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Lattice Kinetic Monte Carlo modeling of germanium solid phase epitaxial growth

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Solid phase epitaxial growth (SPEG) is a common technique used in the manufacturing processes of MOSFET technology. Even though a relatively broad knowledge is found for silicon, there is a greater uncertainty when it comes to germanium, which importance is arising in the last generation of microelectronic devices. To simulate this process, the need of a model which reproduces anisotropic growth and is able to detect and place twin defects becomes relevant, opening the possibility to simulate the interaction of different crystallographies, as it has been observed to be an important factor for some orientations, justifying by this mechanism experimental results.

We present a Lattice Kinetic Monte Carlo (LKMC) model of Ge which is able to give an explanation of the different anisotropy effects in the recrystallization of substrate wafers through a defect formation formalism. An agreement between experimental observations and simulations is found by comparing regrowth velocities for different samples at different anneal conditions with LKMC simulations that consider twin defect formation for specific directions. Different regrowth velocities are found for distinct orientations of a solid phase epitaxial growth process within the annealed sample.

1 Introduction Microelectronic technologies require the development of new materials covering actual properties and applications provided by traditional substrates but adding new functionality. Properties and behavior of silicon have been widely studied and modeled under many different situations and developed for several applications through the past and into the recent years [1–6]. As one of those alternative materials, Ge appears as a valid substitute to silicon [7, 8].

One of the features well characterized for silicon, but not that much modeled in Ge is the SPEG rate dependence on the orientation of the grown substrate. A recent study [9] confirms past observations [10] of strong dependencies on these orientations, not owed to the differences in densities of hairpin dislocations, but to twin defect formation during the recrystallization process.

Consequently, a model similar to silicon [5] but reparametrized to Ge has been developed. It aims to reproduce consistently experimental results for the crucial deca-nano scales that are the main target of the microelectronic processing industries, where the SPEG process is performed within a few nanometers from the surface.

This paper is structured as follows: Section 2 describes the model, dealing with both planar orientation depending on local configurations, and twin defect formation. Section 3 reproduces actual experiments [9] to validate the model when compared with the measured values of SPEG rates and visual observations. Section 4 discusses the results, leaving an open perspective to future work in the field.

2 Model A Lattice Kinetic Monte Carlo (LKMC) model which is able to obtain distinct recrystallization speeds for different planar orientations taking into account

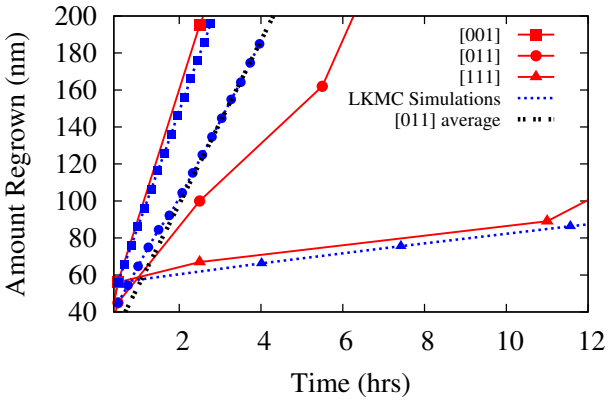

Figure 1 Comparison between experimental results [9] (solid lines) and LKMC simulations (dashed lines) for the three main orientations: [001], [011] and [111]. The first 200 nm of Ge SPEG at 330 °C are shown. A linear regression in the [011] configuration has been done to fit the simulation of that orientation.

facet formation during SPEG by simulating the crystalline lattice is proposed.

Different SPEG velocities are found by carrying out simulations consisting on a full template of crystalline Ge lattice against an amorphous (untemplated) Ge phase. The very next amorphous Ge layer to the α/c interface is progressively crystallized when the number of atoms with two undistorted bonds [11] is the one needed by the planar orientation. These numbers are 1, 2 and 3 for orientations $\{100\}$, $\{011\}$, and $\{111\}$ respectively.

Processes are modeled through three different Arrhenius rates with equal activation energies, and a different prefactor for each one of them. A change in the velocities in the orientations is achieved through these three planar lattice constants, K(100), K(011) and K(111), expressed in atoms/s as:

$$\nu = K\,(site)\exp\left(\frac{-E_{activation}}{k_B T}\right). \qquad (1)$$

As it has been observed in previous works [4,9], it is important to consider a difference in those prefactors depending on the neighbor coordination number encountered at the time of bonding into the lattice. This is modeled by introducing a lower rate in the $\{100\}$ microscopic configurations when less first neighbors are found (6 and 7 in this simulation) making the bond less probable.

Twin defects have also been considered as in Ref. [12], modeled through a 50% probability of forming a twin when a $\{111\}$ configuration is regrown.

3 Results Using an activation energy of 2.17 eV and the prefactors listed in Table 1 the simulations described below have been performed in order to reproduce some of the results showed in Ref. [9].

Configuration	Prefactor(atoms/s)
K(100_h)	2.35 x 10^{18}
K(100_l)	1.18 x 10^{17}
K(011)	2.41 x 10^{16}
K(111)	1.50 x 10^{12}

Table 1 Recrystallization prefactors for the local configurations. *h* and *l* stand for *high* and *low* recrystallization rate, depending on the neighbor coordination number.

Figure 1 presents a comparison between the measured data versus our model for Ge SPEG annealed at 330°C with substrate orientations of $\{100\}$, $\{111\}$, and $\{011\}$, with corresponding angles of 0°, 54.7° and 90° respectively. The experimental first 30 minutes (∼50 nm, depending on the configuration) measured correspond to a planarization process which is not taken into consideration for the results [9]. The calibrated total rates refer to a linear analysis for the whole depth, presented for the $\{011\}$ orientation in the graph to show the fitting performed on the parameters to the average slope. As it has already been pointed out, the average value for thick samples might not be as useful in the microelectronic industry as the values obtained for thin SPEG. In our simulation setup, the cell

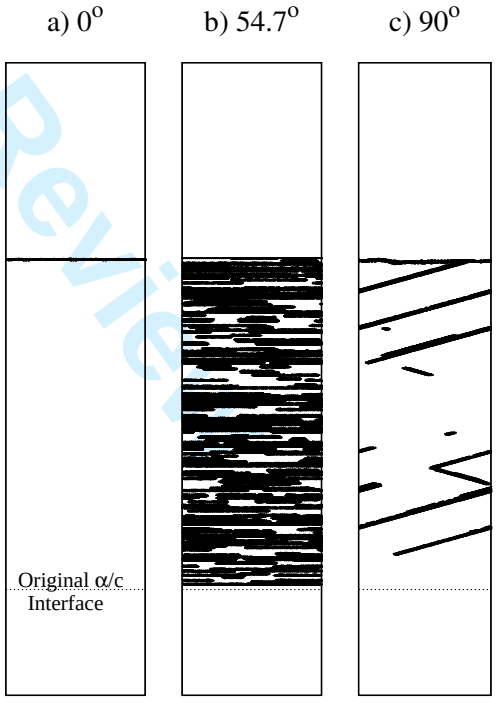

Figure 2 Final atomistic configurations of the 150 nm of simulated SPEG corresponding to the results of Figure 1. Only Ge α/c interface and defective-positioned atoms (twins) are plotted.

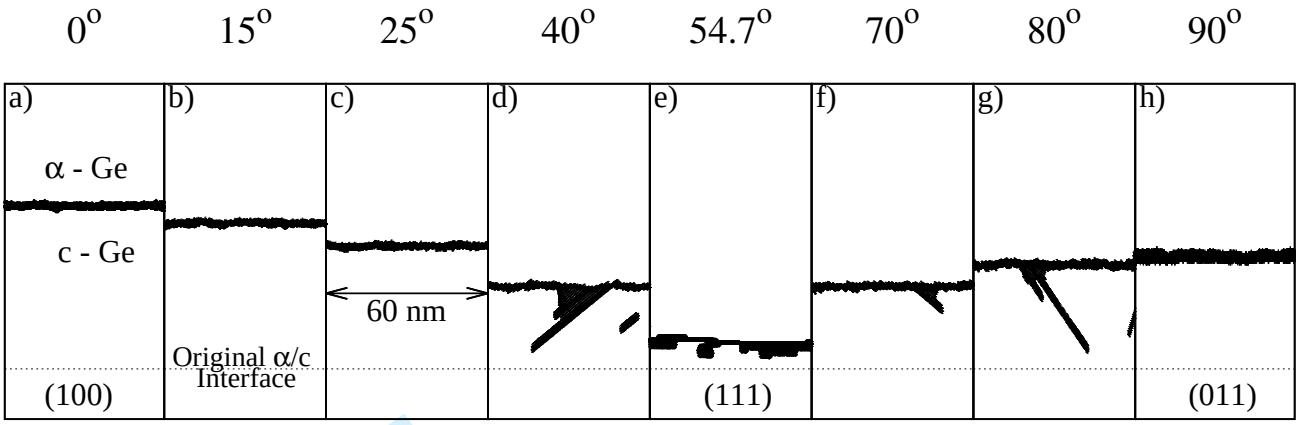

Figure 3 Ge α/c interface and defective-positioned atoms (twins) of an isochronal anneal for eight different configurations at 330°C and 1000s. a) corresponds to the fastest direction, (100) e) to the slowest, (111) and h) is (011). The orientations are a) 0°, b) 15°, c) 25°, d) 40°, e) 54.7°, f) 70°, g) 80°, h) 90°.

has a cuboid geometry with a rectangular base of around 50 nm edge per axis in the YZ plane, depending on the planar configuration due to issues of periodicity in the lattice. Then, the SPEG process was performed through the X axis up to 150 nm. Slight changes in the slope of the experimental results, and differences reported in the literature might be explained as in Ref. [13]: small variations in temperature when performing the experimental procedure have big impacts. An example of the results reported is presented in Figure 2, where a 2D representation of the final regrowth of this process is shown. It can be appreciated that, as expected, {111} configuration is more defective than the others.

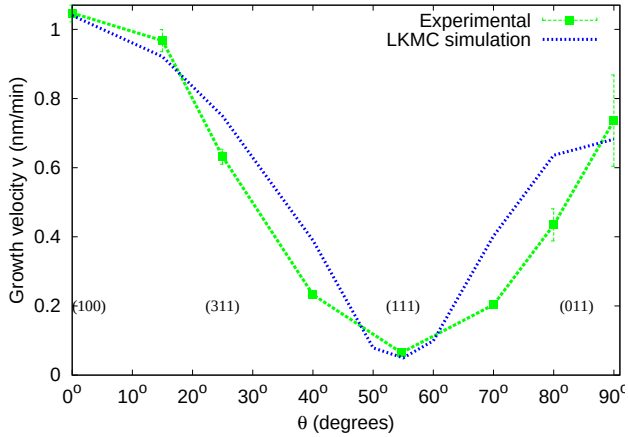

Figure 4 Comparison of experimental [9] Ge SPEG velocities (solid line) and LKMC Simulations (dashed line) for a range of orientations between 0° and 90° at 330°C.

Figure 3 is an atomistic representation of a 1000s isochronal annealing process at 330°C for a wide range of orientations. Position of the Ge α/c interface and defective-positioned atoms of Ge are shown. The low defect roughness for the {100} substrate corresponds to the fastest growing SPEG (a), while the rough {111} substrate corresponds to the slowest orientation. An intermediate roughness between Ge(111) and Ge(100) is also observed for Ge(011).

Figure 4 shows a comparison between experimental and simulated data with the same substrate orientations as in Fig. 3. In the experimental data, a total rate through linear analysis after the first 30 minutes of planarization has been held, proceeding for all orientations in the same way as before. Those planar directions have been simulated with a cell geometry of 180x20 nm^2 with a SPEG amount of 21 nm in the regrowth direction to be recrystallized.

4 Discussion Although the overall match between experiments and simulations in Figs. 1 and 4 is good, the partial disagreement found for the {011} substrate orientation deserves further explanation. On the one hand Csepregi et al. [10] reported a lower velocity for Ge(011) than the one presented in this work. On the other hand, the measured values for {011} recrystallization represented in Fig. 1 seem to present an initial low velocity from 40 to 160 nm, speeding up after that. Does this reflect the true nature of Ge SPEG? Some extra research would be needed to clarify SPEG process on the first nm of regrowth. Other deviations between experimental and simulation results may be a consequence of a mechanism reported by Ref. [14] that we have not seen modeled yet: a process is involved after twin defects are formed in the first seconds of anneal that heals such damage, leaving the structure less defective.

Still, a compromise in the parametrization of the model between the results of Figure 1 for high amounts of material regrowth and for a greater number of orientations (Figure 4) has been made.

It becomes clear in Figure 2 that local configurations of $\{111\}$ are the most important source of defects in Ge, as it is in silicon [3], lowering the velocities of SPEG. Further research in that process might elucidate also the differences in the wide range of orientations, due to the relationship found between the existence of defects and growth velocities.

It is also relevant that a bi-modal growth is not found for the $\{111\}$ configuration in Ge, as it has been demonstrated for silicon [2,5].

5 Conclusions Different growth velocities for each substrate orientation reported for Ge have been modeled successfully using a LKMC algorithm. Simulations match with the results reasonably well for (100) and (111) orientations, while a partial disagreement in the (011) direction is found. Different explanations are given for the disagreement, and further research on this issue is suggested.

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References

[1] A. Claverie, B. Colombeau, B. de Mauduit, C. Bonafos, X. Hebras, G. Ben Assayag, and F. Cristiano, Applied Physics A **76** (7), 1025–1033 (2003).
[2] L. Csepregi, E. F. Kennedy, J. W. Mayer, and T. W. Sigmon, Journal of Applied Physics **49** (7), 3906–3911 (1978).
[3] I. Martin-Bragado, Applied Physics Letters **98** (23), 233109 (2011).
[4] I. Martin-Bragado and V. Moroz, Applied Physics Letters **98** (15), 153111 (2011).
[5] I. Martin-Bragado and B. Sklenard, Journal of Applied Physics **112** (2), 024327 (2012).
[6] I. Martin-Bragado and V. Moroz, Applied Physics Letters **95** (12), 123123 (2009).
[7] A. Toriumi, T. Tabata, C. H. Lee, T. Nishimura, K. Kita, and K. Nagashio, Microelectronic Engineering **86** (7-9), 1571 – 1576 (2009).
[8] D. Kuzum, A. J. Pethe, T. Krishnamohan, and K. C. Saraswat, IEEE transactions on electron devices **56** (4), 648–655 (2009).
[9] B. L. Darby, B. R. Yates, I. Martin-Bragado, J. L. Gomez-Selles, R. G. Elliman, and K. S. Jones, Journal of Applied Physics **113** (3), 033505 (2013).
[10] L. Csepregi, R. Küllen, J. Mayer, and T. Sigmon, Solid State Communications **21** (11), 1019 – 1021 (1977).
[11] R. Drosd and J. Washburn, Journal of Applied Physics **53** (1), 397 – 403 (1982).
[12] I. Martin-Bragado, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms **303** (0), 184 – 187 (2013).
[13] A. Claverie, S. Koffel, N. Cherkashin, G. Benassayag, and P. Scheiblin, Thin Solid Films **518** (9), 2307 – 2313 (2010).
[14] R. Duffy, M. Shayesteh, B. McCarthy, A. Blake, M. White, J. Scully, R. Yu, A. M. Kelleher, M. Schmidt, N. Petkov, L. Pelaz, and L. A. Marques, Applied Physics Letters **99** (13), 131910 (2011).