Level set modeling of the orientation dependence of solid phase epitaxial regrowth

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Level set methods have previously been successfully implemented in interface propagation for etching and deposition processes. In this article, the authors show that level set methods can be used to model solid phase epitaxial regrowth. The model incorporates orientation dependence of regrowth as found by Csepregi *et al.* [J. Appl. Phys. **49**, 3906 (1978)]. The orientation dependent velocity data are taken from Csepregi's paper and fitted to a polynomial function to give the growth velocity for level set methods. Simulations show the capability of our model in predicting the pinching of the corners in ⟨111⟩ direction and humplike shape in ⟨100⟩ direction. This is confirmed by the transmission electron microscope pictures from recent papers. This modeling holds special interest because of the different diffusivities of boron in amorphous and crystalline silicon (approximately five orders of magnitude difference) and because of the various defects forming at the pinching corners which could lead to higher leakage current in scaled devices. The level set model is implemented in FLOOPS. © *2008 American Vacuum Society.* [DOI: 10.1116/1.2823063]

I. INTRODUCTION

Solid phase epitaxial regrowth (SPER) has been one of the most promising techniques for making shallower junctions with highly activated dopants for silicon devices. SPER has been found to be dependent on many factors which include temperature, orientation, dopants and stress.[1,2] For an undoped silicon without any stress applied, SPER is a thermally activated process (for temperature range of ~470–1300 °C) characterized by a single activation energy of ~2.7 eV.[1] There is a strong wafer orientation dependence on regrowth as shown by Csepregi *et al.*[3] Regrowth rate in the ⟨100⟩ direction is almost 25 times faster than that of the ⟨111⟩ and almost four times ⟨110⟩ direction. The effect of this orientation dependence on rectilinear structures was seen in the experiments done by Rudawski *et al.*[4] and Saenger *et al.*[5] They also show that during regrowth, defects form on some sides of a particular orientation. Hence, it becomes necessary to have a model which predicts a two-dimensional (2D) and three-dimensional (3D) image of the regrowth process. Saenger *et al.* also propose a nanofacet model to account for the different shapes of the regrown layers. However, the model is a qualitative one and might not be able to take into account any doping dependence or stress dependence. Hence, we propose to use level set method to account for the orientation dependence of SPER. Adding doping or stress dependence in this model should be much easier than in some of the earlier methods. Our level set model is implemented in Florida object oriented process simulator (FLOOPS) which gives it an advantage of being able to use diffusion capability of FLOOPS. Hence, complex problems of simultaneous regrowth and diffusion of boron in silicon can be better dealt with.

Previously, level set has been used in Ref. 2 for tracking interface of amorphous and crystalline silicon. They used a corrugated amorphous surface and tried to see the effects of stress, curvature, and orientation on regrowth rate. However, even though their velocity function included orientation dependence, their simulations showed no pinching corners in the ⟨111⟩ direction or humplike shape in the ⟨100⟩ direction (as experimentally seen in Ref. 4). This could be probably because of the small amplitude of their amorphous surface (almost like a sine function), or possibly the stress applied being big enough to negate all the effects of orientation. Our model can predict the shapes that transmission electron microscopy (TEM) images have shown for various stages of regrowth (without stress).

A. Level set methods

Level set methods are computational techniques, which can track a moving interface in 2D/3D.[6] These techniques work by embedding the propagating interface as the zero level set of a time-dependent, implicit function, and then solving the resulting equations of motion in a fixed grid Eulerian setting. In FLOOPS, they have been successfully used for etching and deposition commands. Level set methods are based on hyperbolic conservation law as discussed in Ref. 7.

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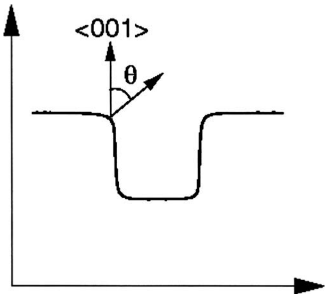

FIG. 1. Surface angle is measured from the ⟨100⟩ direction.

The advantage of level set methods lie in their deftness in being able to propagate different curves based on topological changes, curvature, etc. They have been used in almost every field where interface propagation is required because they can be fine tuned to integrate the physics of the phenomena and at the same time being very stable.

The level set methods are initialized by embedding the interface as a zero level set of a one order higher-dimensional function. This is done by allotting all the points on the level set grid as the signed distances to the original interface [Eq. (1)]

$$\phi(x,y,z,t=0) = \pm d, \tag{1}$$

where ϕ is the higher-dimensional function.

Equation (1) implies that the value of ϕ is zero at the interface. The rest of the grid points get a value of ϕ equal to their distance from the interface (positive on one side and negative on the other side of interface).

The function ϕ then evolves using a convection Eq. (2) which contains a velocity that controls the interface propagation

$$\phi_t + F|\nabla\phi| = 0, \tag{2}$$

where F is the velocity of interface.

$$F = F_A + F_G, \tag{3}$$

where F_A represents the advection velocity (takes the orientation dependence into account) while F_G represents geometric velocity and takes the curvature of the surface into account.

Fast marching method has been implemented in the model to improve the speed of implementation and get better stability. Reference 6 has more information about implementation of fast marching method in level set solutions.

Level set methods approximate very accurately geometric quantities such as curvature, normal, and boundary integrals. This will be very important for our simulations where all these geometric quantities will help relate this mathematical tool with the physics of regrowth.

B. Simulations

For our simulations, we multiply the specified regrowth velocity in the ⟨100⟩ direction with the orientation dependent factor. The data of Csepregi *et al.*[3] was fitted to a fifth order polynomial to get the orientation dependent factor. Figure 1 shows that the surface angle is measured from the ⟨100⟩ direction. Figure 2 shows the data and the fifth order polynomial fit versus surface angle. For our simulations, we have used an amorphous trench region in 2D. The wafer is assumed to be (001) with (110) sidewalls. Hence, the wafer surface sweeps from 0° to 90° as it turns from the wafer bottom up to the sidewalls. Considering the shape of data from Ref. 3, fifth order polynomial was the least order that gives a reasonable fit.

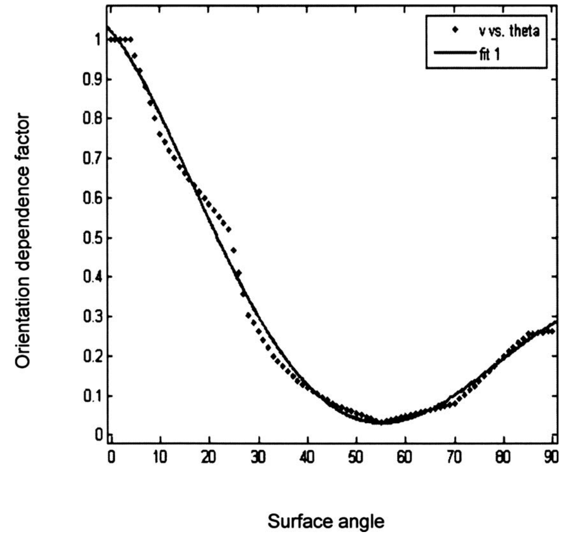

FIG. 2. Data for regrowth velocity and the fifth order polynomial fit vs surface angle.

The polynomial for orientation dependence factor is

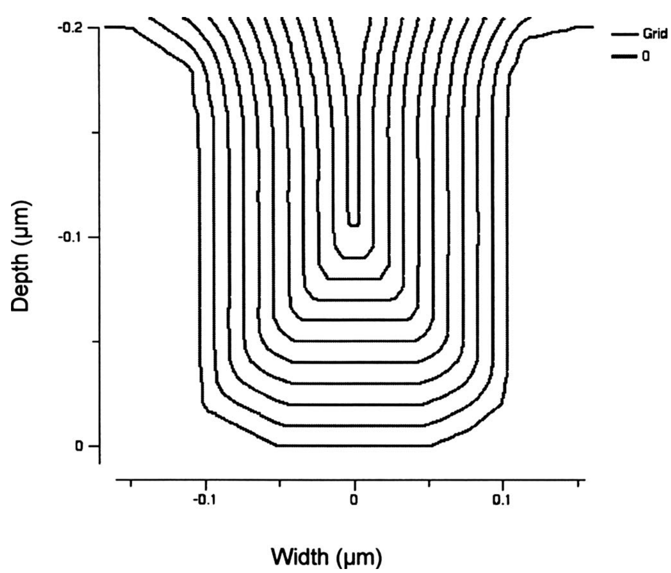

FIG. 3. Regrowth without orientation dependence. The curve represents amorphous-crystalline interface with region below the curve being amorphous. Different curves represent the position of interface at different times.

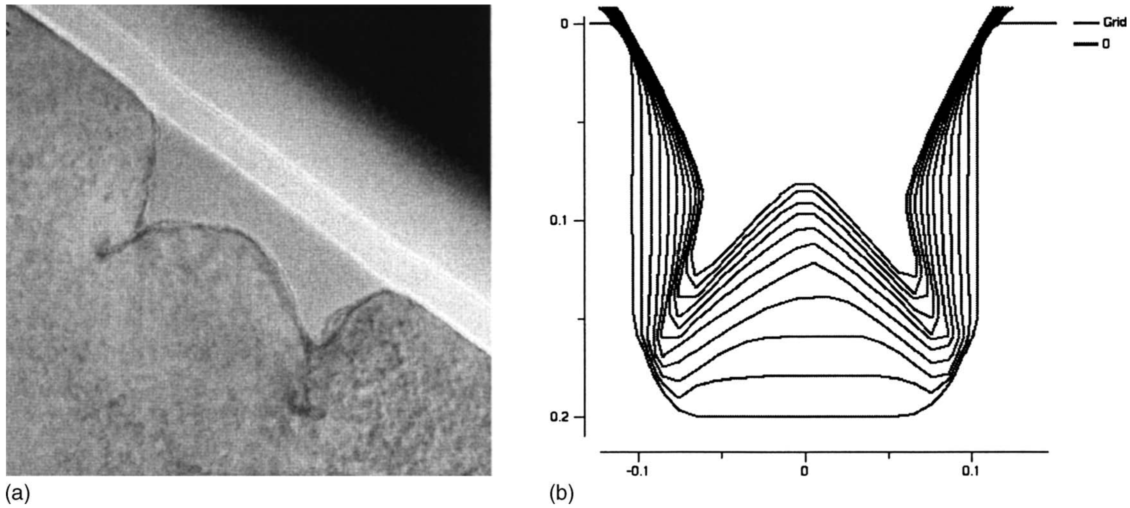

FIG. 4. (a) Cross-sectional transmission electron microscopy image of a partially regrown amorphous-crystalline interface. (b) Simulation of a/c interface (with orientation dependence). The region below the curve is crystalline and above is amorphous. Different curves represent different time points.

$$A_1^*\theta^5 + A_2^*\theta^4 + A_3^*\theta^3 + A_4^*\theta^2 + A_5^*\theta + A_6$$

with $A_1 = 5.3 \times 10^{-10}$, $A_2 = -2.0 \times 10^{-7}$, $A_3 = 2.4 \times 10^{-5}$, $A_4 = -8.9 \times 10^{-4}$, $A_5 = 1.4 \times 10^{-2}$, $A_6 = 1.02$ and θ is the angle in degrees.

We simulated regrowth of a shallow amorphized trench with width and depth equal to 0.2 μm using a constant velocity which was multiplied by the orientation dependence factor. Various stages of regrowth have been shown in our simulations in Fig. 5. Simulations have also been done to see the effect of wider trenches on regrowth and results are shown in Fig. 6.

II. RESULTS AND DISCUSSION

Figure 3 shows regrowth based on isotropic velocity (without any orientation dependence) in the amorphous trench. It is vastly different from what the actual TEM images show.

Figure 4(a) shows a TEM image of partially regrown amorphous trench[4] with the same orientation as used in the simulations. Figure 4(b) is the result of our simulations (orientation dependent) and it shows the evolution of the surface with time. We notice that our model has been able to capture the effects of the pinching in the ⟨111⟩ direction corners and the humplike shape in the ⟨100⟩ direction because of the

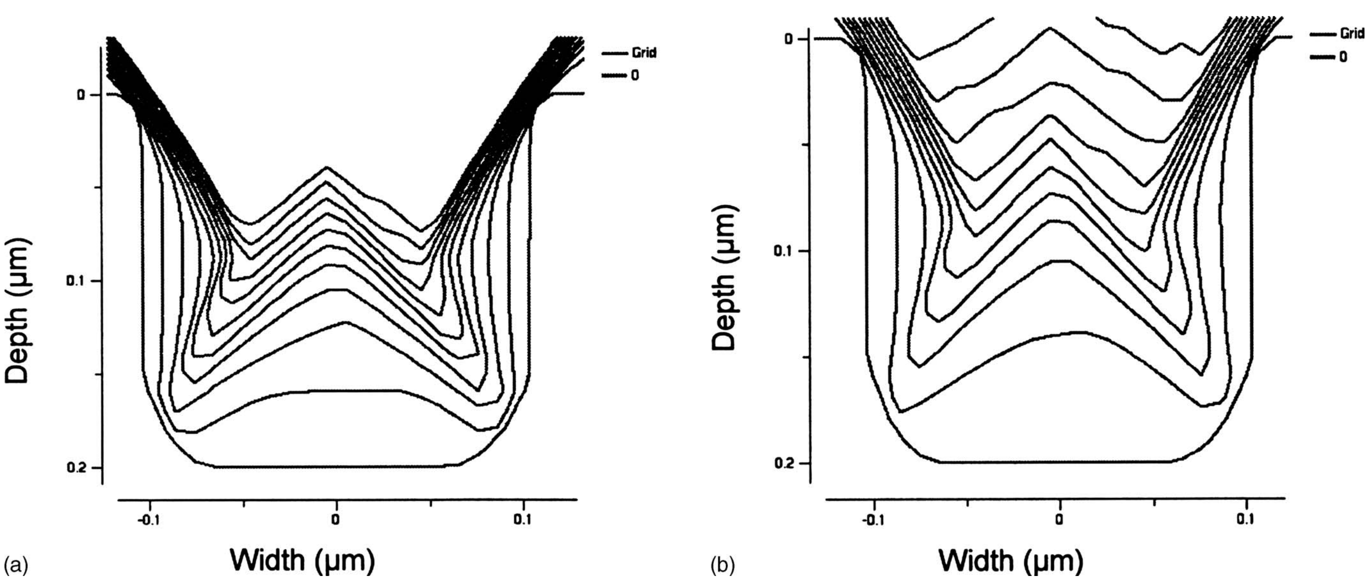

FIG. 5. [(a) and (b)] Simulations of regrowth using level set method for different points in time. (b) is for the smallest time followed by (a) and (b).

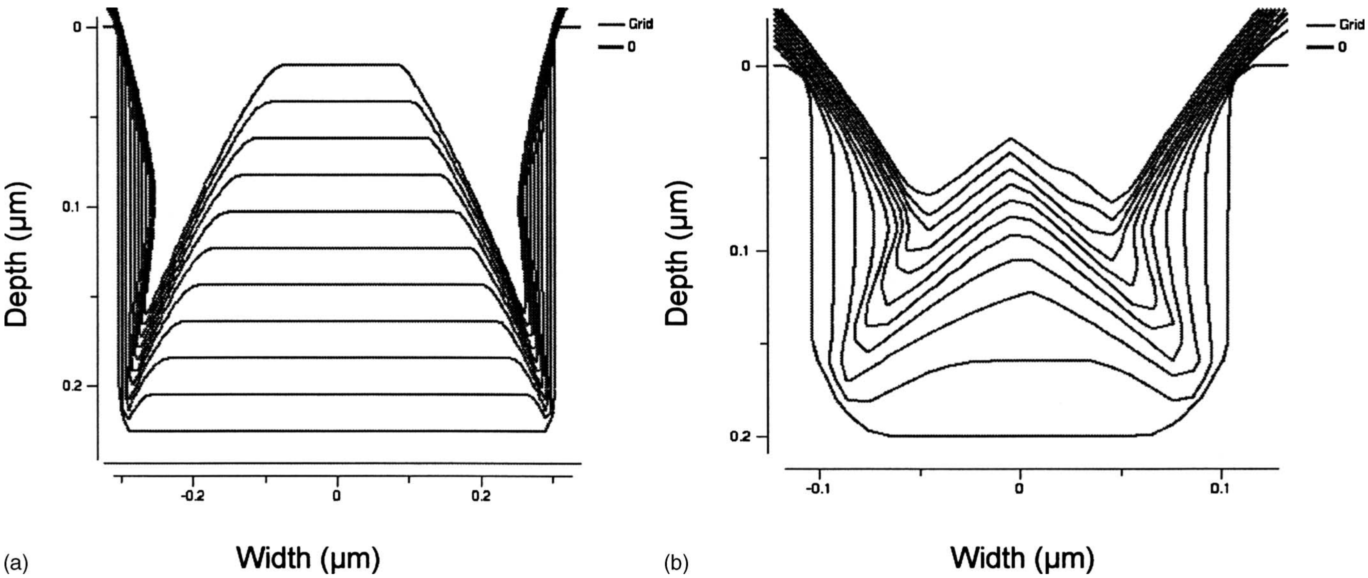

FIG. 6. [(a) and (b)] Simulations of regrowth with wider trenches (each contour represents different time instants).

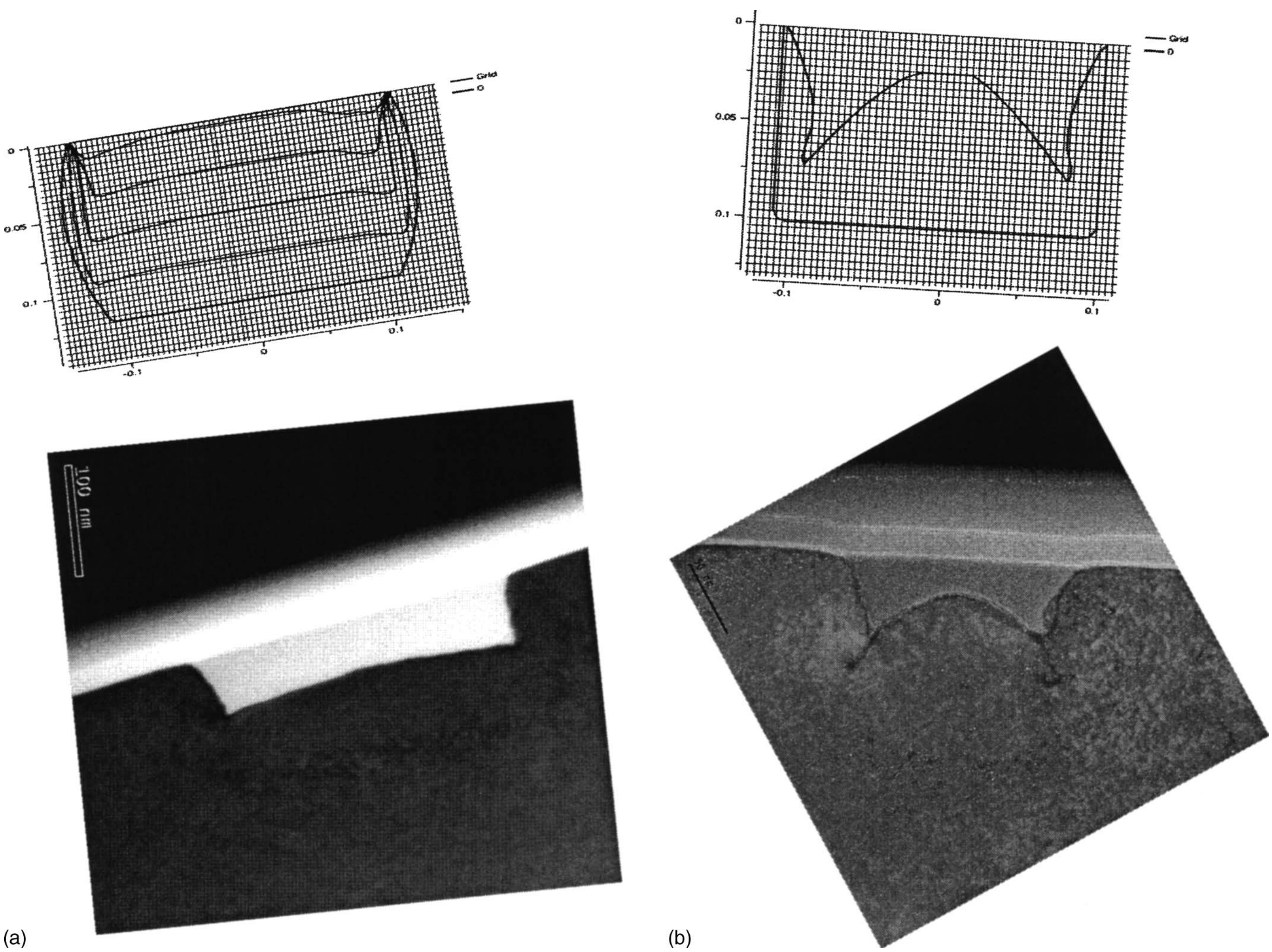

FIG. 7. Simulations placed on top of TEM images (axis and scale matched). (a) shows regrowth without stress while (b) is a compressive stress case.

different velocities in these two directions. The reason we are so much interested in getting these shapes is that there have been experiments[4] which show that the formation of defects during regrowth is strongly dependent on the pinching of corners in the ⟨111⟩ direction. Using stress, this pinching is reduced, defect density can be significantly reduced. The shapes will also be important when diffusion of boron during regrowth is taken into consideration. The diffusivity of boron has been found to be almost five orders of magnitude higher in amorphous silicon as compared to crystalline.[8] We hope to see the effect of nonisotropic velocity on the final boron profiles in future simulations (combining level set methods and FLOOPS' diffusion capabilities).

Figure 5 gives various stages of regrowth. Figures 5(a) and 5(b) are continuations of Fig. 4(b) at higher times. Figure 5(b) shows how finally this would lead to the formation of two separate amorphous packets which will then regrow to complete the crystallization. It also shows the capability of level set method in being able to make two independent surfaces out of one (depending on growth velocity and structure).

Figure 6 shows how the changing of trench width from 0.2 to 0.5 μm changes the shape of regrowth structures. In wider trenches [Fig. 6(a)], the flat portion of the ⟨100⟩ surface reaches the surface before rounding at the top, while Fig. 6(b) is the same case as Fig. 5(a) (trench width of 0.2 μm). These shapes have been confirmed by some TEM images elsewhere.[5]

Another important feature that our simulations predict is that a masked amorphous region (a trench as we have considered) will take more time to regrow than unmasked amorphous layer (like a one-dimensional case for simulation). This is going to have a serious implication since the source/drain in devices is formed by masked amorphous trenches. This is a prediction by our technique and needs to be verified by more experiments.

Figure 7 shows simulations along with TEM images (axis and scale matched). Figure 7(a) shows regrowth without stress while 7(b) is a compressive stress case. Apart from orientation dependence, curvature 4 has been used to match the simulations to TEM images. The role of curvature in regrowth has been shown by Phan *et al.*[2]

III. CONCLUSIONS

We have been successful in simulating the orientation dependent regrowth shapes using level set techniques. The effect of changing trench width on evolving shapes has been shown. TEM images confirm the validity of our model.

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