration, Ge profile, and the presence of extended defects. The details of the sample growth, annealing in inert and oxidizing ambients and characterization techniques can be found from Ref. [15].

5 SIMULATION RESULTS AND DISCUSSIONS

The model was applied to get the diffusion profiles of Ge for the same different anneal times at different temperatures in inert and oxidizing ambients as reported by

Griglione [15]-[16]. The values of D_{Si}^{int} and D_{Ge}^{int} as a function of Ge fraction were used as the fitting parameters in our simulations. We fit these values to match the simulated profiles with the extracted profiles in inert ambient. The simulations were performed for different anneal times keeping these parameters fixed for each temperature. Once these values were fixed for the inert ambient, the diffusion behavior under an oxidizing ambient was completely accounted for by the model with no additional fitting parameters. Figures 1 and 2 show typical fits to the extracted profiles.

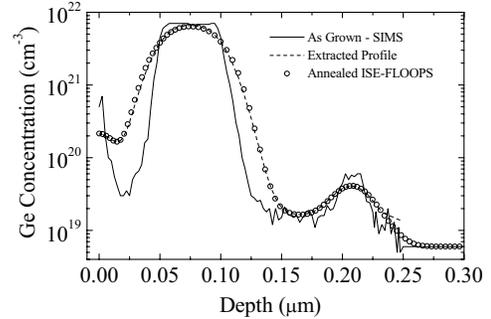


Figure 1: Si-Ge interdiffusion after a 43 min anneal at 1000°C in an inert ambient.

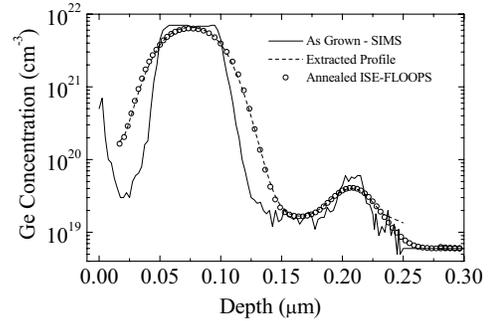


Figure 2: Si-Ge interdiffusion after a 43 min anneal at 1000°C in an oxidizing ambient.

The values of D_{Si}^{int} and D_{Ge}^{int} used in the simulations are compared with the previously published data and are shown in figures 3 and 4. The values of D_{Ge}^{int} are compared with the values reported by Zangenberg *et al.* [24] and Sharma [25]. The values of D_{Si}^{int} are compared with the values reported by Borg *et al.* [26] and Laitinen *et al.* [27]. Below 1100°C, the values of D_{Si}^{int} and D_{Ge}^{int} used in the simulations match published values well. The high diffusivities compared to published values observed for 1100°C anneals may be a result of the rapid relaxation of the SiGe layer expected at that temperature and the presence of a relatively high dislocation density. An alternative explanation may be

that other diffusion mechanisms (e.g. an interstitial mechanism) play a major role at high temperatures.

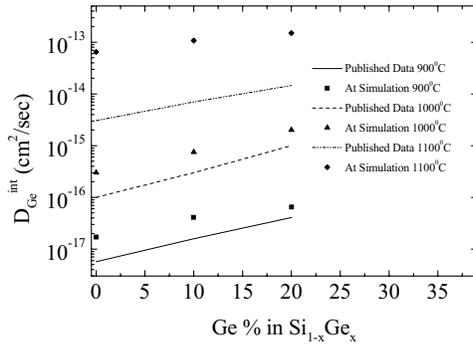


Figure 3: Intrinsic Ge diffusivity values compared with published data.

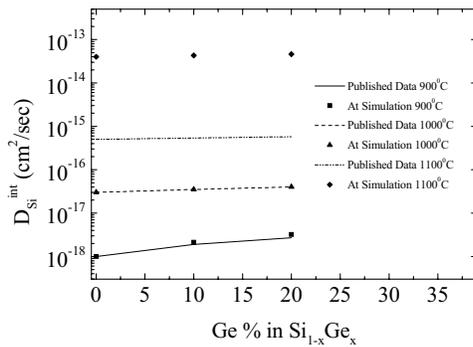


Figure 4: Intrinsic Si diffusivity values compared with published data.

The values of $C_V^{eq,int}$ were varied as a function of Ge fraction. We increased these values in SiGe layer compared to the values in Si and observed the diffused Ge profiles. The diffused Ge profiles initially showed no significant dependence on the increased $C_V^{eq,int}$ values at the SiGe layer. After certain values, the simulated diffused Ge profiles were found to be non Gaussian in nature. The maximum value of $C_V^{eq,int}$ in SiGe up to which the diffused Ge profiles were Gaussian in nature, was taken as the value of $C_V^{eq,int}$ in the simulations and was kept fixed for each temperature.

6 CONCLUSIONS

It is always possible to set an effective diffusivity so that the simulated diffused profiles match with the experimental profiles. However modeling a certain phenomena that satisfies lots different cases is a challenging work. The model used in this work can successfully describe the interdiffusion phenomena of Ge and Si in SQW structures for different anneal times at different temperatures considering the facts that D_{Si}^{int} , D_{Ge}^{int} and $C_V^{eq,int}$

depend on the Ge fraction in $Si_{1-x}Ge_x$. Considering these facts, it is found that keeping these values fixed for each temperature, the vacancy flux model can predict the interdiffusion profile of Ge in Si/Si_{1-x}Ge_x/Si SQW structure both in inert and oxidizing ambients at 900°C, 1000°C and to some extent at 1100°C too.

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