Modeling a Growth Instability in Stressed Boron Doped Silicon

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ABSTRACT

The effects of rate-enhancing dopants and externally applied stress on interfacial growth during silicon crystallization are modeled using advanced numerical methods. The boron doped crystalline Si is modeled as an isotropic linear elastic solid, and the amorphous as a viscous fluid with a time dependent viscosity to reflect structural relaxation. The effect of the dopant is included through its position dependent effect on the rate of crystallization at the interface. Appropriate coupling conditions across the boundary are defined, and both problems are solved using advanced boundary integral methods. The interface is advanced in time using the level set technique. The simulation results match well with experiments and support the fact that both stress and dopant-gradient effects, along with interface orientation effects, must be accounted for to explain the observed behavior. These new effects are of general relevance to the growth of all non-hydrostatically stressed solids, and are therefore important in film synthesis, with potentially significant applications in electronic devices and thin film coatings.

Keywords: growth instability, stressed boron doped silicon, boundary contour method, level set methods, ion-implantation

1 INTRODUCTION

Strained-layer heteroepitaxy is becoming a useful tool for device designers looking to enhance and extend the capabilities of Si-based devices. As a result, an increasing number of Si-based devices involving strained layers are being investigated for use as high-speed field-effect transistors, heterojunction bipolar transistors, and photodetectors. Many of these devices can be made readily with advanced techniques such as molecular beam epitaxy (MBE). The use of such devices would become much more widespread if more cost-effective processes, such as ion-implantation followed by subsequent solid-phase epitaxial growth (SPEG) to restore crystallinity and activate dopants, could be used for their fabrication.

In this work, we investigate the role of stress on interfacial roughening during SPEG of Si, specifically in the presence of ion-implanted boron, a dopant that enhances the local interface velocity relative to that of pure Si. In earlier works, we showed that compressive stress destabilizes the amorphous/crystalline interface during SPEG of Si and allows it to roughen [1]–[3]. The mechanism for this roughening does not arise from energetic concerns, as has been described in references [4] and [5], but instead from the effect of stress on the barriers to local kinetic growth processes [6], [7]. The simulation methods developed to study the Si SPEG are adapted and extended to treat the boron doped Si experiments. Comparison of experiment and simulation shows that a complex interplay between stress, dopant-gradient, and crystalline anisotropy effects determines the interface evolution during growth.

2 EXPERIMENT AND TRANSITION STATE MODEL

An initially 'flat' amorphous/crystalline silicon interface with a roughness of approximately 2 nm and a boron doping profile that varies with depth (distance from the top surface) has a compressive stress σ_1 (< 0) applied mechanically in the plane of the interface at a temperature of 490°C (see Fig. 1). The subsequent crystallization process results in a roughening of the interface. The sample geometry and procedures used to measure the stress effects are described in reference [3]. Transition state theory is used to describe the phase transformation at the silicon amorphous/crystal interface and is described in detail in reference [1].

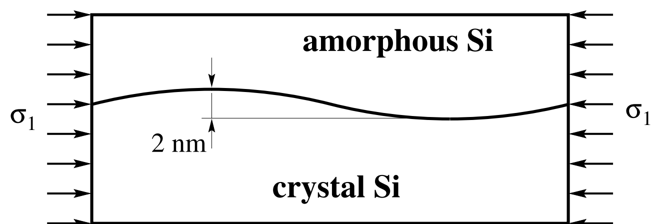

Figure 1: Amorphous/crystalline silicon under compression

3 NUMERICAL METHODS

The simulations are based on a coupling of boundary element and level set methods. The boundary contour version of the boundary element method (BEM) is used to evaluate displacements and boundary stresses on the crystal interface, and tractions on the amorphous interface. Level set methods tract the evolution of this crystalline/amorphous interface. The choice of the boundary contour method (BCM) over the other versions of boundary element method for 2-D simulations is explained in the Simulation section.

3.1 Boundary contour method

The conventional BEM for linear elasticity requires the numerical evaluation of line integrals for 2-D problems and surface integrals for three-dimensional (3-D) ones. By observing that the integrand vector of the boundary integral equation for the Laplace equation is divergence free, Lutz [8] has shown that a further reduction in dimensionality can be achieved. Nagarajan [13] developed this idea into a numerical method that was later termed BCM. Overall, the BCM has been developed for linear elasticity (e.g., [9]–[12]), potential theory [13], and Stokes flow [14]. The divergence free property allows, for 3-D problems, the use of Stokes' theorem to transform surface integrals on the usual boundary elements into line integrals on the bounding contours of these elements (thus the name boundary contour method). For 2-D problems, a transformation based on this divergence free property converts line integrals to path-independent integrals which do not require any numerical integration: integrals are evaluated using potential functions in closed-form. The above transformations are quite general and apply to boundary elements of arbitrary shapes. Thus, the BCM requires only numerical evaluation of line integrals for 3-D problems and simply the evaluation of potential functions at points on the boundary of a body for 2-D cases.

3.2 Level set methods

A traditional technique for tracking moving interfaces is known as the marker particle method for which the interface propagation during incremental time step Δt is monitored by shifting each interfacial marker $\boldsymbol{x}$ in its normal direction $\boldsymbol{n}$ by an amount $v(\boldsymbol{x})\Delta t$. This method can be highly accurate for small-scale motions of the interfaces because of their adaptive nature. However, under complex motions of the interface, the technique can suffer from instability and topological limitations because it follows a local representation of the front, rather than a global one that takes into account the proper entropy conditions and weak solutions.

Level set methods are computational techniques, introduced by Osher and Sethian [15], for tracking moving interfaces in two and three dimensions. These techniques work by first embedding the propagating interface as the zero level set of a time-dependent, implicit higher dimensional function; and second, embedding (or extending) the interface's velocity to this higher dimensional level set function. The resulting equations of motion are then solved in a fixed grid Eulerian setting. Level set methods have been used with considerable success in a wide collection of settings, including fluid mechanics, crystal growth, combustion, medical imaging. This work uses FrontPack (a library for level set methods applied to interface evolution by Adalsteinsson and Sethian) to characterize and advance the evolving interface using a NarrowBand level set formulation [16]. For details about the theory, algorithms, and applications of level set methods, the reader is referred to [17].

4 SIMULATION

Consider a two-phase Si system subjected to nonhydrostatic compressive stress σ_1 as shown in Fig. 1. The interface of the system is modeled as a sine wave with a peak to peak amplitude of 2 nm and a wavelength w. By symmetry only a half wavelength segment needs to be treated (see Fig. 2). The silicon crystal is modeled as an isotropic linear elastic solid with a shear modulus $G_c = 0.6814 \times 10^{11}$ Pa and Poisson ratio $\nu_c = 0.2174$. The amorphous solid is modeled by Stokes flow with a time dependent viscosity to reflect structural relaxation [1]. We assume plane stress for the elastic solids analyses. The interface velocity (normal to the interface) is determined by using Eq. (1) in reference [1]. The velocity is a function of a number of variables, including surface stress, orientation, and curvature at each point on the interface.

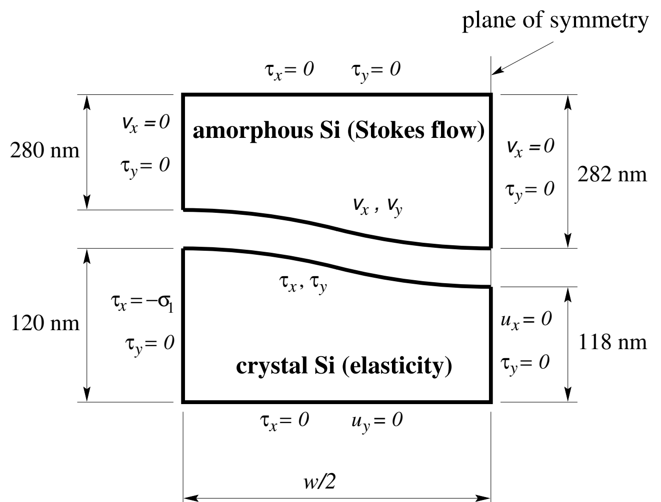

Figure 2: Geometry and BCs for the simulation

The framework employed to determine the interface

growth can be described as follows. First, at time $t = 0$ the traction on the crystal interface is assumed to be $\boldsymbol{\tau}_c = \mathbf{0}$. Then the crystal problem is solved using the BCM for elasticity. A key step in obtaining the traction continuity across the interface is determining the velocity $\boldsymbol{v}_a$ of the amorphous interface at a given time. This velocity results from the relaxation of stress in the crystal due to the change in shape of the interface as it grows. The rate of displacement change du per time step Δt on the crystal interface induces velocity of the amorphous interface

$$\boldsymbol{v}_a \approx \frac{\Delta \boldsymbol{u}}{\Delta t}. \quad (1)$$

Once $\boldsymbol{v}_a$ is determined, traction $\boldsymbol{\tau}_a$ on the amorphous interface can be found by solving the amorphous problem using the BCM for Stokes flow. If $|\boldsymbol{\tau}_c - \boldsymbol{\tau}_a| < \boldsymbol{\epsilon}$ has not been achieved, $\boldsymbol{\tau}_a^{(i)}$ of the current time step is used to update tractions $\boldsymbol{\tau}_c^{(i+1)}$ of the next time step on the crystal interface as follows:

$$\boldsymbol{\tau}_c^{(i+1)} = \boldsymbol{\tau}_c^{(i)} + k_r\, \boldsymbol{\tau}_a^{(i)} \quad (2)$$

where k_r is a relaxation coefficient, and the calculation is iterated.

Upon convergence, the boundary stress on the crystal interface is computed using a post-processing BCM routine. The interface velocity $\boldsymbol{v}_c$ can then be determined by substituting the boundary stress into Eq. (1) in reference [1]. Finally, $\boldsymbol{v}_c$ is supplied to FrontPack in order to advance the crystal interface for the given time step Δt. Note that the mesh of the new interface provided by level set methods could be highly non-uniform. This non-uniformity arises as a result of the fixed grid Eulerian setting employed by level set methods, where two nodes on a new front can be very close to each other. However, this non-uniform mesh can directly be employed by the BCM without degenerating the result accuracy as all boundary integrals are evaluated analytically in the BCM for 2-D calculations.

5 RESULTS AND DISCUSSION

The simulation results match well with experiments. Figures 3 and 4 show plots of the roughness (peak to peak amplitude) vs depth for applied stresses of zero and -0.5 GPa, respectively, for both the simulation and experiment. The zero stress simulation was fit to a wavelength of 150 nm and the -0.5 GPa to a wavelength of 300 nm. These results indicate increasing stress increases overall interface roughening. Matching the boron dopant profile versus depth (not shown) with the roughening profile for the zero stress experiment shows that the roughening increases with increasing dopant concentration. Comparing to the -0.5 GPa stress case indicates that stress tends to sustain the roughening beyond the peak in boron doping. We find that stress, dopant, and kinetic anisotropy effects are all important in determining the roughness evolution during SPEG of boron doped silicon.

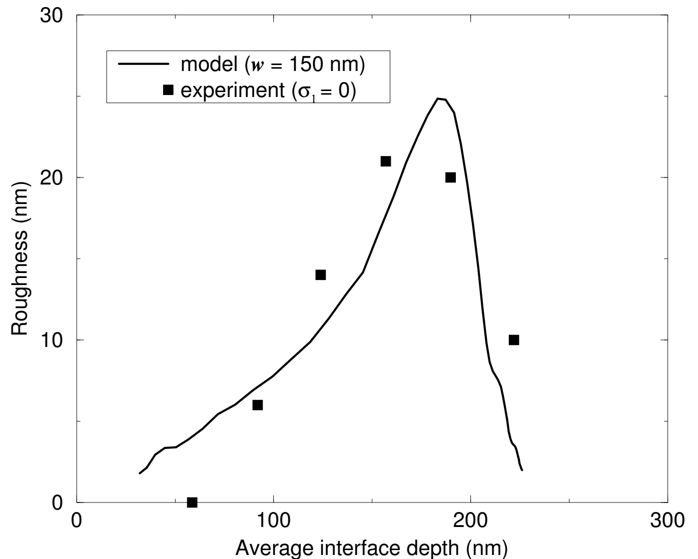

Figure 3: Interface roughness versus depth ($\sigma_1 = 0$)

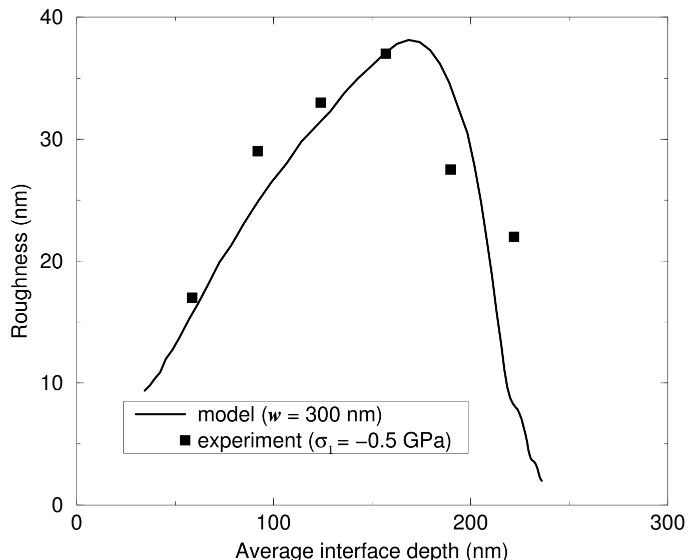

Figure 4: Interface roughness versus depth (σ_1 = -0.5 GPa)

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