

Modeling dopant diffusion in SiGe and SiGeC layers.

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Abstract

Following the development of a unified diffusion model valid for all usual dopants in SiGe layers [1], considering the effect of carbone diffusion on point defects concentrations extends the application of our model to strained SiGeC layers. Using a new SIMS methodology, the study of As intrinsic diffusion in SiGe and SiGeC layers is performed, at low concentration and under equilibrium annealing conditions. Arsenic enhanced diffusion in fully-strained SiGe and SiGeC layers on Si substrates was successfully compared to the unified diffusion model.

1 Modeling

A unified phenomenological diffusion model, based on reliable physical assumptions, was developed [1]. This model, valid to predict the diffusion behavior of all usual dopants in strained and relaxed SiGe layers, summarizes in a single formulation, the influence of the various physical effects acting on the equilibrium concentration of Interstitial (I) and Vacancy (V) point defects and thus on the diffusivity of all substitutional impurities [2].

The unified model was extended to describe the diffusivity evolution of usual dopants in strained SiGeC alloys [3], by considering the effect of supersaturated substitutional Carbon diffusion on point defects concentration [4].

$$\begin{aligned} \left(\frac{[I]}{[I^*]}\right)_C &= \frac{D(I) \cdot [I^*]}{D(Ci) \cdot [Ci^*]} \cdot \frac{[Cs^*]}{[Cs^*] + [Ci^*]} \\ \left(\frac{[V]}{[V^*]}\right)_C &= \left(\frac{D(Ci) \cdot [Ci^*]}{D(V) \cdot [V^*]} \cdot \frac{[Cs^*] + [Ci^*]}{[Cs^*]}\right)^{1/2} \end{aligned} \quad (1)$$

where Ci and Cs are the Interstitial and substitutional carbon atoms, D() is the diffusivity, * implies equilibrium and concentrations are expressed in brackets.

Each physical phenomenon acting on the equilibrium concentration of Interstitials and Vacancies in SiGe alloys is modeled by a single parameter: Q' for the strain effect, Q_{Ge} and Q_C for the chemical effect in alloys (Q_C is related to the Ge content as the same ratio is usually used in strained SiGeC layers) and K_I for the Fermi-level effect.

To explain the different behavior of Phosphorus and Boron in SiGe layers, both diffusing via Interstitial-mechanisms, the hypothesis of BGe coupling is modeled through the parameters K_2 and Q_{BGe} . B retardation is caused by a reaction forming a microscopical-strain-relieving complex of a substitutional Ge next to a substitutional B [5], experimentally detected by Hattendorf *et al.* [6]. Ge and C atoms are believed to be preferentially associated when compared to Boron thus, our model supposes the BGe coupling to be negligible in SiGeC alloys.

The physical parameters of SiGeC alloys vary with Ge and C concentrations and the ratio between the equilibrium concentration of Interstitial (I) and Vacancy (V) point defects in SiGeC alloys, and their standard values in pure silicon, is expressed by:

$$\frac{[I]}{[I]_{Si}} = \left(\frac{[I]}{[I^*]} \right)_C \cdot \exp \left(\frac{Q'^I \cdot \varepsilon + (Q_{Ge}^I + Q_{BGe} + Q_C^I) \cdot 0.042 \cdot x_{Ge} + K_1^I \cdot \Delta E_g}{kT} \right) \quad (2)$$

$$\frac{[V]}{[V]_{Si}} = \left(\frac{[V]}{[V^*]} \right)_C \cdot \exp \left(\frac{Q'^V \cdot \varepsilon + (Q_{Ge}^V + Q_C^V) \cdot 0.042 \cdot x_{Ge} + K_1^V \cdot \Delta E_g}{kT} \right) \quad (3)$$

ε is the biaxial strain, k is the Boltzmann constant and T , the temperature. The change in band gap of strained SiGe and SiGeC layers is $\Delta E_g = -0.96 \cdot x_{Ge} + 0.43 \cdot x_{Ge}^2 - 0.17 \cdot x_{Ge}^3 + 3.4 \cdot y_C$, and is calculated from [7] for relaxed SiGe layers. x_{Ge} and y_C are germanium and carbon molar fractions.

The variation of dopant species diffusivity is directly related to their fraction of Interstitial-mediated diffusion f_i , and the same diffusion mechanisms are supposed in pure silicon, SiGe and SiGeC alloys:

$$\frac{D_{SiGeC}}{D_{Si}} = \frac{1}{1 - K_2 \cdot x_{Ge}} \cdot f_i \cdot \frac{[I]}{[I]_{Si}} + (1 - f_i) \cdot \frac{[V]}{[V]_{Si}} \quad (4)$$

The model calibration was performed on all reliable data from literature on Sb, Ge, B and P diffusion studies in SiGe alloys and on our dedicated set of experiments on B diffusion in SiGe and strained SiGeC layers [3]. The calibrated model leads to the prediction of an important enhancement of As diffusion in SiGe and SiGeC layers, as presented by the theoretical curves of Figure 1 and Figure 2

2 Experimental Results and Discussion

To the knowledge of the authors, equilibrium diffusion data of Arsenic in SiGeC have not been reported to date. Moreover, due to the $^{75}\text{As}^+$ vs. $^{74}\text{GeH}^+$ mass interference, standard SIMS analysis of As in Ge-rich layers is limited to concentrations above 10^{18} cm^{-3} . Arsenic diffusion enhancement in SiGe layers, is clearly identified in [8] and [9] when compared to Si control samples. But, studying a high concentration of implanted

dopants implies considering accurately As clustering, concentration dependent extrinsic diffusion [10] and transient enhanced diffusion effects [11].

A SIMS methodology was developed at CEA-LETI [12], monitoring MCs_2^+ ions (where 'M' stands for Si, Ge or As), in order to avoid the Ge-As mass interference and reach a detection limit lower than 10^{17} cm^{-3} [3].

Full sheet RTCVD SiGe and SiGeC were epitaxially grown on (100) Si substrates having a constant As doping of $2 \times 10^{19} \text{ cm}^{-3}$. Samples were then covered by a 25 nm Si capping layer and heated at 950-1020°C in inert N_2 ambient. For the first time, measuring the intrinsic diffusion of grown-in Arsenic profiles in SiGe and SiGeC layers was performed. The effective diffusivity was analyzed in silicon, in SiGe and SiGeC layers having a germanium content of 7 or 12.3%, and successfully compared to the curves predicted by our calibrated model.

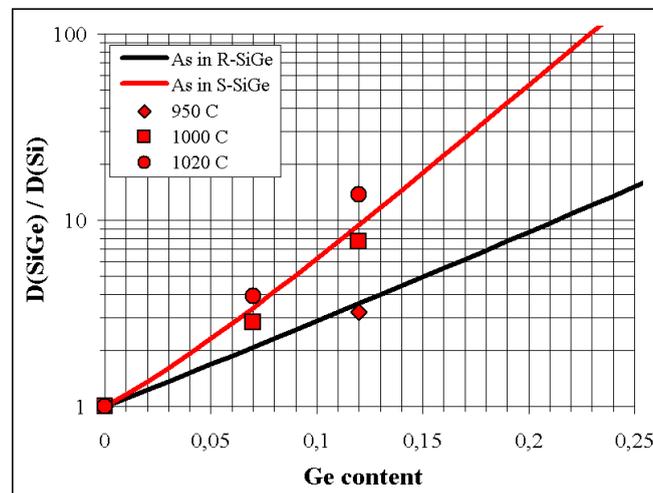


Figure 1 : Arsenic effective diffusivity ratio between SiGe and Si. Curves in grey and black present the model predictions of arsenic diffusion in strained and relaxed SiGe layers, respectively. Symbols are experimental data points.

In Figure 1 and Figure 2, Arsenic experimental measurements confirm the enhancement of As diffusivity, with the Ge and C content of SiGeC layers, predicted by the diffusion model.

As the temperature dependence of our model is very low, in the SiGe samples of Figure 1, the apparent evolution of the arsenic diffusion with temperature is not reproduced. In Figure 2, the low temperature dependence of Arsenic diffusion in strained SiGeC layers is in accordance with the curves from the diffusion model.

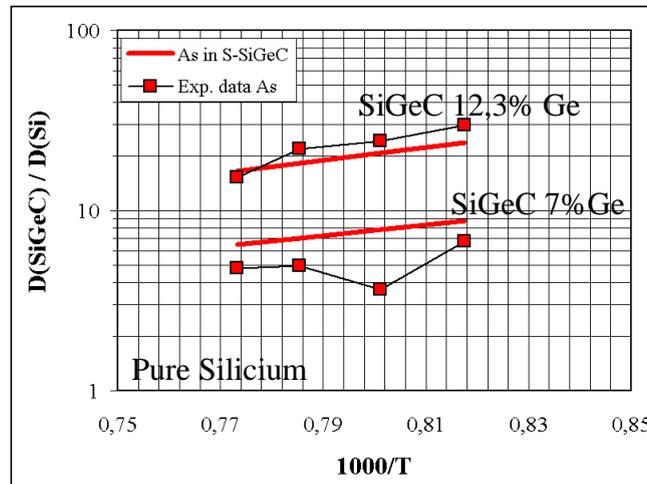


Figure 2 : Arsenic effective diffusivity ratio between strained SiGeC layers and Si. Symbols are experimental data points.

More experimental investigations, analyzing the diffusion of the different dopants in SiGe and SiGeC alloys are needed to improve the model we developed. Nevertheless, considering the variations of point defects concentration, with different physical effects induced by Ge and C atoms, leads to a unified model valid to describe the diffusion behavior of all common dopant atoms in SiGe alloys and strained SiGeC layers.

3 References

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