Atomistic Modeling of Defect Diffusion in SiGe

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Abstract

We have developed an atomistic model for dopant diffusion in SiGe structures and we have implemented it in the kinetic Monte Carlo process simulator DADOS. The model takes into account (i) composition and stress effects on the diffusivity of interstitials, vacancies and dopants, (ii) SiGe interdiffusion, (iii) dopant segregation and (iv) the modifications of band-gap and charge levels. The model has been tested for B and Sb providing a very good agreement with available experimental data.

1 Introduction

SiGe alloys are becoming increasingly important for the manufacture of current high performance devices. In consequence, it is crucial to be able to predict final profiles for dopants in SiGe deep-submicron devices taking into account the many factors that contribute to dopant diffusion. Among these, stress and composition increase the complexity already present in silicon processing modeling [1-3]. Namely, composition and built-in stress can alter formation and migration energies, band-gap and charge levels. As a consequence, they will influence dopant behavior through changes in the effective diffusivity and segregation. Moreover, composition and stress may vary spatially, due to inhomogeneities or to heterostructures, and with time, mainly due to Si-Ge interdiffusion. Given the complexity of such processing scenarios it is important to have a microscopic, physically-based model that can account for every component mechanism. Atomistic kinetic Monte Carlo (KMC) simulators are particularly appropriate for this purpose [4]. Using the KMC simulator DADOS we have developed a comprehensive model and a efficient simulation scheme that reveals the rich phenomenology associated to dopant diffusion in the SiGe system.

2 Implementation and results

As a non-lattice KMC simulator, DADOS follows only the atomistic defects, not the lattice (Si or Ge) atoms. The simulation domain has a 3D grid of small boxes (around 1 nm^3) with varying composition and stress. The Ge content of the $Si_{1-x}Ge_x$ alloy is described by the discrete number of Ge atoms in each box. The composition dependence of the transport capacity of interstitials (I) and vacancies (V) in equilibrium conditions (DC_I^* and DC_V^*) has been modeled through changes in their formation energies and entropies (E_{form} and s_{form}), which have been assumed to scale linearly with Ge content. Figure 1.a illustrates the energy landscape that would see a diffusing particle (with migration energy E_m) when moving through a region where E_{form} changes with the position.

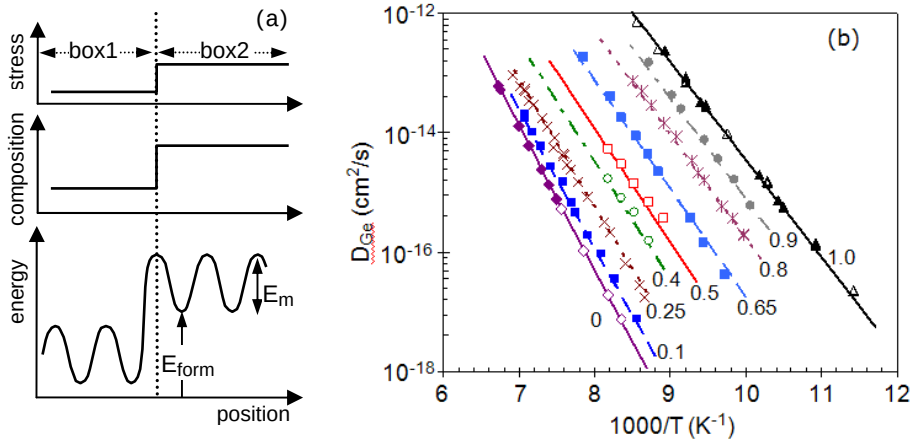

Figure 1: (a) Simplified energy scheme with position-dependent stress and composition. (b) Ge self-diffusivity in $Si_{1-x}Ge_x$ for different values of x. Symbols: experimental data, from Refs.[5-7]. Lines: present model.

We account for the different Si and Ge self-diffusivities by defining the relative probability of an I (or a V) moving a Ge or a Si atom. This relative probability is described by an activation energy and an entropy that, again, scale linearly with the Ge content. These simple assumptions lead to a very good fit of experimental data of Ge and Si diffusivities (D_{Ge} and D_{Si}) in the whole range of SiGe compositions [5-7]. As an example, D_{Ge} is shown in Figure 1.b. In our atomistic scheme, Si-Ge interdiffusion in SiGe heterostructures results from the probabilistic net exchange of Si and Ge atoms between neighbor boxes through the jump of individual Is or Vs form one box to another. The effects of I (or V) supersaturation on Si-Ge interdiffusion are automatically included.

Dopant diffusion is mediated by mobile dopant-defect pairs (such as BI and SbV). Thus, dopant diffusivity and segregation can be successfully fitted to experimental data [2, 8-11] by calibrating the E_{form} of dopants and the charge levels of dopant-defect pairs. The composition dependence of the SiGe band structure plays a role in dopant diffusion, specially in extrinsic conditions, and it has been carefully taken into account in the model.

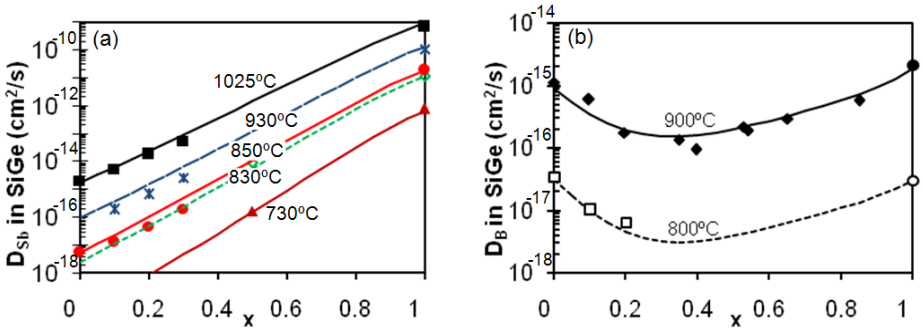

Figure 2: (a) Antimony and (b) boron diffusivities in $Si_{1-x}Ge_x$ as a function of Ge content. Symbols: experimental measurements [2, 8-10, 12]. Lines: model.

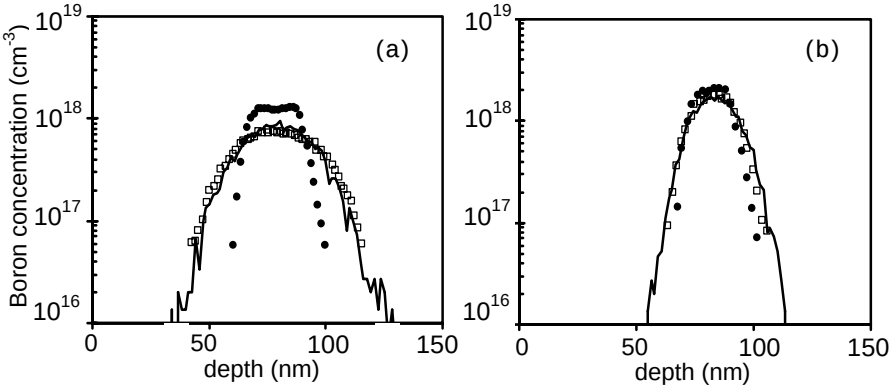

Figure 3: Diffusion of a B spike (a) in Si and (b) in strained $Si_{0.83}Ge_{0.17}$ after a 30 min., 860ºC anneal. Dots: as grown. Squares: experimental data [13]. Lines: simulated

As an example, D_{Sb} and D_B as a function of composition are shown in Figures 2.a and 2.b. In our calibration, microscopic parameter values were kept within the ranges allowed by experimental or theoretical data available.

Stress has been implemented for a biaxial geometry. In this configuration, it is necessary to account for the experimental modification of the diffusivity in the perpendicular direction, characterized by an effective activation volume, and for the anisotropy, inferred from hydrostatic tests [1]. We model these features with an additional change of E_{form} and including the anisotropy in the migration rates of dopant-defect pairs.

Figures 3.a and 3.b illustrate the different B diffusion in Si and in SiGe (strained to Si) [13]. The boron diffusion retardation in the depth direction is due to the joint effect of composition, biaxial compression and reduction of extrinsic diffusivity.

Boron segregation from Si to SiGe is well reproduced in the experiment shown in Figure 4.a [11]. We would like to point-out that: (i) in our model, B segregation is described by a decrease of boron formation energy in SiGe, not by the assumption of Ge-B pairs [11], and (ii) diffusivity and segregation can be calibrated independently.

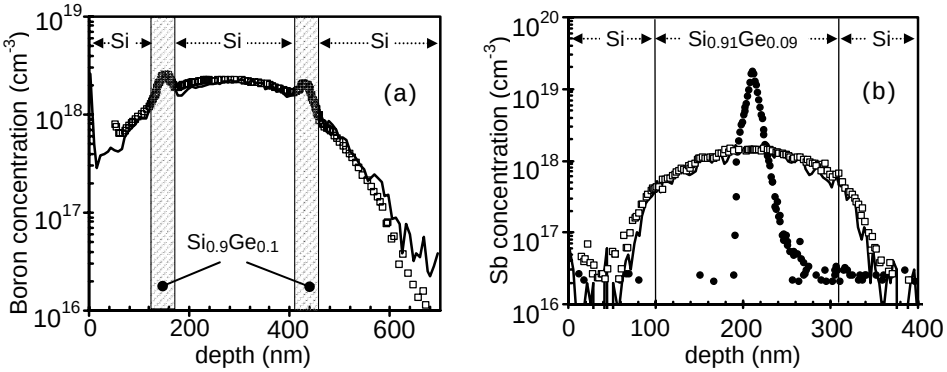

Figure 4: (a) Boron concentration profile, exhibiting segregation to SiGe layers after 96 hours at 850ºC. Squares: experimental data [11]. Lines: simulation. (b) Diffusion of an Sb spike in a Si/SiGe/Si structure after 30 min at 1028ºC. Dots: as grown. Squares: experimental data [2]. Lines: simulation.

Finally, Figure 4.b shows the retardation of an antimony spike diffusion as it enters a Si region in a Si/strained SiGe/Si structure [2].
In conclusion, an atomistic KMC implementation of microscopic, physically-based models can provide a wide-scope simulation environment for the complexities involved in current SiGe device processing. As an improvement over continuum-based implementations, KMC gives direct and easy access to every microscopic parameter and mechanism.

Acknowledgements

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References

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