

Atomistic predictions of substrate orientation impact during SiGe alloys Solid Phase Epitaxial Regrowth

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Abstract—Coupled effects of substrate orientation and germanium concentration during silicon-germanium Solid Phase Epitaxial Regrowth (SPER) is analyzed through lattice kinetic Monte Carlo simulations. Atomistic events depending on the bonding environment allow to replicate the effects of alloying on SPER velocity of (100) substrates. The model is then used to draw predictions of the regrowth anisotropy in SiGe. Whereas Ge increase leads to a well-established SPER rate increase, whatever is the substrate orientation, moving away from (100) substrate orientation leads to a decrease of SPER rate caused by an unavoidable competition between the atomistic recrystallization configurations.

I. INTRODUCTION

Silicon-germanium (SiGe) alloy is widely used in the Semiconductors Industry especially as strain-induced mobility booster [1]. SiGe is indeed integrated in source/drain regions and junction formation can then result from SiGe partial amorphization and Solid Phase Epitaxial Regrowth (SPER) for enhanced doping activation level. In pure Si or Ge the SPER has been closely studied and the influence of substrate orientation [2]–[4], external strain [5] and impurities [6] are well known and modeled.

Unfortunately, SiGe SPER has not been as widely investigated as Si and models correctly describing SiGe SPER are sparse. Moreover, the effect of substrate orientation on SiGe SPER has not yet been studied. This work will address this issue by predicting some aspects of the substrate orientation impact on SiGe alloys SPER. First, the lattice kinetic Monte Carlo model for SiGe SPER [7] will be presented and compared to experimental data on extracted activation energy of SiGe alloys. In a second time, the model will be extended to draw predictions on SiGe SPER on other substrate orientations.

II. MODEL

SPER of SiGe alloys is investigated with an atomistic model within the phenomenological description of ref [8]. The model focuses on the recrystallization kinetics of amorphous atoms (α -atoms) lying at an amorphous-crystalline interface (α -c interface) [9] [10]. For a pure element, thus only considering

Si-Si or Ge-Ge bonds, the recrystallization rate is only ruled by the α -atom local configuration and can be written:

$$r = K \cdot \exp(-E_a/k_B T) \quad (1)$$

where K , prefactor dependent on the local configuration, and E_a , the activation energy for SPER, are listed in tables I and II and $k_B T$ has its usual meaning. Using the kinetic Monte Carlo (kMC) method, recrystallization probabilities of each α -atom are computed. The α -atom that will be recrystallized is randomly selected according to its rate.

In SiGe alloys, the model has to be refined to consider the different atom types in the α -atom surroundings [7]. The model assumes a bond breaking process [11] [12] as the main mechanism for SPER. The K and E_a values are therefore calculated from the chemical bond types of the two bonds linking the considered α -atom to its crystalline neighbors, as highlighted in Figure 1. The values of K and E_a for the Si-Ge bond type are derived from a model calibration on literature-data [3] [4]. In the refined model, the recrystallization kinetics of an α -atom is written:

$$r_{alloy} = K_{alloy} \cdot N_{config} \cdot \exp\left(-\frac{E_{bond_1} + E_{bond_2}}{2 \cdot k_B T}\right) \quad (2)$$

where $K_{alloy} = \sqrt{K_{bond_1} \cdot K_{bond_2}}$ and N_{config} is the number of possible recrystallization configurations in 3D. The latter term must be included in the Equation 2 in order not to break the kMC approach which forces to have an exhaustive list of all the reaction probabilities. For example, in Figure 2, atom 1 can be bound either with atom 2 or atom 3 to form an six-fold ring and recrystallize. The recrystallization probability for atom 1 should be doubled, hence $N_{config} = 2$ for atom 1.

TABLE I
 SPER ACTIVATION ENERGIES FOR CHEMICAL BOND

Chemical Bond	SPER activation energy (eV)
Si-Si	2.7
Ge-Ge	2.17
Si-Ge	2.86

III. RESULTS AND DISCUSSION

A. Germanium content dependence

Considering (100) substrate orientation, the model has been successfully tested against previous experimental results [3] [4]. SPER rates as a function of Ge concentration are extracted for temperatures ranging from 300 to 650°C for activation energy extraction. Figure 3 shows the activation energy extracted from the Arrhenius plot against the Ge content.

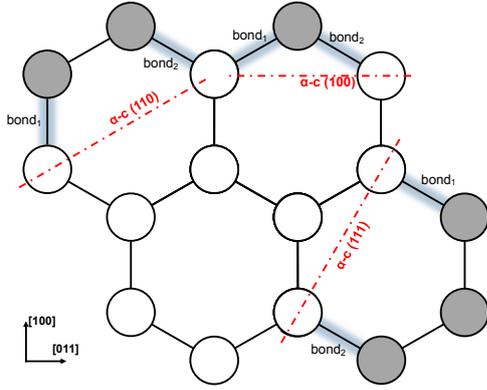


Fig. 1. Schematic of the atomistic configurations for $\{100\}$, $\{110\}$ and $\{111\}$ local configurations. α -atoms are grey. To-be-broken bonds are highlighted.

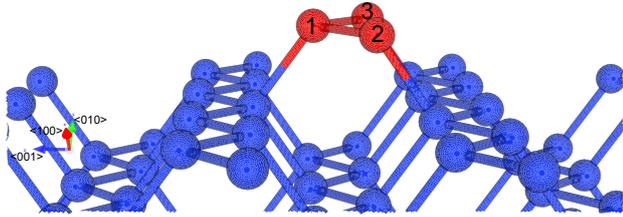


Fig. 2. 3D illustration of two possible $\{110\}$ local configurations for the recrystallization of the atom 1 on a $\{110\}$ plane. Blue atoms are crystalline, red amorphous. N_{config} symbolizes the number of ways that has the atom 1 for being recrystallized, either by forming a hexagon with atom 2 or with atom 3. Here $N_{config} = 2$ for atom 1.

TABLE II
CHEMICAL BOND PREFACTORS FOR MICROSCOPIC(μ)
RECRYSTALLIZATION.

Local config.	$K_{Si-Si}(n)$ (1/s)	$K_{Ge-Ge}(n)$ (1/s)	$K_{Si-Ge}(n)$ (1/s)
$\{100\}_h$	7.425×10^{17}	2.35×10^{18}	4.02×10^{19}
$\{100\}_l$	3.094×10^{16}	1.08×10^{17}	1.81×10^{18}
$\{110\}$	1.325×10^{15}	1.65×10^{16}	2.32×10^{17}
$\{111\}$	8.10×10^{11}	1.50×10^{12}	3.00×10^{13}

The previous model is used on two different cells. For section III-A, a cell of $60 \text{ nm} \times 60a_0 \times 90a_0$ in $\{x, y, z\}$ and periodic conditions along y and z axes. For section III-B $60 \text{ nm} \times 180 \text{ nm} \times 30\sqrt{2}a_0$ with periodic conditions on z -axis only. a_0 is the Si lattice parameter (5.431 Å). The α - c interface evolution is alongside the x -axis. Considering substrate orientation in section III-B, the initial (100) plane is rotated from 0 to 90° around a [001] direction.

From the full Si cell, SiGe alloy is generated by randomly replacing Si atoms by Ge accounting for the specified Ge concentration. The bond distortion brought by the Ge presence is neglected. Initially, all atoms situated between 0 and 55 nm in the x -axis are considered amorphous and the SPER velocities, v , are extracted by a linear interpolation of the α - c interface position for different temperatures.

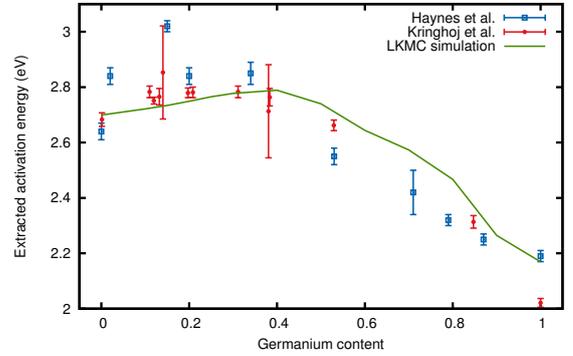


Fig. 3. Composition dependence of extracted activation energy for SiGe alloys SPER. Experimental values from Haynes *et al.* [13] and Kringhøj *et al.* [14].

As the model introduces a value of 2.86 eV for the activation energy of breaking a Si-Ge bond, one could expect that the extracted activation energy maximum will lie for SiGe 50%, at 2.86 eV, where the probability of encountering a Si-Ge bond at the interface is maximum. However, the kMC method is inherently putting into competition all the available events, with their associated probabilities, and the extracted activation energy exhibits this competition.

The fact that, in the competition, there is an event with a relatively low energy (Ge-Ge bond breaking) when compared to the others, tends to lower the extracted activation energy. The more Ge-Ge bonds there are, the more this activation energy lowering there will be. Therefore, for SiGe 50%, the averaged extracted activation energy is lower than for SiGe 40% due to the fact that at SiGe 50% there are enough Ge-Ge bonds to reduce the extracted activation energy below the one of SiGe 40%.

Finally, the introduced value for the Si-Ge bond echoes with the discussion of Haynes *et al.* [13] where they suggested their model might lack an intermediate rate.

B. Coupled concentration/orientation dependence

The model is furthermore used to hypothesize the behavior of SiGe alloys during SPER on different substrate orientations than (100). The results are shown in Figure 4, with SPER rates normalized to allow comparisons between the alloys, and in Figure 5 to complete the image of the Ge influence. Experimental data are plotted when available. This section will juggle between microscopic and macroscopic recrystallizations on several orientations. For the sake of clarity, the former recrystallization will be preceded by μ and the latter by M , for each orientation.

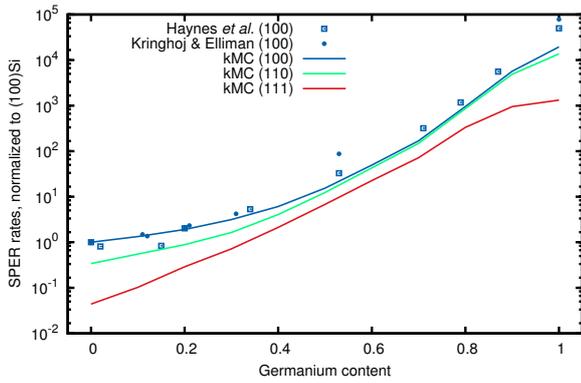


Fig. 4. Experimental [13] [15] and simulated SPER rates dependence on the Ge content on the main orientations during a 450°C anneal.

On the other main orientations, the addition of Ge has the same effect as on (100) alloys. The SPER rate is indeed monotonically increased by the addition of Ge. However, this increase is not the same between the orientations. For (111) alloys, the increase is almost exponential across the whole Ge spectrum. However, the increase is not completely exponential for (100) alloys and they recrystallize almost at the same rate as (110) alloys, thus giving a rate ratio of almost 90% between these orientations, as it can be seen in Figure 5. It can be concluded that, during $M(100)$ recrystallization and especially in the Ge-rich region, the recrystallization is slowed down by some mandatory $\mu(110)$ events, thus reducing the ratio between $M(100)$ and $M(110)$ SPER rates. The more the $\mu(110)$ events there are, the closer the ratio between $M(100)$ and $M(110)$ recrystallization there will be. As $\mu(111)$ event is the slowest, a $M(111)$ recrystallization cannot be furthermore slowed down, hence the quasi exponential rate increase.

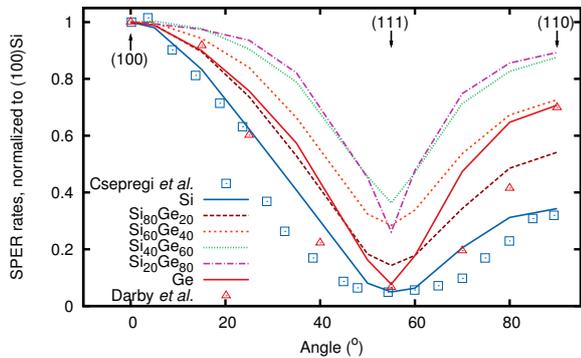


Fig. 5. Available experimental [4] [3] and simulated normalized SPER rates dependence on substrate orientation during SiGe alloys recrystallization.

Figure 5 complements the Ge influence image. Due to the happening of slower events during $M(100)$ recrystallization, the ratio between $M(100)$ and $M(110)$ or $M(111)$ SPER rates are not as strong as in pure Si or Ge. This is especially the case of Ge-rich alloys, e.g. SiGe 60% or 80%, where the ratio between (100) and (110) rates is close to 1:1.

This Ge influence on the SPER rates and their ratios between orientations can also be explained by the competition between the events during SPER. This competition brings an inherent anisotropy at the α -c interface, where some sites have greater recrystallization probabilities than others. This leads intrinsically to a rougher α -c interface in SiGe alloys than in pure elements. The model predicts this behavior as it can be seen in Figure 6. This hypothesis, rose from the kMC calculations, has been tested against experimental data. Pure unstressed Si is known to keep a flat α -c interface during the recrystallization process. The TEM images from references [16] and [17] show indeed relatively flat interfaces, of at most a few nanometers, after recrystallization of several dozens of nanometers.

To compare pure elements to SiGe alloys, a relaxed SiGe 20% sample, grown on a graded buffer, has been implanted at room temperature with Ge^+ ions at 80 keV, to yield 100 nm of amorphous SiGe. The sample was then annealed at 500°C during 7 hours in order to recrystallize 70 nm. The interface roughness is finally extracted via cross-sectional TEM image, and can be seen in Figure 7.

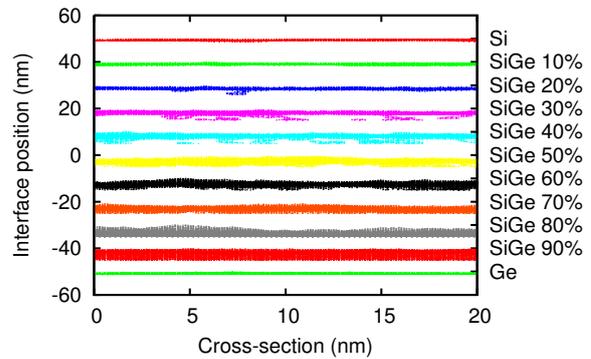


Fig. 6. Cross-section of amorphous-crystalline interfaces after a 70 nm recrystallization with the kMC model at 450°C. Interface are faced up and shifted by 10 nm each to allow comparison. The SiGe alloys exhibit rough interfaces, particularly in the Ge-rich region.

From Figure 7, it is clear that the roughness of the sample is larger than the roughness extracted from pure Si. Several authors have also shown that SiGe SPER exhibits a rougher α -c interface as the Ge content is increased [18]–[20]. However, in these studies, the large roughness is due to the stress brought by the heteroepitaxy and can be explained by the model of Sklénard *et al.* [5]. In the case presented here, the alloy is grown on a graded buffer, therefore eliminating all possible stress. The roughness is thus only due to the local anisotropy brought by the competition between several events. The roughest interface is therefore seen on Ge-rich alloy, where there is a stronger competition between 2.86 and 2.17 eV events, as it can be noticed in Figure 6.

During a $M(100)$ SPER, the rougher the interface is, the more $\mu(110)$ recrystallization sites there will be. This has been assessed by extracting from the kMC simulator the ratio of

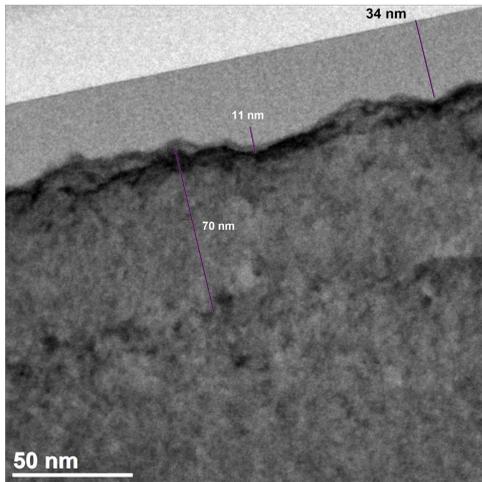


Fig. 7. Bright-field cross-sectional TEM image of a SiGe 20% sample, grown on a graded buffer to avoid stress-related roughness, after a 70 nm recrystallization at 500°C.

$\mu(100)$ and $\mu(110)$ sites that have been recrystallized during a $M(100)$ recrystallization as a function of the Ge content, and can be seen in Figure 8. As hypothesized, the Ge-rich region yields more $\mu(110)$ events due to an increased roughness, thus explaining the low ratios between $M(100)$ and $M(110)$ SPER rates for Ge-rich alloys.

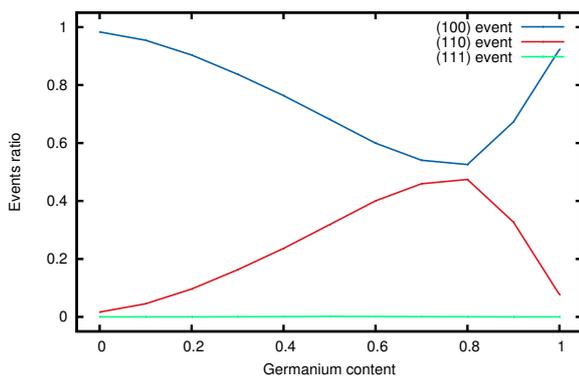


Fig. 8. Ratio of performed events during a $M(100)$ recrystallization. The local anisotropy brought by the competition between events leads to a rougher interface in Ge-rich alloys forcing more $\mu(110)$ recrystallization events to be performed. This impacts the ratios between $M(100)$ and $M(110)$ SPER rates.

IV. CONCLUSION

The influence of Ge addition on both the extracted activation energy and substrate orientation during SiGe alloys SPER has been studied using a kinetic Monte Carlo simulator. The previous model has been refined to include the calculation of the bond type into the recrystallization kinetics and models correctly the Ge content influence on the SiGe alloys extracted activation energy. The Ge addition induces also an increase of the SPER rate on all orientations. However, the increase is less visible on the (100) substrate orientation for Ge-rich SiGe alloys. The inclusion of Ge indeed induces a competition

between recrystallization sites that brings a local and intrinsic anisotropy. This anisotropy leads to a rough interface, rougher than seen in pure elements, and ultimately to weaker ratios between the main orientation SPER rates.

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