Facet formation during solid phase epitaxy regrowth: A lattice kinetic Monte Carlo model

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An atomistic model to account for the formation of facets during solid phase epitaxy regrowth (SPER) is shown. This model relies on a lattice kinetic Monte Carlo approach. The lattice atoms produce different crystalline planes growing with different planar velocities. In particular, the model explains the arrow tip formation during SPER of thin silicon fins typical for fin field effect transistors and the formation of trenches in rectangular-shaped amorphized regions in (001) and (011) silicon, caused by the distortion of the lattice by shear strain and propagated by (111) facets.

Source/drain and source/drain extensions in current transistors are typically produced by ion implantation that, in many cases, partially amorphizes the silicon. Subsequent annealing recrystallizes the damaged sections by solid phase epitaxy regrowth (SPER). It is known that SPER can significantly modify the implanted profiles, as has been reported at least for fluorine, arsenic, and indium. Consequently, the correct simulation of SPER is critical for semiconductor processing.

It is also well known that SPER velocity depends on the substrate orientation, with velocity ratios of 20:10:1 for surface orientations (100), (110), and (111), respectively. Moreover, recent studies of very thin silicon layers in fin transistors have shown the formation of nonplanar recrystallization fronts followed by defect and polycrystalline silicon formation. Also, rectangular (also called line-shaped) amorphized regions have been seen exhibiting a complex time evolution and facet formation, including (111) trenches inconsistent with simple SPER models.

There are existing atomistic models that, by using non-lattice kinetic Monte Carlo (KMC), can accurately predict the one-dimensional amorphization/recrystallization in silicon and even the redistribution of dopants during SPER but unable to simulate the different recrystallization speeds of different planar orientations. Therefore a new model is needed to account for the distinctive facet formation during SPER.

In this paper, we show a model that by introducing the crystalline lattice using lattice KMC (LKMC), is able to reproduce different planar SPER velocities, facet formation, and the peculiar evolution of rectangular amorphized regions.

Standard KMC models discard the lattice and keep track of the defects only. The absence of the lattice in the simulation makes it very difficult for SPER to detect the planar orientation to provide different speed for different planes. Reference 9 assumes that amorphization is created by an accumulation of interstitial-vacancy (IV) pairs and explains recrystallization by assigning a recombination rate to each IV pair that depends on the number of neighboring IV pairs. This assumption is very satisfactory to explain why isolated small amorphous pockets dissolve faster than large amorphous layers and to account for the different recrystallization times of different amorphous pocket shapes. Nevertheless it cannot provide facet formation or different planar recrystallization speeds because the IV pairs do not have any lattice reference.

In contrast, the model we propose introduces the silicon lattice in the crystalline regions and assumes that the recrystallization rate for different orientations depends on the quality of the available crystalline template. In particular, following the qualitative model proposed by Ref. 4, we assume that each atom in the amorphous phase needs to form two undistorted bonds with the crystal. This happens naturally for (100) oriented surfaces. For (110) surfaces, a cluster of two adjacent atoms in the amorphous phase is necessary for each atom to complete two undistorted bonds, and a cluster of three atoms is necessary for (111) surfaces. This is modeled using three different prefactors to simulate the different frequencies at which atoms in the amorphous phase join the crystalline one: \( K(1) \) for atoms that have two undistorted bonds, \( K(2) \) for atoms needing another one to join in a cluster, and \( K(3) \) for atoms needing not one, but two extra atoms to join.

Our model has been implemented by defining the silicon lattice with a particular orientation and assigning each silicon atom in the lattice a “crystalline” or “amorphous” flag according to the initial locations of crystalline and amorphous regions. Each amorphous atom has been given a frequency of...
\[ \nu = K(n) \times \exp\left(-\frac{E + |\varepsilon_{xy}|}{k_B T}\right) \]  

(1)

to be transformed into a crystalline atom, where \( K(n) \) are the \( K(1), K(2) \), and \( K(3) \) prefactors explained previously, and \( E \) is the activation energy. The “quality” of the crystalline template degrades whenever the lattice is distorted, and the amount of lattice distortion is proportional to shear strain \( \varepsilon_{xy} \). This is modeled by increasing the SPER activation energy by \( \lambda|\varepsilon_{xy}| \), where \( \lambda \) is a strain coupling parameter. The absolute value of shear strain is issued because the lattice is distorted regardless of clockwise or counterclockwise shear strain.

Figure 1 shows the (100), (110), and (111) SPER velocities produced by our model after calibrating the prefactors as \( 2.1 \times 10^{16}, 2.0 \times 10^{15} \), and \( 5.6 \times 10^{11} \) s\(^{-1}\). The experimental results, taken from Ref. 4, were all scaled by a factor of \( \approx 8 \) to transform the (100) recrystallization speed into the more accepted value of \( 3.1 \times 10^8 \times \exp(-2.68/k_B T) \) cm/s reported in Ref. 12 and despite the data\(^4\) suggesting an activation energy of 2.9 eV, we took the more common value of \( E = 2.7 \) eV. Figure 1 confirms that the model is able to produce the required recrystallization velocities for different crystal orientations.

Figure 2 compares the experimental amorphous/crystalline interface in thin-body silicon for a (100) substrate pattern in the (110) direction and surrounded by silicon oxide,\(^5\) with our simulation results. After an implant and a 60 s annealing at 600 °C, the regrowth is incomplete but the facets are already formed following (111) planes. Since the silicon is surrounded by Si/SiO\(_2\) interfaces, and these interfaces do not provide a suitable template for recrystallization, it regrows faster in the middle than at the sides. This physical effect is captured in our model without extra assumptions. Since the SiO\(_2\) does not provide valid undistorted bonds, the recrystallization close to SiO\(_2\) has the slowest regrowth. Once the planes begin to form, they are pretty stable because recrystallization on (111) planes is very slow. Finally, since the (111) recrystallization is not just slow but also defect prone, it makes possible a disordered recrystallization, known as random nucleation and growth, to recrystallize the rest of the fin and produce polycrystalline silicon (not shown here).

Figure 3 shows the shear strain distribution, simulated with a process simulator,\(^13\) during the evolution of an initially rectangular amorphized region. The strain is generated by the volume expansion during crystalline silicon conversion into amorphous. \( \varepsilon_{xy} \) is particularly strong at the corners of the amorphous crystalline interface. Since the crystalline

![FIG. 2. Left: arrow tip formation during SPER of a thin fin (16 \times 50 nm\(^2\)). Simulation results (symbols) and the experimental amorphous/crystalline regrowth (line, taken from Ref. 5) after a 60 s, 600 °C annealing. Right: 3D view of the same simulation.](image)

![FIG. 3. Simulated shear strain distribution during the SPER evolution of an originally line-shaped amorphized region in silicon. Notice the sharp gradient at the corners.](image)

![FIG. 4. 3D simulation comparisons of recrystallization of line-shaped amorphized regions in (001) [(a)–(c)] and (011) [(a'–(c')] Si substrates as a function of time \( t \) (up to down), in units of the time required for the SPER to reach the surface (symbols) vs expected results (sketches). Each set contains two simulations; the one in the center assumes that shear strain suppresses SPER velocity while the right one shows SPER without this suppression. The simulations including strain effects are in agreement with the qualitative model reported in Ref. 7, reproduced in the sketches left of the simulation results, and provides the physical reason for the presence of more rounded interfaces shown in experimental results.](image)
lattice is distorted by this shear strain, the atoms close to the corners are not as good a template as atoms far from it.

Figure 4 shows the simulation results for different substrate orientation, times and models compared with the observations reported in Ref. 7. a, b, and c represent the time evolution, normalized to the time required for the SPER to reach the surface, for a (001) oriented substrate, while a’, b’, and c’ show similar results for a (011) orientation. The simulations were performed by amorphizing an initial rectangular area of $200 \times 40 \times 25 \text{ nm}^3$ (of which only half is shown in the figure). For these sizes, the normalized $t=1$ was 14.6 min for (001) and 26 min for (110). The feedback between recrystallization and strain was provided by sending the evolving shape to the mechanics strain simulator every 15 s of simulated time, and loading the updated strain back into the LKMC simulator.

Each set a, b, c, a’, b’, and c’ in Fig. 4 contains three figures. The left one is a sketch representing the data from Ref. 7. The center one assumes that strain inhibits recrystallization ($\lambda=5$). The right ones have no strain-induced growth inhibition ($\lambda=0$). This small correction is able to reproduce the data, as a comparison with the sketches and the strain-free model clearly shows. The somewhat rounded shapes obtained with the strain-dependent model reproduce the apparent rounded shapes exhibited by electron microscopy images on Figs. 2 and 3 from Ref. 7.

We have shown in this work a LKMC model that, based on existing qualitative atomistic ideas, quantitatively explains and reproduces the different planar SPER velocities. It also satisfactory reproduces the facet formation in very thin amorphized fins. Finally it explains the anomalous regrowth patterns and facet formation experimentally seen in rectangular shaped amorphized (001) and (011) silicon substrates, by assuming that shear strain suppresses the recrystallization velocity.