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A FLUID-SOLID INTERACTION MODEL OF THE SOLID PHASE EPITAXY IN STRESSED SILICON LAYERS

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ABSTRACT

The solid phase epitaxy (SPE) in silicon is a well-behaved process that has been extensively investigated by numerous research groups. Recent experimental and modeling work has demonstrated that the effect of stress on the mobility of the amorphous-crystalline Si is responsible for the roughening of this interface during the SPE. In this paper, we present a new technique for modeling the SPE growth in stressed Si layers. The technique is based on the use of a finite-element-based fluid-solid interaction scheme implemented in the ANSYS program. Simulation results show that the model is robust and able to explain the observed interfacial instability during the SPE of stressed Si layers.

1.0 INTRODUCTION

Silicon is the widely used material for most microelectronic applications because it is easily workable, highly integrable and possesses semiconductor properties. This is the most extensively studied electronic material in terms of solid phase epitaxy (SPE) research. SPE is a crystal growth process, which occurs when an amorphous layer in contact with a single crystal substrate crystallizes epitaxially in the solid state by the arrangement of atoms at the interface between the phases [3]. Due to the indirect band gap of Si, pure Si devices are not well suited for optoelectronic applications. However, SPE in Si-Ge alloys has received much attention as electronic and optoelectronic manufacturers are trying to use Si-Ge alloys as the next step to make the Si chips faster. Currently, ion-implantation followed by subsequent SPE (II-SPE) is a popular fabrication technique due to its cost effectiveness [4]. However, when applying this technique to the Si-Ge thin film synthesis, roughening of the amorphous-crystal interface occurs, followed by dislocation and stacking fault generation, leading to severely degraded material not suitable for devices. This observed interfacial roughening has been attributed to the Asaro-Tiler-Grinfeld (ATG) mechanism [1] where the elastic strain energy due to the self-stress caused by Ge is reduced by the roughening. Recent experimental and simulation work on pure Si [2,4,6] has demonstrated that compressive stress alone destabilizes the amorphous-crystalline (a-c) interface and allows it to roughen. The mechanism for this roughening does not arise from the elastic strain energy as described by the ATG instability, but rather from the effect of stress on the interface mobility.

The main objective of this work is to examine the role of stress on the defect formation of pure Si thin films by means of a fluid-solid interaction (FSI) finite element analysis (FEA). This is one of our first steps toward the study of the SPE in a more complex Si-Ge system.

2. PREVIOUS WORK

A complex feature in the formation of Si-Ge thin films is the currently unpredictable interaction between chemical compositions (chemistry) and stress effects (elasticity). Sage *et al.* [6] and Barvosa-Carter *et al.* [2] identified a morphology instability in the SPE growth of pure Si, which was due to the kinetically driven instability, *i.e.* the effect of stress on mobilities. They demonstrated this kinetic effect through both experiments and simulations. These simulations assumed that there is no traction on the interface from the amorphous phase and thus, there is no fluid-solid interaction on the a-c interface. A more accurate model was studied later [4] by not using the above assumption. In all the above simulations, boundary element analysis (BEA) is used for evaluating the stress on the a-c interface. While the boundary-only meshing advantage of BEA in this type of simulation is greatly pronounced, Si had to be treated as an isotropic material in order to avoid anisotropic BEA, which is time-consuming and thus, may offset the benefit of BEA meshing. To estimate the error due to this approximation, a new simulation [5] was carried out for the traction-free amorphous case in which, instead of using BEA, FEA was employed due to its simplicity and effectiveness in treating anisotropic materials.

3. TRANSITION STATE THEORY

A transition-state-theory-based model [4] was developed to evaluate the SPE growth rate and we will adopt this model for our FEA-FSI simulation. The growth velocity normal to the interface at any point can be expressed as

$$\upsilon = \upsilon_0(\theta)\exp[(\sigma V^* - E^*)/k_B T]\sinh(\Delta G_{ac}/2k_B T) \qquad (1)$$

where the prefactor $\upsilon_0(\theta)$ contains factors such as the attempt frequency and defect hopping distance and is a function of interface orientation θ. The first exponential factor in Eq. (1) represents the temperature dependence of the interface mobility. E^* is the activation energy, V^* is the activation strain, σ is the stress tensor at the interface evaluated from the crystal side, T is the temperature, and k_B is the Boltzmann's constant. The second exponential (sinh) factor contains ΔG_{ac} which is the difference in free energy between amorphous and crystalline silicon. This free-energy difference includes contributions from capillarity, elastic strain energy density in both phases, and stress-strain work done on the surroundings. For more details of this transition-state-theory-based model, the reader is referred to Reference [4].

4. FLUID-SOLID INTERACTION SIMULATION AND RESULTS

The novelty of the proposed model compared to the previous work [2,4,5] is that it evaluates the stress on the a-c interface by means of a FEA-based FSI technique. A thin layer of Si, subjected to a compressive stress of 0.5 GPa is considered (see Fig. 1). The amorphous region is modeled as a viscous fluid with a constant density, $\rho = 2.3 \times 10^3$ kg m^{-3} and constant viscosity, $\mu = 10^{13.6}$ Pa·s, and the crystalline region as an anisotropic linear elastic solid. Silicon has a cubic crystal matrix type defined by the following three elastic constants $c_{11} = 1.657 \times 10^{11}$ Pa, $c_{12} = 0.639 \times 10^{11}$ Pa, $c_{44} = 0.796 \times 10^{11}$ Pa. The interface is "preripplled" so that it has a sine-wave shape of amplitude A = 10 nm and wavelength λ = 400 nm. The time-dependent growth of the a-c interface is observed from t = 0 to 7000 sec. Since the interface rippling is in one direction, the problem may be treated using 2-D assumptions.

The simulation is based on the ANSYS's FSI using the sequentially weak coupling analysis. Since the FSI problem cannot be solved without defining any velocity of the fluid interface, a separate FLOTRAN analysis (Fig.2) is performed for the amorphous region to determine this velocity. Note that the velocity of the fluid flow at the a-c interface is not resulted from the crystallization, but rather from the applied compressive stress of 0.5 GPa. The velocity field is then applied to the FSI model at the fluid interface. In the FSI, stress is not applied to the fluid

part since the velocity filed, obtained from the FLOTRAN analysis, produces the same effect as that of the stress applied to the fluid part. Since ANSYS does not allow free surfaces for the fluid, a constraint $v_x = 0$ is applied to the side of the fluid region where the stress is removed.
The basic procedure for the simulation involves the evaluation of stress components σ_x, σ_y, and τ_{xy} for the crystalline Si at the a-c interface. This stress is then required by the transition-state-theory-based model (Eq. (1)) to calculate the growth velocity of the interface. Marker particle methods (MPM) are then applied to track the evolution of the interface for a uniform time step of Δt = 50 sec. In the MPM, the interface propagation during incremental time step Δt is monitored by shifting each interfacial marker (x,y) in its normal direction by an amount $v(x,y)\Delta t$.

The snapshots of the interface front profile are shown in Fig.3 with a time difference of 1000 sec between the successive fronts. These snapshots clearly indicate the growth instability wherein the amplitude of the rippled interface grows as the crystal grows. In Fig. 4, the FEA-FSI results are compared with those from the previous traction-free amorphous BEA [4] and traction-free amorphous FEA [5] models, as well as with the experimental data [2,6]. Here, the calculated amplitude of the a-c interface is normalized by the amplitude of the surface corrugation in order to account for sample-to-sample variations in the latter, and is plotted as a function of the average interface depth. From the figure, it can be observed that while both the results BEA and FEA models for the traction-free amorphous case overestimate the rate of growth instability, the proposed FEA-FSI model appears to provide a better fit to the experimental data.

5. CONCLUSIONS

The proposed FEA-FSI model has shown to be suitable for simulating the SPE in stressed Si layers. The advantage of this model is that it can accurately calculate the stress on the a-c interface while treating anisotropic materials in a simple and effective manner. The MPM, that uses a Lagrangian approximation, can be accurate for small-scale motions of interfaces. However, this method follows a local representation of the front that takes into account only the geometric information and does not consider the entropy conditions or weak solution, so it may face problems from the instability and topological limitations. These problems can be resolved by using level set methods (LSM) which follow a Eulerian partial differential equation approach. Our next step is to model the Si-Ge thin film growth by coupling the proposed FEA-FSI scheme and LSM.

6. ACKNOWLEDGEMENT

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7. REFERENCES

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FIGURES

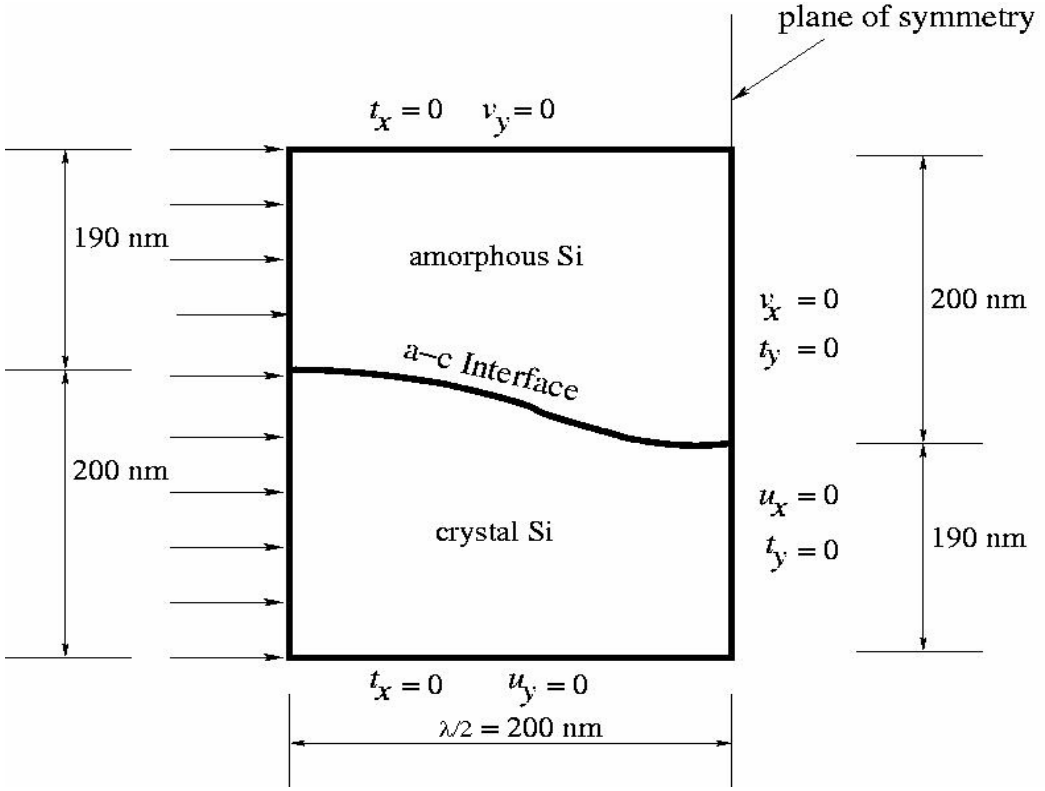

Fig. 1: Geometry and boundary conditions for the FSI model

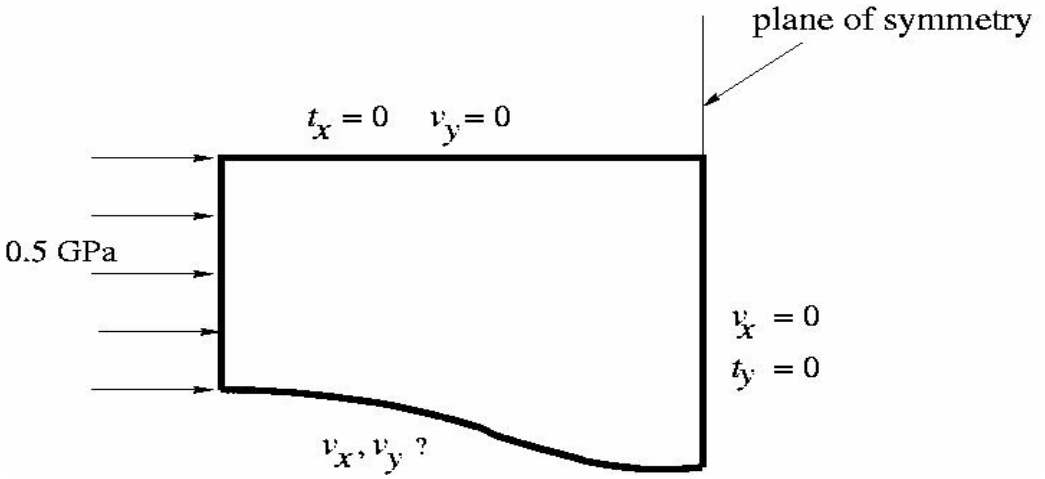

Fig. 2: FLOTRAN Model for the amorphous silicon

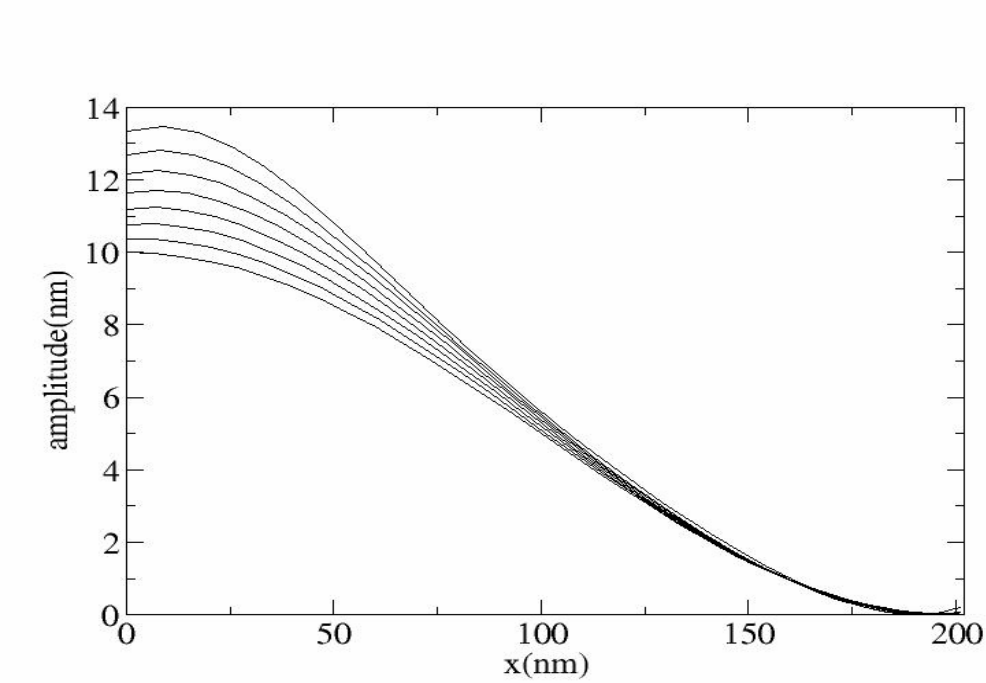

Fig. 3: Snapshots of the interface evolution

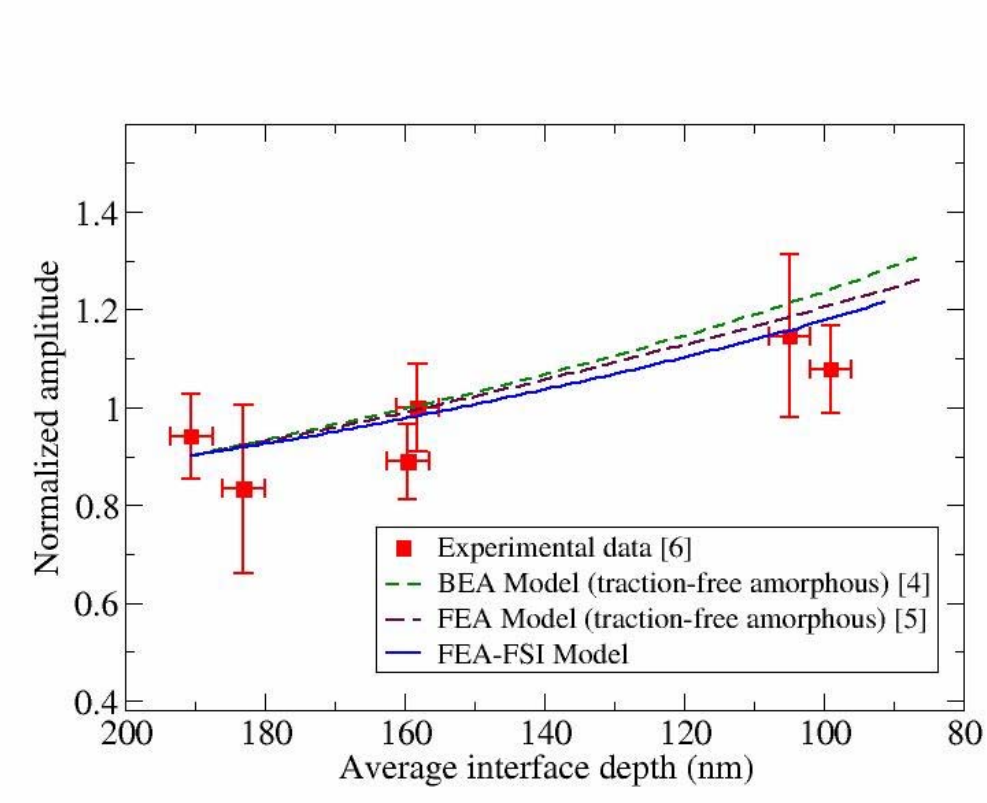

Fig. 4: Average interface depth (nm)