A Unified Model of Dopant Diffusion in SiGe.

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Abstract

The understanding of the effect of each physical mechanism driving dopant and point defect diffusion due to Ge leads to a unified formulation of diffusion for the usual dopants in SiGe material. The model calibration is deduced from a critical synthesis of the theoretical and experimental published studies.

1 Introduction

The control of dopant profiles in SiGe has a direct influence on the electrical characteristics of HBT devices. Furthermore, Ge can be considered as an additional "degree of freedom" for the analysis of the different material parameters on dopant diffusion.

2 Modeling of physical mechanisms

The presence of Ge in Si modifies some of the material physical characteristics with respect to pure Si. The study of the effect of physical phenomena on the equilibrium concentration of point defects is developed, allowing to express the modification of dopant diffusivity as it is proportional to the point defect concentration.

Other phenomena being supposed identical in Si and SiGe, our model considers each physical mechanism acting on dopant diffusion in SiGe as a perturbation of the standard Si diffusion.

2.1 Layer strain effect on diffusion

The synthesis by Zhao et al. [10] on dopant diffusion in strained Si leads to the quantification of the dual effect of strain on the formation energy and thus on the equilibrium concentration of point defects.

A biaxial compression will increase the Vacancies equilibrium concentration (V) and decrease the Interstitials concentration (I). In a SiGe layer, V-mediated dopants like Antimony will diffuse faster in strained than in relaxed SiGe [7] as illustrated in Fig. 1. On the other hand, I-mediated dopants, are believed to have a lower diffusivity in strained than in relaxed SiGe layers as shown in Fig. 2.

2.2 Ge chemical effect

The point defect equilibrium concentrations are closely related to the bonding energy of atoms. In purely covalent crystals, the heat of sublimation corresponds to the rupture of half of the atomic bonds.

Table 1. Material characteristics of pure Si and Ge

Material	Heat of Sublimation ($kJ.mol^{-1}$)	Bonding Energy (eV)
Si	455.6	2.36
Ge	374.5	1.94

In Table 1, we report the lower bonding energy of Ge as compared to Si. As a consequence, the atomic bonding energy in relaxed SiGe is lowered by the presence of Ge, so the formation energy of point defects is decreased with Ge concentration. It explains that both I and V point defects concentration are increased by the Ge chemical effect as suggested by Christensen et al. [2].

2.3 Band gap modification

The strain value is of prime importance on the formulation of the band gap change. The two stress limit values are considered for SiGe layers:

Relaxed (R): $\Delta Eg_R = -0.55\, x_{Ge} + 0.33\, x_{Ge}^2$ from [1]

Strained (S): $\Delta Eg_S = -1.01\, x_{Ge} + 0.835\, x_{Ge}^2$ from [3]

The band gap of Si is lowered by the presence of Ge atoms in the matrix. The equilibrium of charged point defects is modified by this effect and the dopant-defect interactions are reduced, lowering dopant diffusivity.

2.4 B-Ge pairing

For Boron, an other physical mechanism, verified by the dedicated experimentations of Lever et al. [6], has to be considered: a mechanical pairing between Boron and Germanium atoms reducing the number of mobile B atoms.
In a first approximation, we consider the B-Ge pairing parameter as independent of Ge concentration. Indeed, this has to be moderated due to the experiments on B diffusivity in $Si_{0.99}Ge_{0.01}$ of Zangenberg et al. [9] and by the fact that, for a Ge content higher than 50%, no local atomic strain around Ge atoms has to be supposed.

2.5 Formulation

Considering their diffusion mechanism, the diffusivity ratio for all dopants between SiGe and pure Si is expressed in our model with the following formulation:

$$\frac{D(SiGe)}{D(Si)} = \left(\frac{1}{1 + K_2 X_{Ge}}\right) \exp\left(\frac{(Q' + Q_{Ge})\ 0.042 X_{Ge} + K_1 \Delta Eg}{k_b T}\right)$$

Where X_{Ge} is the Ge atomic content of the SiGe layer.
Each basic driving force is introduced through the parameters: K_1 for the effect of the modification of the band gap, Q' for the effect of strain, Q_{Ge} for the Ge chemical effect and finally K_2 for the B-Ge pairing effect in case of Boron diffusion.

3 Discussion

In Fig. 1 and 2, we have gathered all the reliable published data on Antimony in [8] and [4], on Boron in [7], [8] and [9] and finally on Phosphorus diffusion in SiGe strained and relaxed layers in [2] and [5].
In our model, Antimony diffusivity is found to increase rapidly with the Ge content of the layer as both stress and Ge chemical effects enhance V-mediated dopant diffusion.

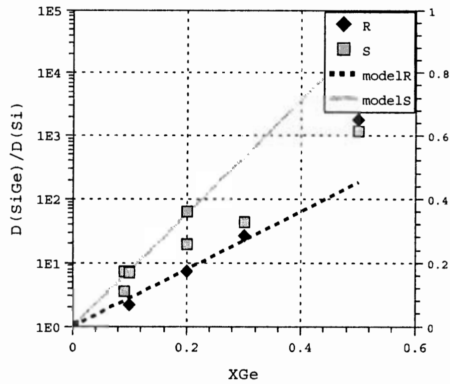

Fig. 1. Antimony diffusivity ratio between SiGe and Si material at 800°C. Squares are experimental data in coherently Strained (S) and diamonds are data in fully Relaxed (R) SiGe. The curves are the model prediction for Strained layer in solid and Relaxed layer in dashed.

The B-Ge pairing is the main effect to consider for Boron diffusion as the effect of the other phenomena on Boron diffusion is weak. Q' and k_2 are on the same order of magnitude than previously published values of [10] and [6].

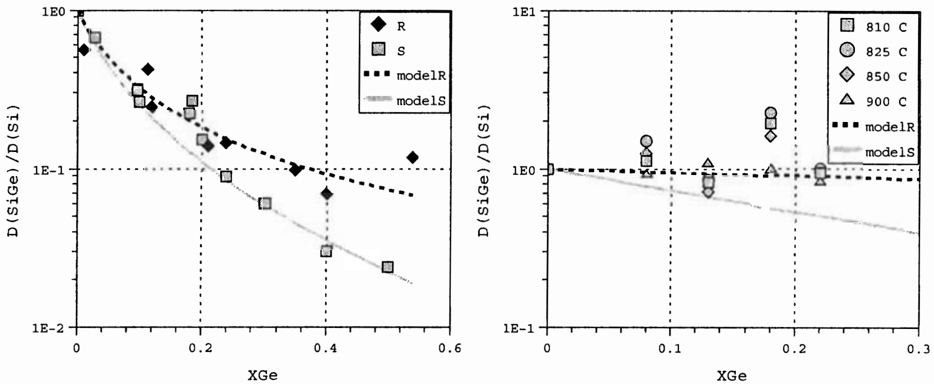

Fig. 2. Boron (left) and Phosphorus (right) diffusivity ratio between SiGe and Si material at 800°C. Legend similar to Fig. 1.

The Phosphorus diffusion in strained and relaxed SiGe, not affected by the pairing effect, is very useful for the study of the different mechanisms acting on Interstitial point defect. P diffusivity is found to be on the same order in Si and SiGe [2] and higher for relaxed layers than for strained ones.

Even if no experimental data of Arsenic diffusion have been reported, our model predicts an enhancement of As diffusivity in Relaxed and Strained SiGe.

4 Conclusion

The understanding of each physical phenomenon involved in the impurity diffusion leads to a unified model for all usual dopants in Strained and Relaxed SiGe in accordance with physical considerations. Despite the dispersion of the experimental data, the diffusion behavior of Sb, P and B in SiGe is well described by our model.
Nevertheless, a detailed atomistic study is needed relative to the behavior of dopant point defects formation energies, and to the B-Ge pairing with the Ge content.

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