Stressed multidirectional solid-phase epitaxial growth of Si

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The study of the solid-phase epitaxial growth (SPEG) process of Si (variously referred to as solid-phase epitaxy, solid-phase epitaxial regrowth, solid-phase epitaxial crystallization, and solid-phase epitaxial recrystallization) amorphized via ion implantation has been a topic of fundamental and technological importance for several decades. Overwhelmingly, SPEG has been studied (and viewed) as a single-directional process where an advancing growth front between amorphous and crystalline Si phases only has one specific crystallographic orientation. However, as it pertains to device processing, SPEG must actually be considered as multidirectional (or patterned) rather than bulk in nature with the evolving growth interface having multiple crystallographic orientations. Moreover, due to the increasingly ubiquitous nature of stresses presented during typical Si-based device fabrication, there is great interest in specifically studying the stressed-SPEG process. This work reviews the progress made in understanding the multidirectional SPEG and, more importantly, stressed multidirectional SPEG process. For the work reviewed herein, (001) Si wafers with (110)-aligned, intrinsically stressed Si3N4/SiO2 patterning consisting of square and line structures were used with unmasked regions of the Si substrate amorphized via ion implantation. It is revealed that the stresses generated in the Si substrate from the patterning, both in line and square structures, alter the kinetics and geometry of the multidirectional SPEG process and can influence the formation of mask-edge defects which form during growth to different degrees as per differences in the substrate stresses generated by each type of patterning. Likewise, it is shown that application of external stress from wafer bending during SPEG in specimens with and without patterning can also influence the geometry of the evolving growth interface. Finally, the effect of the addition of SPEG-enhancing impurities during multidirectional stressed growth is observed to alter the evolution of the growth interface, thus suggesting that stress influences on growth are much less than those from dopants. Within the context of prior work, attempts are made to correlate the prior observations in single-directional stressed SPEG with the observations from patterned stressed SPEG reviewed herein. However, as is argued in this review, it ultimately appears that much of the research performed on understanding the single-directional stressed-SPEG process cannot be reasonably extended to the multidirectional stressed-SPEG process. © 2009 American Institute of Physics. [DOI: 10.1063/1.3091395]

TABLE OF CONTENTS

I. INTRODUCTION .................................................. 2
II. SINGLE-DIRECTIONAL SPEG PHENOMENA. ........... 2
   A. Atomistic considerations .................................. 2
   B. Temperature dependence .................................. 3
   C. Substrate orientation dependence ....................... 4
   D. Impurity dependence ...................................... 4
       1. Electrically active impurities ....................... 5
       2. Electrically inactive impurities ................... 5
   E. Stress dependence ......................................... 5
       1. Macroscopic kinetics ................................... 5
       2. Morphological instability ............................ 7
       3. Dopant-stress synergy .................................. 7
III. MULTIDIRECTIONAL SPEG PHENOMENA ....................... 7
   A. Mask-edge defect formation .............................. 7
   B. Growth interface pinning ................................ 8
   C. Growth interface curvature .............................. 9
IV. EXPERIMENTAL .................................................. 10
   A. Masking and ion implantation ............................ 10
   B. Application of stress ..................................... 10
       1. Pattern-induced stress ............................... 10
       2. Externally applied stress ............................. 11

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I. INTRODUCTION

Solid-phase epitaxial growth (SPEG) of Si following amorphization via ion implantation has been a phenomenon of fundamental and technological importance for several decades since first being reported more than 40 years ago.1–4 Basically, SPEG is the epitaxial crystallization process of a continuous amorphous (a) Si layer in direct contact with a single-crystal Si substrate at an elevated temperature. The crystalline phase grows at the α-crystalline interface, consuming the α-Si ultimately resulting in a single crystal of Si. The process is also interchangeably referred to as solid-phase epitaxy, solid-phase epitaxial regrowth, solid-phase epitaxial crystallization, and solid-phase epitaxial recrystallization.

SPEG is most often studied as a single-directional phenomenon where amorphization via ion implantation has created an α-Si layer of finite thickness and effectively infinite lateral extent. Single-directional SPEG is also referred to as blanket, single orientation, or bulk growth with a schematic of single-directional (001)-oriented SPEG presented in Fig. 1. The roles of growth temperature,5–7 substrate orientation,8 and impurities9–15 have been widely studied for this case with more recent work investigating the effects of stress on single-directional SPEG.16

The study of multidirectional SPEG has been far less studied relative to the single-directional counterpart. Multidirectional SPEG refers to situations where amorphization has created an α-Si layer of finite thickness width and finite lateral extent. This is also referred to as multiorientation or patterned SPEG. Additionally, within the classification of multidirectional SPEG are the subclasses of two-dimensional (limited in one lateral dimension) and three-dimensional (limited in two lateral dimensions) growths. A schematic of a two-dimensional multidirectional SPEG process is shown in Fig. 2.

SPEG is most commonly employed in front-end processing of integrated circuit (IC) devices. Nonbulk α-Si layers are typically created as the result of selectively masking certain portions of wafers prior to ion implantation. The SPEG process in such circumstances often results in imperfect growth and the subsequent generation of defects which can degrade device performance17–19 and is therefore of great technological relevance. Given this, it is perplexing and somewhat counterintuitive that multidirectional SPEG has been studied far less than the single-directional counterpart.

It is often assumed that the extensive knowledge of single-directional SPEG can be directly applied to multidirectional SPEG but due to the general lack of knowledge about multidirectional SPEG, it is not clear that this is reasonable. More importantly, it is becoming increasingly relevant to study the role of applied stress on patterned SPEG not only due to the increasing presence of stress in IC devices but also as a possible means to circumvent defect formation associated with imperfect multidirectional growth.20–22

This work reviews the progress made in understanding multidirectional SPEG and, more specifically, the role of stress on multidirectional SPEG. Emphasis is placed on understanding the roles of pattern-induced and externally applied stress on multidirectional growth. Further consideration is given to the combined presence of impurities and stress during growth. Ultimately, these studies aim to answer fundamental questions regarding stress influences on the evolution of the α-crystalline interface during growth and the formation/suppression of defects associated with multidirectional growth.

II. SINGLE-DIRECTIONAL SPEG PHENOMENA

A. Atomistic considerations

Before discussing the many important phenomena that occur in single-directional SPEG, it is necessary to discuss the atomistic processes responsible for growth. It is important to note that while SPEG is analogous to liquid-phase epitaxy (LPE), the issue of atomic flux or diffusion of atoms to the growth interface (pertinent to LPE)23 is not relevant to SPEG as the atoms used for growth are already bonded to the growth interface and atomic motion is considerably more hindered compared to the liquid-solid phase transformation.

Starting from an atomically sharp α-crystalline growth interface with no steps, ledges, or islands, atoms in the α-Si phase bonded to the adjacent crystalline phase rearrange to nucleate small crystal islands with monolayer height h.24 This is the case for (001)-, (011)-, and (111)-oriented interfaces. Following nucleation, atoms in the α-Si phase bonded to the island ledges preferentially add to the ledges and the islands grow laterally in the growth interface. Once the island reaches a minimum size Amin, a new island can begin nucleating on top of it. It is believed the ledges have <110>-type normal directions (in the case of Si) as this would minimize the number of α-crystalline bonds generated by adding an atom to an island.14 Classical crystal growth theory holds that the macroscopic growth velocity should be governed by the relation

\[ v = h \left( \frac{J \pi v_{m1} v_{m2}}{3} \right)^{1/3}, \]

where J is the rate of nucleation per unit area and \( v_{m1} \) and \( v_{m2} \) are the ledge migration velocities. By convention, 1 and 2 are the in-plane Cartesian axes and 3 is the axis aligned with the growth direction. In the case of LPE, J, \( v_{m1} \), and \( v_{m2} \) are all governed by the rate of attachment of atoms to
the growth interface and thus Eq. (1) predicts growth to be a single-timescale process.23,25–27

However, it is uncertain if Eq. (1) is also applicable to the case of SPEG. In particular, it has been advanced by some28,29 that SPEG may be a multitimescale process, the origins of which are still not entirely understood. In classical crystal growth theory, it is assumed that a new island with infinitely small initial size (smaller than the critical size to be thermodynamically stable) begins nucleating on top of another island instantaneously after $A_{\text{min}}$ is achieved. Thus, it would be reasonable to assume essentially instantaneous nucleation for such a case. On the other hand, in the case of initial nuclei forming with non-negligible size (perhaps such that a nucleus is thermodynamically stable), it is conceivable that such a process would take a finite amount of time. Particularly in the case of SPEG, atomic movement at the interface is hindered considerably compared to the case of LPE which may give rise to such an issue. Thus, it has been advanced16,28 that after an island reaches $A_{\text{min}}$, nucleation does not begin immediately and requires additional time to form a nucleus with nonzero size.

This process is shown schematically in Fig. 3 for (001)-oriented Si SPEG. If this sequential approach is taken to model growth kinetics, the functional form for $v$ of an advancing $\alpha$-crystalline growth front is given by

$$v = \frac{h}{\tau_n + \tau_m},$$

(2)

where $\tau_n$ is the timescale for island nucleation once the underlying island reaches $A_{\text{min}}$ (referred to as the nucleation timescale) and $\tau_m$ is the time scale required for an island to reach $A_{\text{min}}$ after initial nucleation with $\tau_m$ (referred to as the migration timescale) governed by $A_{\text{min}} = \pi(r_0 + v_m \tau_m)(r_0 + v_m^2 \tau_m)$ where $r_0$ is the initial radius of the nucleated island.

The most important characteristic of Eq. (2) is that SPEG is a multitimescale process as was first suggested by Williams et al.29 Interestingly, work on isolating the nucleation and migration kinetics has suggested that the nucleation timescale is much longer than the migration timescale.16 This is analogous to the energetics associated with formation and migration processes of point defects in bulk Si.30 Thus, in the absence of any other factors, $v \sim h/\tau_n$. However, under different circumstances, the migration timescale is not negligible and must be considered to explain other phenomena associated with single-directional Si SPEG.

**B. Temperature dependence**

The most prominent and well-known attribute of single-directional SPEG is that $v$ for a (001)-oriented $\alpha$-crystalline growth front (in the absence of any other factors) is highly temperature sensitive and exhibits classical Arrhenius-type behavior11 given by

$$v = v_0 \exp \left( \frac{-\Delta G^*}{kT} \right),$$

(3)

where $v_0$ is a temperature-independent prefactor, $\Delta G^* = 2.7$ eV is the activation energy for macroscopic growth, $k = 8.62 \times 10^{-5}$ eV/K is Boltzmann’s constant, and $T$ is the absolute temperature.5–7 Measured $v$ versus reciprocal of $kT$ behavior is presented in Fig. 4. Equations of the form of Eq. (3) also describe the growth kinetics in LPE of pure materi-

![FIG. 1. Schematic of the bulk (001)-oriented SPEG process showing (a) the as-implanted state, (b) partial growth of an epitaxial Si layer, and (c) completed SPEG resulting in a single Si crystal (Ref. 16). Reproduced and modified with permission from Rudawski, Mater. Sci. Eng. R. 61, 40 (2008). Copyright © 2008 by Elsevier. Reprinted by permission of Elsevier.](image1)

![FIG. 2. Schematic of a two-dimensional patterned SPEG process showing (a) the as-implanted state, (b) partial growth of an epitaxial Si layer, and (c) completed SPEG resulting in a single Si crystal.](image2)
als which is somewhat analogous to the SPEG process.\textsuperscript{25,32} It is important to note that SPEG kinetics of deposited $\alpha$-Si films are greatly different from those created via ion implantation and thus this review is limited in scope to $\alpha$-Si created via ion implantation.\textsuperscript{5}

The most important implication of Eq. (3) is that intrinsic SPEG can be reasonably modeled as the result of a single atomistic process which, as per Eq. (2), is the timescale required for island nucleation following achievement of $A_{\text{min}}$ of the underlying layer.

C. Substrate orientation dependence

After discovery of the Arrhenius-type behavior of $v$, it was then revealed by Csepregi \textit{et al.}\textsuperscript{8} that the substrate orientation has a profound influence on SPEG kinetics. They studied the SPEG kinetics as a function of substrate orientation angle ($\theta$) from [001] toward [110] as shown in Fig. 5 and discovered that $v$ is a complicated function of $\theta$. In particular, SPEG kinetics are maximized and minimized for (001)- and (111)-oriented substrates, respectively. A simple bond-rearrangement model by Csepregi \textit{et al.}\textsuperscript{8} was advanced to explain these results based on the assumption that an atom in the adjacent $\alpha$-Si can only add to the Si if bonded to two crystalline atoms. This approach was successful at qualitatively explaining the $v$ versus $\theta$ behavior between the [001] and [111] directions but could not be extended any further.

It is possible to explain all of the results of Csepregi \textit{et al.}\textsuperscript{8} by recognizing that any $\alpha$/crystalline interface oriented away from (001), (011), or (111) orientations (major orientations) will inherently have ledges and steps. Thus, since the atoms preferentially add at ledges, growth becomes dominated by the projection of the ledge velocity onto the growth direction the more tilted the growth direction is from the nearest major orientation. Thus, migration kinetics are more influential in the macroscopic growth kinetics for off-axis directions compared to the major directions.

D. Impurity dependence

The influence of impurities on SPEG kinetics has been extensively studied for many different types of impurities. However, the basic influence a particular impurity has on growth kinetics is determined primarily by whether or not it becomes electrically active.
1. Electrically active impurities

In the case of electrically active impurities, SPEG kinetics are enhanced approximately linearly with impurity concentration which is shown for the case of P in Fig. 6.9–14 For dilute impurity levels, all dopants are incorporated substitutionally and become electrically active during SPEG due to the epitaxial nature of the process, and thus dopant-enhanced growth is attributed to electronic processes occurring at the growth interface.14,33 In particular, it appears that individual crystal nuclei may possess charge states such that the overall nucleation kinetics (given by the addition of charged and uncharged nucleation kinetics) are enhanced. It should also be noted that the study of dopant-influenced SPEG is of high technological relevance as dopant activation during SPEG occurs. It should also be noted that the study of dopant-influenced SPEG is of high technological relevance as dopant activation during SPEG can be achieved which is well in excess of equilibrium solubility. 34–36

2. Electrically inactive impurities

The influence of electrically inactive species on growth kinetics is very different compared to electrically active impurities. In this case, \( v \) decreases with increasing impurity content which is shown for the case of O in Fig. 7.5,6,15 The nucleation kinetics are expected to be unaltered by electrically inactive species and thus SPEG-retarding effects are attributed to slowed migration kinetics. Presumably, this effect occurs as the result of the additional time required to incorporate an impurity atom into a growing island ledge since inactive impurities tend to cause significant local lattice distortions when incorporated nonsubstitutionally.37,38

E. Stress dependence

1. Macroscopic kinetics

Due to the increasingly prevalent nature of stresses during many crystal growth processes, stress-influenced SPEG has become a topic of greater technological interest.39–42 The first studies of stress-influenced (001)-oriented SPEG studied the influence of pure hydrostatic stress (\( \sigma \)) and produced compelling evidence that \( v \) was exponentially enhanced with \( \sigma < 0 \) (compression) as shown in Fig. 8.43–47 Thus, \( v \) as a function of \( \sigma \) was observed to take the form

\[
v = v(0) \exp \left( \frac{\Delta V_n^* \sigma}{kT} \right),
\]

where \( v(0) \) is the \( \sigma = 0 \) (zero stress) growth rate and \( \Delta V_n^* = -0.28 \pm 0.03 \) \( \Omega \) is the activation volume for SPEG under hydrostatic stress and \( \Omega = 12.1 \) cm\(^3\)/mol is the atomic volume of Si. From the form of Eq. (4), it appears that the assumption of SPEG being controlled only by nucleation is reasonably extended to the hydrostatic stress results.

The influence of nonhydrostatic stresses on SPEG kinetics is especially relevant as typical stresses involved in crystal growth are of this nature. Aziz et al.48 were the first to study the effect of uniaxial stress in the plane of the growth interface (\( \sigma_{11} \)) on \( v \) as shown in Fig. 9. The data produced were, as a whole, somewhat weakly ordered and significantly scattered. However, it appears that application of \( \sigma_{11} > 0 \) causes SPEG enhancement while application of \( \sigma_{11} < 0 \) causes retardation. Thus it was suggested that

\[
v = v(0) \exp \left( \frac{\Delta V_{11}^* \sigma_{11}}{kT} \right),
\]

where \( \Delta V_{11}^* = 0.15 \pm 0.01 \) \( \Omega \). In an attempt to unify the results from hydrostatic stress experiments, Aziz et al.48 ad-
advanced the concept of an activation strain tensor ($\Delta V'_{ij}$) which could be used to describe the expected influence of an arbitrary stress state ($\sigma_{ij}$) on $v$ as given by

$$v = v(0) \exp \left( \frac{\Delta V'_{ij} \sigma_{ij}}{kT} \right),$$

where it was assumed that SPEG could be approximated as being the result of a single-timescale process. Physically, $\Delta V'_{ij}$ is the volumetric deformation associated with going from the initial state ($\alpha$-Si) to the transition state during growth as given by transition state theory.\(^{31}\) Due to the strong Arrhenius-type behavior of $v$, this was a reasonable assumption.\(^{5-7}\) Therefore, $\Delta V'_{ij}$ then takes the form

$$\Delta V'_{ij} = \begin{pmatrix} \Delta V'_{11} \\ \Delta V'_{11} \\ \Delta V'_{33} \end{pmatrix}$$

for the $\alpha$-Si/(001) Si interface. Thus, in conjunction with the hydrostatic stress experiments, $\Delta V'_h = 2 \Delta V'_{11} + \Delta V'_{33}$ and $\Delta V'_{33} = -0.58$ $\Omega$. Therefore, it was predicted that uniaxial stress normal to the growth interface ($\sigma_{33}$) would cause greater changes to the growth kinetics than pure hydrostatic stress. Barvosa-Carter\(^{45}\) performed this experiment and reported an exponential enhancement of $v$ with compressive $\sigma_{33}$, as shown in Fig. 10, which is in qualitative agreement with the predictions of the activation strain tensor. However, it was experimentally determined that $\Delta V'_{33} = -0.35$ $\Omega$ which is much less than the predicted value of $-0.58$ $\Omega$ but very similar to $\Delta V'_h = 0.28 \pm 0.03$ $\Omega$. Thus, it appears that normal uniaxial stress causes the same changes to growth kinetics as hydrostatic stress\(^{43-47}\) which is not predicted by the activation strain tensor.\(^{44}\)

Recently, Rudawski et al.\(^{28}\) also studied SPEG with the application of $\sigma_{11}$ and produced results which were in striking contrast to those observed by Aziz et al.\(^{48}\) More specifically, they observed that application of $\sigma_{11} > 0$ did not measurably alter $v$ while application of $\sigma_{11} < 0$ reduced $v$ to be one-half the value observed for $\sigma_{11} \geq 0$ as shown in Fig. 11. Thus, $v$ as a function of $\sigma_{11}$ can be shown\(^{50}\) to be of the form

$$v = \frac{h}{\tau_0 + \frac{1}{\tau_{m,1}(0)} \left[ A_{\min} \pi r_0 \right] \left[ 1 + \frac{2\pi(A_{\min} - \pi r_0^2)}{r_0(\pi A_{\min} - \pi r_0)} \exp \left( \frac{\Delta V^{m,11}_{11} \sigma_{11}}{kT} \right) \right]^{-1}}.$$

where $\tau_0$ is the $\sigma_{ij}=0$ nucleation timescale, $\tau_{m,1}(0)$ is the stress-free ledge velocity along 1, and $\Delta V^{m,11}_{11} = 12 \pm 1$ $\Omega$ is the longitudinal activation volume for ledge migration along $1$. The basis for Eq. (8) is the justification that $\sigma_{ij}$ alters nucleation and migration processes differently depending on the geometry of the deformation associated with the transition state of each process. More specifically, it was rationalized that crystal island nucleation should not be influenced by $\sigma_{11}$ while island ledge mobility in the direction of $\sigma_{11}$ would be altered due to differences in the volumetric deformation associated with each transition state.\(^{31}\) Thus, since nucleation is inherently limiting with $\sigma_{ij}=0$, enhancing migration along one direction (with $\sigma_{11}>0$) does not greatly change the growth kinetics. However, retarding migration along one direction ($\sigma_{11}<0$) increases the time required for an island to reach $A_{\min}$ and thus decreases $v$.

In fact, Eq. (8) can be readily and reasonably fitted to the data reported by Aziz et al.\(^{48}\) in Fig. 9, but it is quite evident that Eq. (5) cannot be reasonably fitted to the data reported by Rudawski et al.\(^{28}\) in Fig. 11. Recently, it was also shown that Eq. (8) can be extended for generalized $\sigma_{ij}$ to explain the


hydrostatic stress and normal uniaxially compression data. Also, work by Phen et al. in SPEG of tensile, biaxially stressed Si did not observe any changes to the growth kinetics which is, in fact, predicted by the model of Rudawski et al. Thus, it appears that the model of Rudawski et al. provides a more accurate overall explanation of all stress-influenced bulk SPEG.

2. Morphological Instability

An interesting result of SPEG with \( \sigma_{11} < 0 \) is interfacial roughening during growth, as shown in the weak-beam dark-field cross-sectional transmission electron microscopy (WBDF-XTEM) images presented in Fig. 12. At first glance, it may appear that the application of in-plane compression simply changes the growth mode from Frank–van der Merwe to Stranski–Krastanow or Volmer–Weber modes. However, the primary driving forces for growth mode transitions of films are the interfacial energy between the film and substrate and the strain energy of the film. In the case of Si SPEG, the film and substrate are identical, so no interfacial energy consideration exists. Also, there is effectively no strain energy consideration since the film and substrate are stressed to equal magnitude. Thus, the morphological instability is kinetically driven.

The model of Rudawski et al. readily predicts this very type of instability. It is important to note that the mechanical properties of \( \alpha \)-Si are much different from the crystalline counterpart. Specifically, Young’s modulus of \( \alpha \)-Si is almost one-half that of the average crystalline value and \( \alpha \)-Si exhibits some viscoelastic behavior (though this is mostly negligible at temperatures where SPEG occurs). Thus, if there is a perturbation in the \( \alpha \)/crystalline interface, the localized stress \( \sigma_{ij}^{\text{local}} \) along the perturbation may be greatly different from the macroscopic stress \( \sigma_{ij} \) depending on how the stress is applied. In the case of application of \( \sigma_{11} < 0 \) applied via wafer bending, it can be shown that \( \sigma_{ij}^{\text{local}} \) in the troughs of the interface will be different than \( \sigma_{ij}^{\text{local}} \) at the peaks of the interface such that the peaks grow faster than the troughs, therefore causing interfacial roughening. In the reverse case, application of \( \sigma_{11} > 0 \) alters \( \sigma_{ij}^{\text{local}} \) at the troughs and peaks such that the troughs grow faster than the peaks, thereby resulting in the dampening of any perturbation in the interface. This is shown schematically in Fig. 13.

3. Dopant-stress synergy

Until recently, it was assumed in all stressed-SPEG studies that any effect of stress on growth kinetics was independent and separable from any other effect. More specifically, this was extended to experiments where both dopants and stress were present. However, recent work by Rudawski et al. suggested that dopants and stress may be synergistic in influencing the growth kinetics. In particular, it appeared that this was the case with in-plane compression, though no synergy appeared to be present for the tensile case. Advancement of this idea was based primarily on prior extensive work of stress-induced changes to the Si band structure since it appears that electronic processes occurring at the growth interface are responsible for dopant-enhanced SPEG.

III. MULTIDIRECTIONAL SPEG PHENOMENA

A. Mask-edge defect formation

Typical IC device layouts have (110)-aligned features on (001) wafers and this configuration will be reviewed in this work. Of course, that is not to say that other configurations are not worth investigating. In particular, there is growing interest in the use of (011) wafers with different crystallographic feature alignments due to possible increases in inherent and stress-enhanced charge carrier mobility. There has been some initial, interesting research into multidirectional SPEG in layouts besides the typical (110)-aligned/(001)-oriented layout, but for purposes of clarity, these layouts have been omitted from this review.

Cerva and Küsters were the first to study the multidirectional SPEG process by forming a two-dimensional \( \alpha \)-Si layer via ion implantation into a (001) wafer with...
(110)-aligned SiO$_2$ lines.\textsuperscript{71-73} This created an $\alpha$-Si layer with rounded corners beneath the mask edges as shown in the high-resolution on-axis phase-contrast XTEM (HR-XTEM) image presented in Fig. 14(a). Following annealing to partially complete SPEG, they observed a sharp notch in the resulting growth interface near the initially round corner of the $\alpha$-Si region, as shown in Fig. 14(b). End of range (EOR) damage is present near the initial $\alpha$/crystalline interface.\textsuperscript{74} With further annealing to complete SPEG, a defect was observed to form which nucleated near the notch in the growth interface and propagated upward to the surface as shown in Fig. 14(c). HR-XTEM suggested the defects to be vacancy-type dislocations or microtwin arrays. However, due to the lack of plan-view TEM (PTEM) analysis, the exact nature of the defects was inconclusive at the time of the initial studies.

It was suggested by Cerva and Küsters\textsuperscript{74} that the mask-edge defects formed as the result of the growth interface on opposite sides of the notch [Fig. 14(b)] folding inward and advancing on itself. However, atomistically, it was unknown exactly why the defects formed as a result of this process.

The notching and subsequent self-advancing of the growth front are somewhat similar to the formation of clamshell or type-IV defects reported by Jones \textit{et al.}\textsuperscript{74} In this case, formation of a buried $\alpha$-Si layer from ion implantation produces two growth interfaces which advance on each other as SPEG proceeds. When the two interfaces meet after SPEG is complete, dislocation loops form at the meeting point. From an atomistic standpoint, this defect formation occurs at the meeting of two migrating island ledges on opposite growth interfaces. If the top crystal layer is slightly displaced relative to the bottom layer, the two ledges will be out of registry and form a dislocation when meeting.

In the case of mask-edge defect formation, there is no way for one portion of the self-advancing front to be displaced relative to the other since the two are connected by a continuous, single $\alpha$-Si crystal. However, as the two portions of the growth front advance, the atoms in the encompassed $\alpha$-Si layer are forced to effectively add to both sides of the growth front almost simultaneously. If the atoms do not add perfectly to both sides of the interface, this could lead to defect formation.

Recently, the nature of mask-edge defects has been studied using $g_{220}$ bright-field PTEM (not presented).\textsuperscript{75} The defects appear to be linear in nature (characteristic of dislocations) and aligned along (110)-type directions and there is no evidence of stacking fault or microtwin contrast. Standard diffraction analysis revealed the dislocations to be either shear- or 60°-type with Burgers vectors of type $b = a/2(110)$ where $a = 5.43$ Å is the Si lattice parameter. Thus, as per the initial observations of Cerva and Küsters,\textsuperscript{74} it appears that the mask-edge defects are, more specifically, composed of shear- or 60°-type perfect dislocations rather than microtwins or stacking faults.

### B. Growth interface pinning

The formation of two-dimensional $\alpha$-Si layers typically results in a portion of the resulting $\alpha$-Si region being formed in contact with a SiO$_2$, Si$_3$N$_4$, or other non-Si layer. In this case, SPEG is inhibited at the point of attachment.

The case of multidirectional SPEG of a two-dimensional $\alpha$-Si region bounded by SiO$_2$-filled trenches, shown in Fig. 15(a), was studied by Burbure \textit{et al.}\textsuperscript{76} During SPEG, the growth interface was pinned at the initial points of contact with the trenches which resulted in the growth interface re-orienting to (111)-oriented SPEG. Thus, a triangular region of $\alpha$-Si bound by the surface, SiO$_2$-filled trench, and (111) plane was formed. In this case, SPEG can only template off the (111)-oriented front, which is known to be highly defective,\textsuperscript{8} as shown in Fig. 15(b).

From Fig. 15(b), it appears that the presence of the SiO$_2$-filled trench is frustrating growth at the point of attachment. This is further substantiated by additional work by Burbure \textit{et al.}\textsuperscript{76} where SPEG was affected with the SiO$_2$ removed from the trenches, as shown in Fig. 15(c). In this case, the size of the resulting triangular $\alpha$-Si region was smaller than the one observed with the SiO$_2$ left intact. Thus, the region of defective Si present after the completion of SPEG was much smaller than the case shown in Fig. 15(b). Presumably, growth at a free surface is allowed since the atoms are not bonded to any other material. Thus, some
growth up the SiO₂-free trench occurs before the formation of a thermally grown SiO₂ layer occurs, which stops further growth.

C. Growth interface curvature

In the absence of any other factors, it is known that a bulk α-Si layer will remain planar during SPEG. In fact, a growth interface which initially has perturbations, shown in Fig. 16(a), will become planar upon annealing and thus the perturbed state is not stable, as shown in Fig. 16(b). This observation has been explained using several different arguments. From standard, classical theory of polycrystalline growth, there is thermodynamic driving force to minimize interfacial free energy. Thus, the direction of motion of the growth interface between two crystals is determined by the sign of the curvature of the interface. This may be analogously applied to SPEG since forming a perturbed growth interface results in excess α/crystalline interfacial area. Therefore, a trough in the interface should grow faster while a peak should grow slower, eventually dampening the perturbation. Such an argument is based on the idea of the α/crystalline interface having an interfacial energy and influencing driving force considerations. Simulation work in fairly simple structures by Phan et al. advanced

\[ v \propto \sinh \left( \frac{\gamma k \Omega}{kT} \right), \]

where \( \kappa \) is the local interfacial curvature, but arrived at the conclusion that curvature did not appreciably influence the SPEG process. Additionally, it is worth noting that to date, there has been no experimental evaluation of \( \gamma \) and only simulation-type work has been used to study such effects. Typically, the derived values of \( \gamma \) are relatively small, on the order of \( \sim 0.5 \) J/m².

Recent work by Morarka et al. also studied the influence of interfacial curvature in SPEG but arrived at the conclusion that curvature significantly alters the process. Specifically, it was determined using level set simulations that the local growth velocity was linearly dependent on the local curvature. At present, the physical explanation for such dependence is unknown, but it has been postulated that the existence of \( \gamma \) between the two phases may be playing a role. Specifically, the stress exerted on the growth interface by the interfacial tension will be greater in the case of a curved interface which, in conjunction with the knowledge of stress-
influenced SPEG, may be the origin of this influence. Work is in progress in an attempt to gain greater insight into the curvature effect.

IV. EXPERIMENTAL

A. Masking and ion implantation

A layer of ~150 nm thick Si$_3$N$_4$ on ~10 nm of SiO$_2$ (both deposited using chemical vapor deposition) was used to form a mask on an ~750 µm thick (001) Si wafer. The residual stress in the continuous Si$_3$N$_4$/SiO$_2$ layer was estimated to be ~1 GPa (tensile) as determined using wafer curvature measurements. The Si$_3$N$_4$/SiO$_2$ layer was then reactive ion etched to form line- or square-type patterning aligned to the ⟨110⟩ in-plane wafer directions as shown in Fig. 17. In the case of the lines, the spacing between adjacent line edges was ~500 nm with a line width of ~250 nm while in the case of the squares, the spacing between edges was ~250 nm with a square width of ~500 nm as shown in Fig. 17.

The Si regions unmasked by the line and square structures were amorphized via ion implanted at room temperature using Si$^+$ implantation at 40 keV to a dose of 1 × 10$^{15}$ cm$^{-2}$ (single implant) or Si$^+$ implantation at 20 and 60 keV with doses of 1 × 10$^{15}$ cm$^{-2}$ (double implants) as shown in Fig. 18. Additionally, some samples receiving double Si$^+$ implantation were subsequently As$^+$ implanted at 7.5–50 keV to doses of 5 × 10$^{14}$–1.6 × 10$^{15}$ cm$^{-2}$. Samples receiving only Si$^+$ implantation are referred to as intrinsic while samples receiving subsequent As$^+$ implantation are referred to as As doped.

B. Application of stress

1. Pattern-induced stress

In the case of a continuous thin film on a very thick Si substrate, the stresses generated in the substrate will be exceedingly small compared to those in the film. However, when the film becomes discontinuous (as in the case of the masking used in this work) significant stresses can be generated in the substrate. As was the case for stress applied during single-directional SPEG, the coordinate system is defined with 1 and 2 Cartesian axes as [110] and [110] in-plane wafer directions and the 3 axis as [001] (the wafer normal). Thus, in the case of $\sigma_{ij}$ generated in the substrate,

$$\sigma_{ij} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{pmatrix},$$

where diagonal elements of $\sigma_{ij}$ are referred to as normal stresses and off-diagonal elements are referred to as shear stresses. By convention, positive (negative) elements of $\sigma_{ij}$ are referred to as tensile (compressive).

Figure 19 presents cross-sectional contour plots of the normal stresses generated in the Si substrate using both line and square structures as simulated using the Florida object-oriented process simulator (FLOOPS). In the case of the line structure for all three normal stress components, tensile stresses are apparent in most of the Si substrate in the area between the maskings. However, in the near vicinity of the

FIG. 17. Plan-view scanning electron microscopy images of (a) line and (b) square structures.

FIG. 18. HR-XTEM images of as-implanted (a) line and (b) square structures Si$^+$ implanted at 20 and 60 keV to doses of 1 × 10$^{15}$ cm$^{-2}$.
mask edge, there is a rapid transition from compressive to tensile normal Si substrate stresses moving from under the masking to the open area.

The normal stresses generated in the Si substrate are very different in square structures compared to the line structures. In particular, the spatial variations in each normal stress are quite different. In the case of $\sigma_{11}$, most of the unmasked area is in tension while the rapid transition from compression to tension moving out from under the mask edge is once again apparent [Fig. 19(f)]. However, in the case of $\sigma_{22}$, the areas both under and out from under the mask edge are compressive (in the mask-edge vicinity) and only the middle portion of the unmasked area is tensile in nature. In the case of $\sigma_{33}$, the behavior is similar to that of $\sigma_{11}$, with the unmasked area in tension and the rapid transition from compression to tension upon moving from under to out from under the mask edge.

Thus, the main difference in the Si substrate stresses generated by line and square structures is that the $\sigma_{22}$ component is entirely compressive both under and out from under the masking for the square structures while it is compressive (tensile) under (out from under) the masking for the lines.

In some certain circumstances, as will be revealed, the patterning was removed after implantation via etching with a solution of 49% HF for 30 min (referred to as etched samples). This effectively removes all substrate stresses previously generated by the masking.

Also, it is important to note that additional stresses may possibly be generated due to thermal mismatch of the materials at high temperatures. However, due to the similarities in the thermal expansion coefficients of Si$_3$N$_4$ and Si, this is likely not a concern.  

Finally, it should be noted that the stress simulations did not address the possibility of stresses in the crystalline phase induced from the ~2% volumetric expansion associated with Si amorphization. Such a possibility is analogous to the well-known phenomenon of stresses induced in a transistor which has SiGe source and drain regions. However, during ion irradiation, the a-Si is subject to viscous flow which could presumably allow for accommodation of the volumetric expansion and minimal resulting substrate stresses in patterned material. Thus, the possibility of stresses in the crystalline phase existing as a result of the amorphization process in patterned material needs further investigation but for purposes of clarity has not been addressed here.

2. Externally applied stress

Another means of applying stress in the Si substrate was achieved using a novel quartz four-point bending apparatus as shown in Fig. 20. The (001) Si wafers were cleaved along (110)-type in-plane directions into strips with approximate dimensions of $0.5 \times 6.0 \text{ cm}^2$. Then, the pieces were inserted into the bending apparatus. A graphite screw was used to push a small piece of glass slide against the underside of the wafer strip. Thus, the two outer bending points are generated by the quartz apparatus and exert a downward force with magnitude $F$ while the two inner bending points are generated by the edges of the glass piece in contact with the graphite screw and generate an upward force with magnitude $F$. This generates an internal bending moment $M$, which varies along the length of the strip. Specifically, within the two inner bending points, $M$ will be constant and maximized as given by

$$M = FL,$$  

(11)

where $L$ is the distance from the inner to outer bending points. As one moves from an inner bending point toward the nearest outer bending point, $M$ decreases linearly with displacement from the inner bending point, $l$, as given by

$$M = FL\left(\frac{L-l}{L}\right),$$  

(12)

and thus $M$ vanishes at the outer bending points and beyond. In the near vicinity of the surfaces of the strips (where the implanted regions are located), $M$ generates $\sigma_{11}$ (uniaxial stress) as given by

$$\sigma_{11} = \frac{Mc}{I},$$  

(13)

where $c$ is the wafer half-thickness and $I$ is the cross-sectional moment of inertia. Thus, uniaxial stress is generated along the in-plane [110] direction using this method. In the case of the top wafer surface, $\sigma_{11}$ will be tensile while in the case of the bottom surface $\sigma_{11}$ will be compressive of the same magnitude. Since $M$ is constant within the two inner bending points, this section of the strip will exhibit a constant radius of curvature, $r$, and the magnitude of $\sigma_{11}$ in the near vicinity of the wafer surfaces in this strip section will be given by

$$\sigma_{11} = \frac{Ec}{r},$$  

(14)

where $E=170 \text{ GPa}$ is Young’s modulus of Si along (110)-type directions at the annealing temperature. Measurement of $r$ was achieved using a Philtec laser displacement system. Since $M$ decreases linearly on moving from the inner to outer bending points, $\sigma_{11}$ will correspondingly decrease as given by
\[ \sigma_{11} = E \left( \frac{L - l}{L} \right) . \]  

Thus, by determining the value of \( \sigma_{11} \) between the inner bending points (the maximum value), \( \sigma_{11} \) can be calculated at any point on the strip.

It is important to note that in cases when the patterning is still present on the wafer strip (referred to at etched samples), \( \sigma_{11} \) generated from bending is additive with that generated from the masking. Of course, in cases where the strips were etched prior to bending, \( \sigma_{11} \) generated is only from bending.

C. Temperature calibration and annealing

All specimens were annealed in N2 ambient using a tube furnace. In the case of specimens not subjected to application of wafer bending, pieces were placed in a quartz tray which was inserted into the furnace. In the case of specimens subjected to bending, only the quartz bending apparatus with a bent strip was inserted into the tube furnace. The furnace was precalibrated to the desired annealing temperature prior to annealing. In the case of nonbending (bending) specimens, the empty quartz tray (quartz apparatus) was inserted into the furnace with N2 flow at room temperature and a thermocouple was used to measure the temperature of the tray (apparatus) at equilibrium (this is the reported \( T \)). For this work, \( 500 \leq T \leq 550 \) °C was used with the error in all \( T \) measurements estimated at \( \pm 1 \) °C. For all temperatures, the quartz tray (apparatus) reached thermal equilibrium with the furnace very quickly (<2 min) such that it is reasonably assumed that the samples were given isothermal processing.

D. TEM/focused ion beam sample preparation

A focused ion beam (FIB) system was used to prepare site-specific TEM samples from the strips. In this method, a focused beam of Ga+ ions is accelerated to 30 keV and used to mill away small portions of the wafer. Ultimately, a 100–200 nm thick 10 \( \mu \)m long, electron-transparent membrane (specimen) is produced which is then removed from the wafer surface \textit{ex situ} and placed on a grid for imaging. Prior to FIB processing, the wafer pieces were placed on Al stubs with C adhesive and subsequently evaporated coated with \( \sim 30 \) nm of C. The thin C film was used to make the surface conductive for imaging and for surface protection during the initial stages of preparation. Subsequently, a layer of \( \sim 1 \) \( \mu \)m thick Pt was FIB-deposited over the area of interest to protect the area from further beam damage during the main stages of sample preparation. Thus, negligible FIB-induced damage to the specimens was experienced.

A JEOL 200CX TEM operating at 200 keV was used for XTEM analysis of samples. High-resolution on axis and \( g_{120} \) bright-field imaging conditions were used in this work.

V. RESULTS

A. Intrinsic two-dimensional multidirectional SPEG with pattern-induced stress

1. Lines

The case of two-dimensional multidirectional SPEG with applied stress from line structures is now considered. Samples were Si+ implanted at 40 keV to a dose of \( 1 \times 10^{15} \) cm\(^{-2} \) and subsequently annealed at 550 °C for up to 15 min. Figures 21(a)–21(e) present a sequence of HR-XTEM images of the SPEG process near the mask-edge region of etched line structures while Figs. 21(f)–21(j) present the corresponding sequence of HR-XTEM images of the SPEG process in unetched line structures.

In the as-implanted case, shown in Figs. 21(a) and 21(f), the initial \( \alpha \)-Si layer was \( \sim 80 \) nm thick as measured from the surface to the (001)-oriented \( \alpha \)/crystalline interface. Af-
ter annealing for 5 min, the etched and unetched samples exhibited similar amounts of growth with rounded growth interfaces beneath the mask edge as shown in Figs. 21(b) and 21(g). However, after annealing for 10 min, the etched sample, shown in Fig. 21(c), has started to produce a sharp notch in the growth interface under the mask edge while the unetched sample, shown in Fig. 21(h), still exhibits a somewhat rounded growth interface in the same region. Annealing for 13 min in etched samples produced a very sharp notch in the growth interface just under the mask edge, shown in Fig. 21(d), while the unetched sample, shown in Fig. 21(i), still exhibits a notch-free growth interface. It also appears that SPEG in unetched samples has been enhanced compared to the etched samples as the surface to (001)-oriented growth interface depth is appreciably smaller in the unetched sample. Finally, after annealing for 15 min, the notch in the growth interface of the etched sample, shown in Fig. 21(e), remains incomplete with the SPEG process while the SPEG process has been completed in the unetched case, shown in Fig. 21(j). However, a mask-edge defect has formed in the unetched sample (indicated by arrow). Also, though it is not shown here, a mask-edge defect also formed after completion of SPEG in the etched line structure.

2. Squares

The case of two-dimensional multidirectional SPEG with applied stress from square structures is now considered. Samples were Si⁺ implanted at 40 keV to a dose of 1 × 10¹⁵ cm⁻² and subsequently annealed at 550 °C for up to 15 min. Figures 22(a)–22(e) present a sequence of HR-XTEM images of the SPEG process in etched square structures while Figs. 22(f)–22(j) present the corresponding sequence of HR-XTEM images of the SPEG process in unetched square structures.

Similar to the case of line structures, the as-implanted square structure, shown in Figs. 22(a) and 22(f), exhibits an initial α-Si layer that was ~80 nm thick as measured from the surface to the (001)-oriented α-crystalline interface. After annealing for 5 min, both etched and unetched square structures, shown in Figs. 22(b) and 22(g), displayed similar amounts of growth. However, after 10 min of annealing, the etched sample, shown in Fig. 22(c), has begun to form a notch in the growth interface under the mask edge while the unetched sample, shown in Fig. 22(h), still exhibits a rounded corner region. Interestingly, the SPEG process also appears to be enhanced in the unetched structure as the surface to (001)-oriented growth interface distance is less in the unetched sample. After annealing for 13 min, the notch in the growth interface of the etched sample, shown in Fig. 22(d), has become more pronounced while the corner region of the unetched sample, shown in Fig. 22(i), remains rounded. Finally, after annealing for 15 min, the etched sample, shown in Fig. 22(e), still exhibits a sharp notch in the growth interface. In contrast, the SPEG process has nearly completed in the unetched sample, shown in Fig. 22(j), and no mask-edge defects are evident. Once again, though it is not shown here, completion of SPEG in the etched square structure resulted in mask-edge defect formation.

3. Considerations

Observing the SPEG process in both line and square structures both with and without pattern-induced stress, two things are very apparent: (1) the presence of pattern-induced stress alters the SPEG process (both the shape of the growth interface and the growth kinetics) and (2) the nature of the pattern-induced stress (lines versus squares) alters the SPEG process. However, there are several finer points of consideration which must be addressed in order to fully understand the nature of the SPEG process under pattern-induced stress.

Foremost, as discussed earlier, the growth interface has a continuum of different orientations which significantly impacts the patterned SPEG process even without any applied stress. Thus, part of determining the nature of patterned SPEG requires detailed knowledge of the response of each different growth orientation with applied stress. For purposes of clarity, this continuum can be reduced to just two growth
interface orientations: a (001)-oriented front and {110}-oriented fronts, though this is, in reality, a somewhat significant deviation from the actual nature of the multidirectional SPEG process.

The stressed (001)-oriented SPEG process has been extensively studied since the mid-1980s and thus the response of (001)-oriented growth to an arbitrary applied stress can be somewhat reliably predicted. Of course, many different studies utilizing different applied stress states were necessary to fully understand stress (001)-oriented SPEG. In terms of (110)-oriented growth, very little is known about the response of this growth orientation to applied stress, though some initial work has been conducted. Thus, it would be a tremendous undertaking requiring a similarly large body of research to fully understand the nature of the stressed (110)-oriented SPEG process. This lack of knowledge regarding stressed (110)-oriented growth makes understanding of the patterned SPEG process under application of pattern-induced stress (let alone any type of stress) extremely challenging. Moreover, reducing patterned SPEG to consisting of only two growth fronts is an oversimplified version of the actual structure of interest and it would certainly be worthwhile to determine the nature of the stressed-SPEG process for the many different growth orientations between (001)- and (110)-oriented growths. Furthermore, it may or may not be the case that that any knowledge of single-directional stressed SPEG can be somehow applied to the patterned SPEG process. It may very well be the case that SPEG of this continuum of growth fronts is inherently different from bulk SPEG and that discretization of this continuum is not a valid approach.

An added consideration comes from the complicated Si substrate stress states generated by the patterning, as shown in Fig. 19. Specifically, the large spatial variation of the stress state within the Si substrate implies the stress dependence of each growth orientation will suffer similar spatial variability which makes understanding of the nature of the patterned SPEG process under pattern-induced stress challenging. Also, the issues with growth interface pinning at the SiO2 interface as well as growth interface curvature effects likely play a role in the overall nature of patterned SPEG. In the case of growth interface pinning, this effect may be reasonably assumed to be independent of stress, but the same may not be the case for interface curvature effects.

Thus, it is clear that pattern-induced stress can significantly alter the SPEG process, but there are many different considerations necessary to fully understand and predict the patterned SPEG process in such cases. Specifically, the issues regarding combined stress/growth orientation dependence, complicated substrate stresses, growth interface pinning, and growth interface curvature represent the many building blocks necessary to understand the stressed patterned SPEG process.

B. Intrinsic two-dimensional multidirectional SPEG with external stress

Studying multidirectional stressed SPEG using patterning is certainly of high technological relevance, but the stress states generated in the Si substrate in such cases are often quite complicated. Thus, by studying multidirectional stressed SPEG using etched samples subjected to wafer bending, only σ11 from externally applied stress is present. Ultimately, this significantly simplifies the analysis of the system and, in principle, allows for greater, more fundamental examination of the growth process.

Both line and square structures were used for this portion of work with all patterning layers removed prior to annealing. Si+ implantation at energies of 20 and 60 keV with doses of $1 \times 10^{15}$ cm$^{-2}$ produced an amorphous layer $\sim 120$ nm deep with rounded corners beneath mask edges as shown in Fig. 18. External stress along [110] to a magnitude of $\sim 200$ MPa was applied via wafer bending with both tensile and compressive σ11 studied. Samples were annealed at T=500 °C. For each value of σ11, the (001)-oriented growth velocity $v_{[001]}$ was calculated by measuring the amorphous layer thickness from the EOR damage at the center of the implant profile while the (110)-oriented growth velocity $v_{[110]}$ was calculated by measuring the amorphous layer thickness from the EOR damage at a depth of 25 nm at different anneal times. Additionally, evolution of the interface angle $\theta_i$ between the (001)- and (110)-oriented growth fronts as a function of σ11 was investigated. The parameters $v_{[001]}$, $v_{[110]}$, and $\theta_i$ are displayed schematically in Fig. 23.

Figures 24(a)–24(c) show HR-XTEM images of samples annealed with σ11=0 up to 3 h. After 1 h of annealing, the rounded corner of the as-implanted profile has started to disappear and the corner begins to appear square in nature as shown in Fig. 24(a). After 2 h of annealing, shown in Fig. 24(b), the corner has become quite sharp, though no meeting of the two growth interfaces has occurred. However, after 3 h of annealing, the two interfaces have met and a mask-edge defect has formed as shown in Fig. 24(c). Plots of $\theta_i$ versus stress for 1 and 2 h anneal times are presented in Figs. 25(a) and 25(b), respectively. As shown in Figs. 25(a) and 25(b), as SPEG proceeds, $\theta_i=90^\circ$ after 1 h and then $\theta_i$ decreases to 76° after 2 h, indicative of the two interfaces meeting.

HR-XTEM images of samples annealed up to 3 h under σ11=−200 MPa are presented in Figs. 24(d)–24(f). There is little difference compared to the stress-free sample after 1 h.
of annealing as shown in Fig. 24(d) and \( \theta \) after 1 h is similar as shown in Fig. 25(a). However, after 2 h of annealing shown in Fig. 24(e), meeting of the interfaces has occurred. After 3 h of annealing, significant defect evolution has occurred as shown in Fig. 24(f). Compared to the stress-free case, the evolution of the mask-edge defect begins earlier in the SPEG process at \( \sim 2 \) h of annealing when \( \sigma_{11} = -200 \) MPa is applied which agrees with similar work of Shin et al. where defect nucleation was accelerated with compression. This is further supported by Fig. 25(b) as \( \theta \) has decreased significantly after 2 h of annealing, suggesting impingement of the two interfaces which would cause defect formation.

Finally, HR-XTEM images of samples annealed up to times of 3 h under \( \sigma_{11} = 200 \) MPa are presented in Figs. 24(g)–24(i). Once again, the amorphous layer shows little difference compared to compressive or stress-free samples after 1 h of annealing as presented in Fig. 24(g) which is further supported by Fig. 25(a). However, after 2 h of annealing, the corner of the amorphous layer has not started to come to a point or become sharp, suggesting significant separation of the two interfaces as displayed in Fig. 24(h). Up to 3 h of annealing, as presented in Fig. 24(i), there is no meeting of the interfaces or defect evolution evident in contrast to stress-free and compressive samples. This was observed to be the case for tensile stresses exceeding 100 MPa. At values of 50 and 25 MPa, defect evolution was evident. Furthermore, in tension \( \theta \) is much larger than in compression after 2 h of annealing, as shown in Fig. 25(b). The larger values of \( \theta \) are indicative of greater separation of the growth interfaces which presumably prevents mask-edge defect formation.

A plot of \( v_{[110]} \) and \( v_{[001]} \) versus \( \sigma_{11} \) is presented in Fig. 26(a) with published values of stress-free bulk growth provided for comparison. From Fig. 26(a), enhancements to \( v_{[001]} \) along with retardation of \( v_{[110]} \) in tension are observed. However, the nature of these trends is far from conclusive. In fact, observing the HR-XTEM images of samples annealed with tension and without stress for 3 h [Figs. 24(c) and 24(f)] indicates very similar amounts of growth. Thus, even though the velocity calculations indicate enhanced (001)-oriented SPEG with tension, portions of the HR-XTEM data suggest little if any enhancement in tension, which is consistent with the observations of bulk stressed SPEG. The reason for this discrepancy is due to the fact that it is difficult to prepare FIB samples directly across the middle of a square structure. Thus, slight misorientation of the squares could easily account for the discrepancy between the measured growth velocities and portions of the HR-XTEM data.

Furthermore, it is important to consider the ratio of (001)- and (110)-oriented growth velocities as a function of \( \sigma_{11} \) since ultimately it is the relative difference between the two which controls defect nucleation. It appears that the ratio increases with increasing tension and retards with increasing compression, as shown in Fig. 26(b). Of course, it is difficult to determine in an absolute sense how the application of \( \sigma_{11} \) is changing each growth velocity. There is inherent difficulty in measuring different growth velocities within a two-dimensional structure compared to bulk material. However, if it is reasonably assumed that \( \sigma_{11} \) alters \( v_{[001]} \) similarly to bulk SPEG, it thus appears that \( \sigma_{11} \) is enhancing (retarding)
face being significantly different from the nominal macro-
larger separation between the two interfaces
defect evolution. Specifically, larger velocity ratios suggest
consistent with the observations regarding stress-influenced
stressed SPEG.\textsuperscript{16,28}
interface being pinned\textsuperscript{76} at the surface would presumably
ing of the amorphous layer during SPEG resulting from the
applied
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Intrinsic two-dimensional multidirectional SPEG
The multidirectional SPEG process. In the case of square
structures, the patterning generates sufficient stress such that
growth is altered to avoid mask-edge defect nucleation. This
also happens with externally applied tension (etched samples). However, it was also shown that externally applied compression (etched samples) accelerates defect nucleation.

Another important consideration to note is that of the
presence of the \(\alpha\)-Si phase since the elastic properties of \(\alpha\)-Si are vastly different from the crystalline counterpart.\textsuperscript{55} Presumably this could lead to the stresses on the growth inter-
face being significantly different from the nominal macro-
scopic stress as measured.

Most importantly, the trend observed in Fig. 26(b) is
consistent with the observations regarding stress-influenced
defect evolution. Specifically, larger velocity ratios suggest
larger separation between the two interfaces (larger values of \(\theta_i\)) and, subsequently, suppression of defects. Comparing this
to the trends observed with the stress dependence of the
evolving interface angle, this is exactly what was observed.

C. Intrinsic two-dimensional multidirectional SPEG
with pattern-induced and external stresses

From the previous two sections, it is apparent that both
pattern-induced stress and externally applied stress can alter
the pattern-induced stress component can be spe-
cifically altered to influence the SPEG process and, ulti-
mately, mask-edge defect formation. Thus, it appears that the
magnitude of the SPEG-altering effect from the pattern-
induced stress is similar to that for the case of externally
applied stress. Presumably, annealing a specimen with
both square pattern-induced stress and externally applied ten-
sion would produce the same result of suppressed mask-edge
defect formation. However, the case of square pattern-
induced stress with externally applied compression is not as
straightforward since both applied stimuli are directing the
system toward different ultimate endings.

Square structures were used for this portion of work. \(\text{Si}^+\)
implantation at energies of 20 and 60 keV with doses of 1 \(\times 10^{15}\) \text{cm}^{-2} produced an amorphous layer \(\sim 120\) \text{nm} deep
with rounded corners beneath mask edges as shown in Fig.
27(a). External stress along [110] of \(\sigma_{11} = -325\) MPa (com-
pression) was applied via wafer bending. In addition to the
externally applied stress, the square patterning was left intact
to generate additional substrate stresses in some samples. Samples were annealed at \(T = 525^\circ\)C for 3 h.

Figures 27(b) and 27(c) present BF-XTEM micrographs of the completed SPEG process in square structure with the patterning left intact both without and with externally applied \(\sigma_{11}\) after annealing for 3 h, respectively. It is evident that no mask-edge defects have formed in the case without externally applied compression while substantial mask-edge defects have formed in the case where externally applied compression was present.

Within the context of the previous sections where only
pattern-induced stress or externally applied stress were used,
these results imply that the \(\sigma_{11}\) stress component can be spe-
cifically altered to influence the SPEG process and, ulti-
mately, mask-edge defect formation. Thus, it appears that the
magnitude of the SPEG-altering effect from the pattern-
induced stress is similar to that for the case of externally
applied stress.

D. As-doped two-dimensional multidirectional SPEG
with pattern-induced stress

Until now, the issue of impurity-influenced SPEG has
been specifically removed from the study of stressed multi-
directional SPEG allowing for a cleaner, less complicated
analysis of the patterned SPEG process. However, considerations of combined dopant and stress influences are actually far more technologically relevant than the intrinsic case (already quite relevant) due to the use of dopant ion implantation into source and drain regions. Thus, using As+-implanted material, the combined effects of dopants and pattern-induced stress is examined in square structures.

In this portion of work, all samples were Si+ implanted at 20 and 60 keV with doses of $1 \times 10^{15}$ cm$^{-2}$ to produce an α-Si layer $\sim 120$ nm deep. Subsequently, some samples were additionally implanted with As$^+$ using energies of 7.5, 15, 30, or 50 keV with doses of $5.0 \times 10^{14}$, $7.3 \times 10^{14}$, $1.1 \times 10^{15}$, or $1.6 \times 10^{15}$ cm$^{-2}$, respectively. These combinations were utilized to produce a peak As concentration of $\sim 5.0 \times 10^{20}$ cm$^{-3}$ at different depths as predicted using simulations. Samples were annealed at $T=525$ °C for times of 0.8–3.0 h. Anneal times were chosen so that the SPEG process was observed after half the annealing time required for completion, $t_{0.5}$, and after the full time required for completion, $t_{1.0}$. The anneal times were estimated based on bulk (001)-oriented SPEG rate as enhanced by the presence of As.

Figure 28 displays BF-XTEM images of the evolution of the SPEG process in intrinsic square structures with and without the patterning. The as-implanted samples are shown in the BF-XTEM images in Figs. 28(a) and 28(d) and exhibit an α/crystalline interface with rounded corners beneath the SiO$_2$/Si$_3$N$_4$ mask edges. When the patterning was removed (unstressed) and the samples annealed for $t_{0.5}=1.5$ h, the (001)- and (110)-oriented SPEG interfaces converge at a depth of $\sim 60$ nm as shown in Fig. 28(b). In contrast, when the patterning was left intact (stressed) and the sample annealed to $t_{0.5}=1.5$ h, shown in Fig. 28(e), convergence is delayed until the (001)-oriented growth interface was $\sim 20$ nm deep. After annealing for $t_{1.0}=3.0$ h, the unstressed sample exhibits mask-edge defects extending $\sim 70$ nm deep as shown in Fig. 28(c) while the stressed specimen shows no mask-edge defects as displayed in Figs. 28(f) and 29(a).

Small EOR defects are observed near the original α/crystalline interface in all annealed specimens. As previously discussed, pattern-generated substrate stresses alter the relative SPEG velocities and prevent defect formation. Interestingly, annealing for $t_{1.0}=2.6$ h in stressed specimens As$^+$ implanted at 7.5 keV produced mask-edge defects $\sim 52$ nm deep, as shown in Fig. 29(b). Thus, it is evident that the presence of As during SPEG influences mask-edge defect formation.

The case of SPEG with the addition of As$^+$ implantation at various energies in stressed (unetched) square structures is now considered. Figures 30(a)–30(c) present BF-XTEM micrographs of the evolution of multidirection SPEG in stressed samples additionally As$^+$ implanted at 7.5 keV. The predicted As concentration ($C_{As}$) profile is schematically superimposed on the as-implanted image in Fig. 30(a) which indicates a projected range of $R_p \sim 10$ nm. After annealing for $t_{0.5}=1.3$ h, shown in the BF-XTEM micrograph presented in Fig. 30(b), there is still significant separation of the (001)- and (110)-oriented SPEG fronts, presumably since the (001)-oriented front did not approach the peak of the As profile. A small protrusion in the (110)-oriented growth interface near $R_p$ (indicated by arrow) is evident, suggesting local SPEG enhancement as indicated in Fig. 30(a). Annealing for $t_{1.0}=2.6$ h, shown in Fig. 30(c), reveals mask-edge defects $\sim 52$ nm deep.

Figures 30(d)–30(f) display BF-XTEM micrographs of multidirectional SPEG in stressed samples additionally As$^+$ implanted at 15 keV. A predicted $R_p$ of $\sim 16$ nm is shown schematically in Fig. 30(d) on the image displaying the predicted As profile in the as-implanted structure. The BF-XTEM image of SPEG completed to $t_{0.5}=1.2$ h, shown in Fig. 30(e), shows a small protrusion (indicated by arrow) in the (110)-oriented growth interface near $R_p$ of the As, indicating a localized SPEG enhancement. Completion of SPEG after 2.3 h, shown in Fig. 30(f), reveals the existence of mask-edge defects at a depth of $\sim 56$ nm, similar to the 7.5 keV As$^+$-implanted specimen. It is interesting to note the smaller protrusion in the (110)-oriented growth interface near $R_p$ for the 7.5 keV As$^+$-implanted sample. This observation may be related to interface pinning at the SiO$_2$/Si/α-Si
the SiO2 boundary which may have had a significant retarding effect near $R_p$ for the 7.5 keV implant energy as discussed earlier.

Images depicting multidirectional SPEG evolution in stressed specimens additionally As$^+$ implanted at 30 keV are shown in Figs. 30(g)–30(i). Again, the predicted As profile is superimposed on the as-implanted structure which indicates $R_p$ of $\sim$26 nm as shown in Fig. 30(g).$^{102}$ Annealing for $t_{0.5}$=1.0 h produced a very distinct protrusion in the (110)-oriented α-Si crystalline interface near $R_p$, again indicating a local SPEG enhancement, as shown in Fig. 30(h). In this case, the protrusion (indicated by arrow) is more pronounced compared to the 7.5 and 15 keV As$^+$-implanted samples, as shown in Fig. 30(b), presumably due to greater distance from the SiO2/α-Si boundary. Completion of SPEG after 2.0 h, shown in Fig. 30(i), reveals substantial mask-edge defects at a depth of $\sim$56 nm, similar to the 15 keV As$^+$-implanted case.

Lastly, the sequence of multidirectional SPEG evolution in stressed samples additionally As$^+$ implanted at 50 keV is presented in Figs. 30(j)–30(l). The As profile superimposed on the as-implanted structure, presented in Fig. 30(j), indicates $R_p$ of $\sim$39 nm.$^{102}$ Annealing for $t_{0.5}$=0.8 h reveals that mask-edge defect formation has already commenced, as presented in Fig. 30(k). Completion of SPEG after 1.5 h, shown in Fig. 30(l), reveals clear mask-edge defects with a depth of $\sim$60 nm, similar to the other samples.

Comparing the different As implants suggests that even with the application of stress from the patterning, the (110)-oriented SPEG enhancement from the dopants is large enough to overcome the retardation from the stress though the stress effect is not negligible as evidenced by the deeper defects observed in unstressed Si$^+$-implanted samples. Furthermore, the defect depth apparently is not very sensitive to As$^+$ implant energy. In the case of shallower As$^+$ implantation, the (001)-oriented growth front is far from $R_p$ until it nears the surface and thus suffers minimal dopant enhancement. Correspondingly, the (110)-oriented SPEG front is enhanced enough to produce an interface geometry favorable for defect formation, though it is somewhat retarded by the presence of the SiO2/Si/α-Si boundary.$^{76}$ In the case of deeper implantation, the (001) SPEG orientation is enhanced at greater depths compared to shallower implantation. Meanwhile, the (110) growth orientation is less affected by the surface in this case and suffers greater enhancement. However, the enhancement to (001)-oriented SPEG is great enough to keep the interface geometry unfavorable for defect formation until the growth process has partially completed. Thus, increasing the implant energy tends to enhance (001)-oriented SPEG which somewhat compensates for the enhanced (110)-oriented SPEG. In contrast, decreasing the implant energy causes (110)-oriented SPEG to be somewhat retarded by the presence of the surface, allowing the (001)-oriented SPEG to occur appreciably. This is evident in the BF-XTEM images presented in Fig. 31.

VI. CONCLUSIONS AND FUTURE WORK

In summary, studies of multidirectional (patterned) SPEG and, more specifically, stressed multidirectional SPEG of Si were reviewed. In the case of two-dimensional multidirectional growth in (001) Si wafers with (110)-aligned features, it was shown that many different phenomena influence the nature of the multidimensional epitaxial growth process.
Specifically, the inherent anisotropic nature of the SPEG process plays a key role in multidimensional growth. However, issues with growth interface pinning at SiO₂/Si/α-Si interfaces as well as interface curvature effects may also be playing roles. Most importantly, it was shown that the shape of the evolving growth interface is responsible for controlling the formation of mask-edge defects. The stressed two-dimensional multidirectional growth process was studied under many different stress states. Specifically, it was shown that the use of intrinsically stressed Si₃N₄ patterning with both line and square geometries to generate stresses in the Si substrate can influence the multidirectional growth process to different degrees. However, it appears that only the use of square structures can influence the geometry of the evolving growth interface such that mask-edge defect formation can be avoided. At present, it is unclear why this is the case since it is very difficult to compare the results of stressed growth in bulk material with that of pattern material. Specifically, the high degree of spatial variation of each stress component within the Si substrate generated by pattern-induced stresses and the lack of knowledge of stressed growth for growth orientations other than (001) Si are major challenges. Moreover, coupling these considerations with the inherent issues of growth kinetics anisotropy, growth interface pinning, and curvature effects makes understanding the stressed multidirectional SPEG process extremely complicated.

As a possible means to circumvent the issues with pattern-induced Si stresses, externally applied uniaxial stress along the in-plane [110] direction was applied via wafer bending in specimens with the patterning removed. Similarly to the case of growth under pattern-induced stress, it appears that externally applied in-plane uniaxial stress can alter the multidirectional growth kinetics and influence mask-edge defect nucleation. Specifically, it appears that the geometry of the growth interface under the mask edge is altered as well as the ratio of (001)- and (110)-oriented growth velocities with externally applied tension (compression) resulting in mask-edge defect suppression (formation). Again, comparison of these results to single-directional stressed growth results is not necessarily valid or reasonable as was the case in multidirectional growth under pattern-induced stress.

Interestingly, the combined presence of pattern-induced and externally applied stress appears to alter the multidirectional growth process. Specifically, it was shown that the ability of square patterning to suppress mask-edge defect formation can be counteracted by the simultaneous application of externally applied in-plane compression.

Finally, the multidirectional growth process was studied in As-doped material under pattern-induced stress from squares. It appears that the introduction of dopants, known to enhance growth in bulk material, exerts a sufficient enhancing effect on (110)-oriented growth such that the ability of the square patterning to suppress defect nucleation is avoided. Interestingly, this effect appears to be independent of the depth of the implanted As profile, possibly due to a compensating effect from (110)-oriented growth retardation from the presence of the surface SiO₂ layer. Within a larger context, it appears that electrically active impurities exert much greater effects on growth kinetics compared to applied stress since SPEG is inherently nucleation limited and dopants drastically reduce the nucleation timescale associated with growth.

In terms of future work, there are still many unanswered questions regarding the multidirectional SPEG process as well as the stressed multidirectional growth process. In this work, the two-dimensional case was discussed, but that does not mean that the three-dimensional case is not worth considering or technologically irrelevant. Of course, characterizing such a system would be more challenging than the already challenging two-dimensional case and requires extensive experimental work. Moreover, simulation work regarding the nature of the two-dimensional growth processes has not yet been able to successfully predict the experimentally observed growth interface geometries. Again, this raises the issues of interface pinning and curvature effects during the growth process.

Furthermore, it may be useful to study the stressed single-directional growth process in different orientations, but it is uncertain if any of the knowledge ascertained from such work would be applicable to the stressed multidimensional growth process. In this work, only one particular orientation was used, but future work investigating other orientations would certainly be interesting as well as technologically important.

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The scientific papers of J. W. Gibbs (Dover, New York, 1961).


Philos. Mag. 50, 238 (1900).


Harvard University, 1997.


J. Appl. Phys. 95, 967 (1994).


