

SPER-Driven Dislocation Nucleation and Uphill Diffusion Modeling for Semiconductor Processing

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Abstract—We present a physics-based modeling framework for Solid Phase Epitaxial Regrowth (SPER) in crystalline semiconductors, with explicit focus on two critical phenomena: (i) dislocation nucleation at amorphous-crystalline interfaces, and (ii) dopant uphill diffusion driven by phase-boundary motion. By incorporating orientation-dependent regrowth kinetics and a stress-modulated activation barrier, we model dislocation formation via a critical resolved-normal-stress threshold on the $\{111\}$ habit plane: accumulated tensile stress exceeding the threshold triggers vacancy-type Frank partial nucleation. Simultaneously, we couple the SPER phase-field evolution with a generalized Fickian diffusion model featuring a phase-dependent chemical potential gradient to capture uphill transport.

Index Terms—SPER, dislocation nucleation, uphill diffusion, phase-field, epitaxial regrowth, semiconductor processing

I. INTRODUCTION

Solid Phase Epitaxial Regrowth (SPER) is a frequently used process in advanced CMOS manufacturing, enabling the low-temperature crystallization of amorphous silicon layers. While SPER kinetics have been widely modeled using level-set approaches [1]–[3], a predictive description of dislocation nucleation and uphill diffusion has remained elusive. This work addresses this gap by formulating a minimal yet physics-based model that captures the core physics of SPER-driven defect and dopant evolution.

II. MODEL FORMULATION

A. SPER Kinetics

The SPER level-set equation is expressed as [1]:

$$\frac{d\phi}{dt} = v |\nabla \phi|, \quad (1)$$

$$v = v_0 f \exp\left(-\frac{E_a + \Delta E_s}{kT}\right), \quad (2)$$

where ϕ denotes the phase (0: amorphous, 1: crystal), v the orientation-dependent recrystallization velocity, v_0 the recrystallization velocity prefactor, f the sum of the orientation weight factors, E_a the recrystallization activation energy

($E_a = 2.68$ eV [6]), and ΔE_s the stress-induced change in the activation barrier.

The factor f is calculated using

$$f = a w_{001} + b w_{110} + c w_{111}, \quad (3)$$

$$\hat{n} = a \hat{e}_{001} + b \hat{e}_{110} + c \hat{e}_{111}, \quad (4)$$

where $\hat{n}$ is the surface normal vector of the a-c interface, $\hat{e}_{ijk}$ is the unit vector in the $\langle ijk \rangle$ direction, w_{ijk} is the relative velocity factor for the three major orientations, and (a, b, c) are the components of $\hat{n}$ decomposed in the non-orthogonal basis of the principal directions, evaluated within the angular sector bounded by the adjacent principal directions. With this construction f reduces exactly to w_{hkl} when $\hat{n}$ is along $\langle hkl \rangle$ and interpolates linearly in between, so that w_{111} being the smallest weight directly produces a velocity minimum along $\langle 111 \rangle$. The single-direction regrowth-rate ratios measured by Csepregi *et al.* [7], $v_{001} : v_{110} : v_{111} = 19.7 : 7.5 : 1$, provide the reference ordering. Since those were obtained for planar (single-direction) regrowth, we treat the weights as calibration factors for the present multi-directional, confined geometry.

The regrowth rate depends on the interface orientation and on the local stress. Following Aziz [3], stress couples to the regrowth barrier through an activation strain tensor Ω_{ij}^* , giving the stress-induced barrier change

$$\Delta E_s = -\Omega_{ij}^* \sigma_{ij}, \quad (5)$$

where σ_{ij} denotes the local stress tensor and Ω_{ij}^* the activation strain tensor. We retain the in-plane component $\Omega_{11}^* = +0.15 \Omega$ (Ω : the Si atomic volume), measured directly under applied in-plane stress σ_{11} by Aziz *et al.* [3]; in-plane tension accelerates regrowth, consistent with the observed faster growth of the central $[001]$ front.

In a confined patterned structure, the stress effect should be treated more rigorously. Only Ω_{11}^* has been measured directly, under in-plane uniaxial σ_{11} along $[110]$; the remaining tensor components are not independently established. The

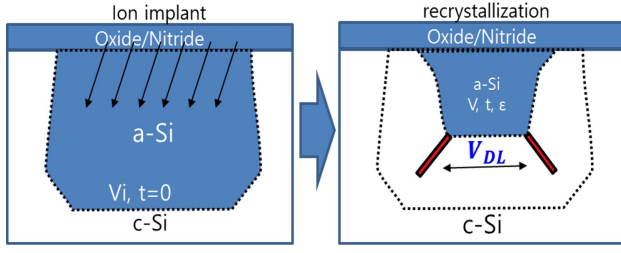


Fig. 1. SPER stress model.

activation-strain-tensor framework moreover does not fully account for the measured response. Assuming in-plane isotropy ($\Omega_{22}^* = \Omega_{11}^*$), the trace relation $\Delta V_h^* = 2\Delta V_{11}^* + \Delta V_{33}^*$ predicts $\Delta V_{33}^* = -0.58\Omega$ from $\Delta V_{11}^* = +0.15\Omega$ and $\Delta V_h^* = -0.28\Omega$ [4], whereas the directly measured value is $\Delta V_{33}^* = -0.35\Omega$ [2], [5]; reconciling the two instead requires $\Delta V_{22}^* \approx -0.08\Omega$, i.e. the in-plane response is not isotropic and the line-direction ($[1\bar{1}0]$) coupling differs in sign and magnitude from Ω_{11}^* . We therefore retain only the directly measured in-plane component $\Omega_{11}^* \sigma_{11}$, which alone gives the best agreement with the observed front shape, and absorb the residual orientation dependence into a modest orientation dependence of the prefactor v_0 . A more rigorous stress model for confined geometries is left to future work.

B. Dislocation Nucleation and Evolution

The stress that drives Eq. (5) is self-generated during regrowth. Amorphous silicon prepared by ion implantation has about 1.8% lower atomic density than crystalline silicon [8]; the crystallization contraction therefore generates an increasing tensile stress as SPER proceeds under a constraining capping layer.

Because α -Si is atom-deficient, the accumulated tensile stress is relieved by the nucleation of vacancy-type Frank partial dislocations, formed by the removal of a $\{111\}$ atomic half-plane (Burgers vector $\mathbf{b} = \frac{a}{3}\langle 111 \rangle$, sessile, with $\mathbf{b}$ normal to the fault plane). The formation of such a climb-type partial is driven by the resolved normal stress on the fault plane,

$$\sigma_{NN} = \hat{n}_i \sigma_{ij} \hat{n}_j, \quad \hat{n} \parallel \langle 111 \rangle, \quad (6)$$

rather than by a resolved shear stress: removal of a half-plane produces a local volume reduction, so it is the tensile normal stress on the $\{111\}$ plane—not shear—that provides the driving force, consistent with the dilatational origin of the stress. A dislocation nucleates where σ_{NN} on a $\{111\}$ plane first exceeds a critical value. Once formed, the dislocation produces a local stress field that compresses the adjacent amorphous side of the interface, locally retarding regrowth at the corner and reproducing the corner slowdown observed experimentally. The process is modeled by coupling the diffusion solver (stress-dependent regrowth) with the stress solver (phase-dependent stress evolution and dislocation formation).

Fig. 1 depicts the model concept, and the physical terms are defined as:

$$\epsilon = 1 - \left(1 - \frac{\Delta V_{total}}{V}\right)^{\frac{1}{3}}, \quad (7)$$

$$\Delta V_{total} = \alpha(V_i - V) - V_{DL}, \quad (8)$$

$$\sigma_0 = 3K\epsilon, \quad (9)$$

where α denotes the volume expansion ratio of amorphous relative to crystalline silicon ($\sim 1.8\%$), V_i the initial amorphous volume, V the current amorphous volume, V_{DL} the volume change associated with the stacking fault from dislocation formation, σ_0 the SPER stress source, and K the bulk modulus. Measurements give an elastic modulus of implant-amorphized Si within a few percent of the crystalline value [9]; we therefore use the same single-crystal Si elastic constants for both phases. The as-implanted amorphous layer is taken to be stress-free, so no initial strain term is included.

At a given time, σ_0 is calculated based on the volume change due to recrystallization and dislocation formation during SPER. The resulting σ_0 is then used as a stress source in the stress solver, and stress equilibration is performed.

C. Uphill Diffusion

During the SPER process, implanted dopants are swept along the moving amorphous-crystalline interface—a phenomenon known as uphill diffusion [10]. In conventional diffusion modeling, an amorphous region is typically assumed to be instantaneously recrystallized during the pre-diffusion step. To explicitly simulate both SPER and uphill diffusion while minimizing disruption to the existing diffusion solver framework, we apply a separate diffusion step to the implanted dopants before the conventional diffusion step. Because uphill diffusion is highly localized at the amorphous-crystalline (a-c) interface and completes within a low thermal budget, it is reasonable to simulate uphill diffusion separately from conventional diffusion. In the separate uphill diffusion model, only the drift term originating from the free energy gradient is considered. Conventional diffusion is performed afterward. Using the generalized Fick's law [16], the drift term is incorporated by defining a phase-dependent chemical potential:

$$\mu^* = \phi \times \Delta G, \quad (10)$$

$$C_{eq} = C_0 \exp\left(-\frac{\mu^*}{kT}\right), \quad (11)$$

where ΔG is the Gibbs free energy difference between the amorphous and crystalline phases, C_{eq} is the equilibrium dopant concentration, and C_0 is a reference concentration (its absolute value is irrelevant).

Accordingly, the total flux becomes:

$$J_A = -D_A C_{eq} \nabla \left(\frac{C_A}{C_{eq}} \right), \quad (12)$$

$$= -D_A \nabla C_A - D_A C_A \frac{\Delta G}{kT} \nabla \phi. \quad (13)$$

The first term represents pure diffusion, while the second term accounts for drift driven by the free energy gradient at the a-c

interface. The free energy difference ΔG between the phases comprises three physically distinct contributions:

$$\Delta G = \Delta H_{\text{strain}} + zq\Delta\psi - T\Delta S_{\text{config}}, \quad (14)$$

namely (i) a *volume/strain* term from the dopant size misfit and the density difference between the amorphous and crystalline phases, (ii) an *electrostatic* term, the product of the dopant charge state z and the electrostatic potential difference $\Delta\psi$ between the two phases (the Fermi level being constant in equilibrium, $\Delta\psi$ arises from the band offset across the a-c interface), and (iii) a *configurational entropy* term, the amorphous network having higher entropy than the ordered crystal.

The strain term is geometry-dependent. Let $\Delta\varepsilon$ denote the lattice strain induced by substituting the dopant for a Si atom (the dopant size misfit), so that the strain-compensation energy follows $\Delta H_{\text{strain}} = -V_0 \Delta\varepsilon : C : \varepsilon$ in the notation of Ref. [11]. In a one-dimensional blanket geometry with a free surface, the volume change on dopant incorporation relaxes along the growth direction and no macroscopic stress builds up; the strain contribution then reduces to the dopant self-energy, scaling as $\Delta H_{\text{strain}} \propto \Delta\varepsilon^2$. In a volume-confined region, however, recrystallization cannot relax freely, so a macroscopic stress develops. This stress couples linearly to the dopant ($\propto \Delta\varepsilon\sigma$), modifies the local equilibrium concentration, and adds to the SPER crystallization stress, making the confined case considerably more complex.

III. RESULTS AND DISCUSSION

Figure 2 shows the simulated SPER evolution, from the initial amorphous profile (a) through intermediate stages (b,c) to the final state with dislocation formation (d). We used the orientation weights $w_{001} : w_{110} : w_{111} = 4.0 : 2.8 : 1$, which make the corners of the [110] and [001] fronts align along the [111] direction. The simulation qualitatively reproduces the formation of (111) facets near the active edge and at the intersection of the [110] and [001] fronts. The in-plane activation-strain coupling of Eq. (5) accelerates the central [001] front, where the in-plane tensile stress is largest, in agreement with the experimentally observed faster central growth. The snapshots in Fig. 2 correspond to annealing at 600 °C for 0, 160, 240, and 320 s, with a regrowth prefactor $v_0 = 3 \times 10^5$ m/s. At the material interface, regrowth is impeded by an additional energy barrier of 0.5 eV applied as a penalty. A dislocation nucleates where the resolved normal stress σ_{NN} on a {111} plane (Eq. (6)) first exceeds a critical value of 0.5 GPa; the predicted nucleation site coincides with the mask-edge corner.

The model also captures the effect of an externally applied strain, imposed as a fixed-displacement boundary condition on the x -faces ($x_{\min}, x_{\max}$) of the domain. Figure 3 compares the regrowth at 600 °C and 240 s under an applied uniaxial strain of -0.5% , 0, and $+0.5\%$. Tensile strain ($+0.5\%$) lowers the activation barrier through Eq. (5) and accelerates crystallization, while compressive strain retards it, consistent with the in-plane activation-strain coupling.

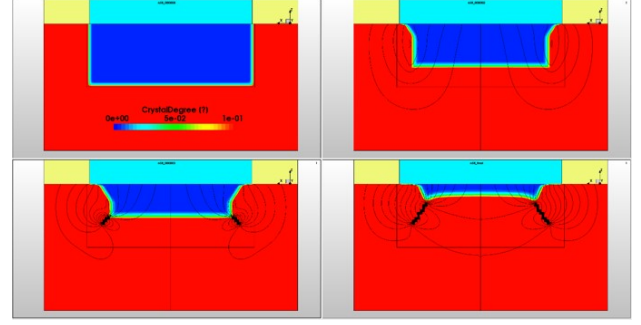


Fig. 2. Simulated SPER evolution at 600 °C: (a) initial (0 s), (b) 160 s, (c) 240 s, and (d) 320 s (final state), showing dislocation formation at the corner. Contour lines are iso-X-displacement and indicate the locations of dislocations and stacking faults.

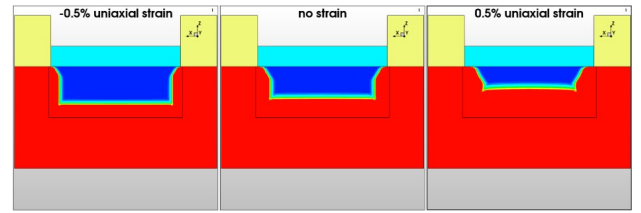


Fig. 3. Effect of an externally applied uniaxial strain on regrowth (profiles at 600 °C, 240 s): -0.5% (compressive), 0, and $+0.5\%$ (tensile). Tensile strain accelerates crystallization.

The present model is intended as a qualitative framework. A numerical caveat arises because SPER is implemented as an advection term within the diffusion solver: a reasonable result requires the phase gradient to vary smoothly over several mesh elements across the interface; otherwise the solution exhibits a strong mesh dependency and a noisy interface. The absolute regrowth velocity is not predicted quantitatively: the prefactor v_0 and the orientation weights w_{hkl} act as calibration factors, chosen through their relative values to make the stacking fault of the nucleated dislocation follow the corner trace, rather than to reproduce measured rates. The pattern-induced stress effect—the experimentally observed difference between line and square geometries, and between etched and unetched structures—is not resolved in detail here; a faithful treatment requires the full film-edge stress field and its temperature history. The simulated amorphous-crystalline boundary is also noticeably flatter than observed experimentally, reflecting the limitations of the linear stress coupling together with the limited accuracy of the activation-strain-tensor description of SPER: only the in-plane component Ω_{11}^* is directly measured, the in-plane isotropy assumption is inconsistent with the hydrostatic data, and the growth-normal component is not well reproduced by the tensor framework. Applying the model to multi-directional recrystallization in confined structures will therefore require more precise stress and activation-strain data; a more complete stress model incorporating the remaining tensor components and higher-order contributions is expected to sharpen the corner morphology and is left to future work.

Dopant redistribution at the moving a-c interface during

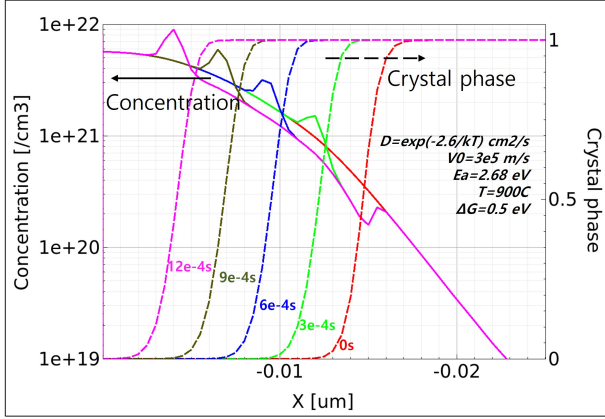


Fig. 4. Demonstration of uphill diffusion using a fictitious dopant species A. The same prefactor $v_0 = 3 \times 10^5$ m/s is used; the remaining parameters are annotated in the figure.

low-temperature SPER has been observed experimentally for B [10], As [13], and B, As, and In [14]. Isolating the uphill sweeping for direct comparison with experiment is difficult, because several effects occur together: amorphizing implants generate end-of-range damage, and the measured profile reflects the combined effects of interface sweeping, fast amorphous-phase diffusion, and conventional diffusion. This is most pronounced for B, whose diffusivity in α -Si is several orders of magnitude higher than in c-Si [12]. The In case is the clearest, being well resolved in Ref. [14]. We therefore restrict ourselves to the sign of each contribution (Table I).

For the electrostatic term, the ionized dopant feels the interfacial band bending as a potential difference $\Delta\psi$ [15]. For a donor the charge is positive and the bending is that of an n -type region; for an acceptor both the charge and the bending reverse, so the product $zq\Delta\psi$ has the *same* sign for donors and acceptors, driving both toward the amorphous side (+). The configurational entropy term ($S_a > S_c$) is likewise common to all species (+). The strain term scales with the size misfit $\Delta\epsilon$: it is weak for the nearly size-matched As, but promotes pile-up for the size-mismatched dopants. We note that this sign is not fixed: *if* a tensile stress builds up preferentially on the amorphous side in a volume-confined region, a small dopant (B, P) would be accommodated more comfortably on the crystalline side, and its strain contribution could reverse.

IV. CONCLUSION

We have presented a physics-based modeling framework for SPER combining orientation-dependent regrowth kinetics, a stress-modulated activation barrier, and interface-driven dopant redistribution. The principal finding is that the location of dislocation nucleation is predicted by the resolved normal stress on the $\{111\}$ habit plane: a vacancy-type Frank partial nucleates at the amorphous-crystalline corner where this stress is largest, in qualitative agreement with the observed mask-edge defect positions. The in-plane activation-strain coupling reproduces the faster central $[001]$ growth, and the dislocation

TABLE I
SIGN OF EACH CONTRIBUTION TO DOPANT PILE-UP AT THE MOVING A-C INTERFACE

Dopant	Strain ($\Delta\epsilon$)	Electrostatic	Entropy	Net
Sb	+	+	+	+
P	$+(-^\dagger)$	+	+	+
B	$+(-^\dagger)$	+	+	+
As	o	+	+	+

+: promotes pile-up, -: opposes, o: weak/neutral. Redistribution of B, As, and In is experimentally established [10], [13], [14]. † The strain contribution of a small dopant (B, P) can change sign once a tensile stress develops during regrowth.

stress field locally retards corner regrowth. The uphill diffusion is treated separately: rather than solving the dopant strain self-consistently with the stress field, we prescribe the Gibbs free energy difference ΔG between the phases and show, for a model dopant, that the drift term of the generalized Fick's law captures the dopant pile-up at the moving a-c interface.

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