Effects of hydrostatic pressure on dopant diffusion in silicon

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A point-defect-based model for the stress effects on dopant diffusion in silicon is presented. Variations in binding energies and diffusivities of dopant-defect pairs under hydrostatic pressure are modeled, and a pressure-dependent dopant diffusion equation is derived. New experimental work was performed on boron pileup near dislocation loops, and compared to the model. Qualitative agreement is possible, which suggests that stress might be a significant effect in scaled modern device structures. © 1995 American Institute of Physics.

I. INTRODUCTION

Stress is inevitable in the materials used in the fabrication processes of silicon integrated circuits. As the device dimensions are reduced and the packing density of circuits is increased, the stress induces more and more significant effects. It can cause severe degradation of device characteristics by generating and propagating dislocations in the silicon substrate. Furthermore, the stress in silicon also causes dopant redistribution and changes in the doping profile in the active regions to an extent that is no longer negligible in modern scaled-down devices.

Major sources of stress can be traced in the stages of the IC fabrication sequences. It has been observed that the important sources of stress in the silicon substrate are deposition of films with intrinsic stress and thermal oxidation of nonplanar surfaces. For example, very large stresses are usually built up in the silicon area near the edges of nitride films. Also, a high stress is built up at the corner of the device isolation regions, such as trench isolation. Extended defects such as edge dislocations and stacking faults are induced by the stress from the oxide as well as deposited films. Moreover, the dislocations can glide a significant distance in the stress field. As devices are scaled, the active transistor regions are nearer to the edges of the isolation structure. Stress-induced dislocations have become a critical factor to consider in designing short-channel metal-oxide semiconductor field-effect transistors (MOSFETs) and shallow junction bipolar devices.

In addition, extended defects such as dislocation loops are naturally accompanied by the stress field around them. High-dose ion implantation creates dislocation loops in the substrate. Theoretical calculation of the stress around the dislocation loops with observed density and size shows that the pressure around the loop layer can be locally in the order of $10^9$ dyne/cm$^2$, a value near to the nitride film stress. The formation of dislocation loops during the subsequent thermal annealing is also considered to be catalyzed by the high stress from nitride films and isolation structure.

The stress from these sources, whether it is from dislocations or from film materials with lattice constants different from silicon, may affect the doping profile enough to make an appreciable change in device characteristics. It is thermodynamically reasonable that the diffusion of solutes in crystalline silicon is affected by the stress field. There has been experimental evidence of stress-induced anomalous dopant diffusion, such as boron gettering$^2$ and phosphorus$^4$ and boron$^5$ retarded diffusion. Thus, the extended defects induced by the stress in silicon should be accounted for in advanced diffusion modeling for scaled devices. In a previous work, we developed a model for the evolution of dislocation loops based on the effect of pressure on point defect diffusion. The growth of dislocation loops during oxidation was modeled on the basis of the number of silicon atoms captured by the distributed loops. In this paper, the model is extended to account for the effects of hydrostatic pressure on dopant-defect pairs. Through the investigation based on the dopant-defect pairing theory described in our previous work$^8$, a physics-based atomistic model for the stress effects on dopant diffusion in silicon is accomplished.

II. A THERMODYNAMIC MODEL FOR STRESS EFFECTS ON DOPANT DIFFUSION

Under the theory of dopant diffusion mediated by point defects, the diffusion of dopant-interstitial and dopant-vacancy pairs is naturally affected by the pressure field. First, the pressure changes the concentrations of point defects in equilibrium.$^{10-13}$ For example, compressive pressure tends to attract vacancies and repel interstitials. When the pressure $P$ is positive, the formation enthalpy of an interstitial increases by the amount of $P \Delta V_P$, whereas that of a vacancy decreases by $-P \Delta V_V$. $\Delta V_P$ and $\Delta V_V$ are the values of the elastic volume expansion susceptible to the external pressure effect on the silicon interstitial and vacancy, respectively. The effects on equilibrium concentrations are formulated as described by Borucki.$^{6,7,10}$

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Under compression, therefore, $C^*_{I(P)}$ decreases while $C^*_{V(P)}$ increases with respect to the nominal values $C^*_{I(P=0)}$ or $C^*_{V(P=0)}$ without the pressure. On the other hand, tensile pressure has the opposite effects on the point defects. The gradient of pressure results in point defect movement in the neighborhood of the dislocation loop layer. This produces a driving force for the dopant diffusion, and enhances the diffusion where the point defect population is increased.

The pressure field also changes the binding energy of a dopant-point-defect pair. Figure 1 shows this schematically. The binding energy of dopant-defect pairing is defined as the difference in thermodynamic potentials of paired and unpaired point defects. A free interstitial (at far right of the figure) has its formation enthalpy increased due to the compressive pressure. As the interstitial approaches the dopant through the lattice sites, there is a net energy loss corresponding to the binding energy of the dopant-interstitial pair. This energy can also be shifted by the change in thermodynamic potential of the dopant-interstitial pair, which is the interaction energy of the pair with dislocation loops if the pressure is due to the loops. The situation is reversed for dopant-vacancy pairing. Thus, the pressure-dependent binding energies $E^b_{AI(P)}$ and $E^b_{AV(P)}$ are

$$E^b_{AI(P)} = E^b_{AI(P=0)} - P\Delta V_A + P\Delta V_I,$$  

$$E^b_{AV(P)} = E^b_{AV(P=0)} + P\Delta V_A - P\Delta V_V,$$  

where $P\Delta V_A$ and $-P\Delta V_V$ are the potential shift for dopant-interstitial and dopant-vacancy pairs. The values for the effective volumes of elastic inclusion for the dopant-defect pairs, $\Delta V_A$ and $\Delta V_V$, are not established experimentally. It is reasonable that the dopant-vacancy pairs will be affected by the pressure in the same direction as free vacancies. The pressure may vary spatially, as around dislocation loops. Their interaction with the unpaired point defects and the pairs leads to local variation of the potential shift. More generally, the change in formation enthalpy $\Delta H^f_{AX(P)}$ of the $AX$ pair is equal to $P\Delta V_{AI}$ and $-P\Delta V_{AV}$ for dopant-interstitial pair $AI$ and dopant-vacancy pair $AV$, respectively, whatever the source of pressure $P$ is. Similarly, $\Delta H^f_{X(P)}$ is the notation for $P\Delta V_A$ and $-P\Delta V_V$ for unpaired interstitial and vacancy, respectively. Then, Eqs. (3) and (4) can be summed up as one equation:

$$E^b_{AX(P)} = E^b_{AX(P=0)} - \Delta H^f_{AX(P)} + \Delta H^f_{X(P)}. \tag{5}$$

The changes in binding energies lead to a local variation of the pairing coefficient $K_{AX(P)}$ and the concentration of the pair $C_{AX(P)}$ under pressure. Since the pressure effect can be assumed to be equal for the pairs with different charge states, the effective binding energy $E^b_{AX(P)}$ is affected by the same amount due to the pressure. From Eq. (5) and the definition of pairing coefficient as described in Refs. 9 and 6, we obtain

$$K_{AX(P)} = K_{AX(P=0)} \exp \left(-\frac{\Delta H^f_{AX(P)} - \Delta H^f_{X(P)}}{kT} \right). \tag{6}$$

The pressure-dependent pairing coefficient $K_{AX(P)}$ is now a function of location in contrast to the constant $K_{AX(P=0)}$, because the pressure can vary locally, as around the dislocation loops. This should be considered in deriving the diffusion equation including the pressure effect. Accordingly, the concentration of dopant-defect pairs is affected by pressure. If the magnitude of the pressure in the silicon substrate is less than $5 \times 10^9$ dyne/cm$^2$, which is the typical case, it can be shown that the value $(K_{AX(P)} C^*_{X(P)})^{-1}$ for phosphorus and boron under pressure is much larger than unity. In this case, we can safely assume that the unpaired dopant concentration $C^*_{AX}$ in equilibrium is the same with or without the pressure. Combining Eqs. (1), (2), (6), and Eqs. (2)–(6) in Park and Law,$^9$ we can evaluate the pressure effect on the total concentration of $AX$ pairs in equilibrium:

$$C^*_{AX(P)} = C^*_{AX(P=0)} \exp \left(-\frac{\Delta H^f_{AX(P)} - \Delta H^f_{X(P)}}{kT} \right). \tag{7}$$

Thus, the equilibrium concentration of dopant-interstitial pairs $C^*_{AI(P)}$ decreases in a compressive medium, while that of dopant-vacancy pairs $C^*_{AV(P)}$ increases. The pair concentrations in nonequilibrium are accordingly affected by the pairing coefficients in Eq. (6) as well as the point-defect distribution changed due to the pressure.

The change in the pair concentration due to pressure should be reflected on diffusion equations. A dopant diffusion model accounting for concentration of pairs in the absence of pressure has been established.$^8$ The diffusion equation should now incorporate the pressure effects on pairing coefficients in the framework of the pair diffusion model. Moreover, it is necessary to account for an additional pair flux due to the local variation of the formation enthalpy of the pair $\Delta H^f_{AX(P)}$. With all these changes, the equation for dopant diffusive flux $-J_A$ under pressure $P$ can be rederived starting from the following equation:
where the subscript \((P)\) denotes the pressure dependence, \(Z_{AX_c}^*\) is the sign of net charge of the pair \(AX_c^*\), \(\Psi\) is the electric potential, \(q\) is the electron charge, and \(C_{AXc}^{*}(P)\) is the concentration of dopant-defect pair \(AX_c^*\) under pressure. It is assumed that the intrinsic diffusivity of the dopant-defect pair \(d_{AXc}^*\), which is related with lattice vibration and entropy of migration\(^{15}\) is not affected by the external pressure, although it should be confirmed experimentally. The summation is for both defect \(X\) (interstitial \(I\) or vacancy \(V\)) for each charge state \(c\) of the pair. The last additional term accounts for the flux of the pairs induced by the variation of the stress field in terms of the change in formation enthalpy of the pair \(\Delta H^{f}_{AXc}(P)\). This additional term is theoretically consistent with a few previous works on diffusion of point defects in the presence of a strain gradient.\(^{16-18}\) Equation (8) is based on the assumption that the migration entropy of the dopant-defect pair is not significantly affected by the pressure, which is reasonable considering a theoretical estimation of point defect migration enthalpy in strained metals.\(^{18}\)

Equation (8) is now further developed for a donor dopant of singly positive charge state. A similar derivation can be achieved for the case of an acceptor dopant with proper consideration of charge states. The concentration of \(AX_c^*\) pairs under pressure and under nonequilibrium defect conditions can be expressed in terms of the unpaired substitutional dopant concentration \(C_{A}(P)\), defect concentration \(C_{X}^{c-1}\), and the pressure-dependent pairing coefficient shown in Eq. (6). Following Eq. (5) in Park and Law\(^9\) for the noncR case, we have

\[
-C_{AXc}^{*}(P) = K_{AXc}(P)C_{X}^{c-1}C_{A}^{+}(P) \quad \text{or} \quad C_{AXc}^{*}(P) = K_{AXc}(P)C_{X}^{c-1}C_{A}^{+}(P).
\]

The gradient of Eq. (9) is evaluated by incorporating the variation of the pairing coefficient \(K_{AXc}(P)\) in Eq. (6):

\[
\nabla C_{AXc}^{*}(P) = \frac{C_{AXc}^{*}(P)}{C_{A}^{+}(P)} \left[ \nabla C_{A}^{+}(P) + \frac{C_{A}^{+}(P)}{C_{X}^{c-1}} \nabla C_{X}^{c-1} \right]
\]

Substituting Eq. (10) into Eq. (8), we obtain

\[
-J_c = \sum_{X_c} d_{AXc} \left[ \frac{C_{AXc}(P)}{C_{A}^{+}(P)} \nabla C_{A}^{+}(P) + C_{A}^{+}(P) \left( \nabla \log C_{X}^{c-1} - \frac{q \Psi}{kT} \right) \right] + Z_{AXc}^* \frac{q \Psi}{kT} + \frac{\Delta H^{f}_{AXc}(P)}{kT}. \quad \text{(11)}
\]

The formation enthalpy changes the same amount for defects of different charge states. Thus, the concentration of defect \(X\) in the inert intrinsic condition under pressure \(C_{X}^{c-1}(P)\) is expressed in a manner similar to Eqs. (1) and (2):

\[
C_{X}^{c-1}(P) = \frac{C_{X}^{c-1}(P=0)}{\exp \left( \frac{-\Delta H^{f}_{AXc}(P)}{kT} \right)}. \quad \text{(12)}
\]

Combining this equation with Eqs. (2) and (3) in Park and Law,\(^9\) we can describe the nonequilibrium concentration of charged defects \(C_{X}^{c-1}\) in terms of the equilibrium concentration under pressure \(C_{X}^{c*}(P)\) and the carrier concentrations:

\[
C_{X}^{c-1}(P) = G_{X}^{c} C_{X}^{c-1}(P) \frac{C_{X}^{c*}}{C_{X}^{*}(P) n_i} \quad \text{(13)}
\]

where \(G_{X}^{c}\) is the charge state term \((n/n_i)^{1-c}\), where \(c\) denotes the charge state of the pair \((0\) for neutral pairs, \(-1\) for negative pairs, and \(+1\) for positive pairs).

When the pressure is not originated from extended defects, the electric potential term \(\Psi\) in Eq. (11) can be described in terms of carrier concentrations as simply as in the nonpressure case. For the case of dislocations, however, it is possible that the dangling bonds around the core of dislocations are charged due to gettered impurities and defects. In order to model the potential gradient thoroughly in this case, it will be necessary to solve Poisson’s equation around the dislocations. The significance of this effect may be estimated by calculating the upper bound of the potential variation by numerical solution of Poisson’s equation in a simplified distribution of dislocations. In the present derivation, however, the potential variation due to the possibly charged dislocations is not considered, for the nature of the charge states is not characterized experimentally under the high-temperature diffusion conditions. Under this simplifying assumption, we have the following relationship between potential and electron concentration for the donor dopant, as in the nonpressure case described by Law:\(^{19,20}\)

\[
\log G_{X}^{c} + Z_{AXc}^* \frac{q \Psi}{kT} = \log \left( \frac{n}{n_i} \right)^{1-c} + Z_{AXc} \log \left( \frac{n}{n_i} \right).
\]

Equation (14) is valid for any charge state \(c\) of the donor-defect pair. Now the term inside the brackets of Eq. (11) is simplified by incorporating Eqs. (12), (13), and (14). Also the term outside the brackets can be expanded by using Eqs. (9) and (13). In short, Eq. (11) becomes

\[
-J_c = \sum_{X_c} d_{AXc} K_{AXc}(P) G_{X}^{c} C_{X}^{c-1}(P) C_{A}^{+} \times \frac{C_{X}^{c*}}{C_{X}^{*}(P) n_i} \nabla \log \left( \frac{C_{A}^{+}(P)}{C_{X}^{*}(P) n_i} \right). \quad \text{(15)}
\]

Equation (15) is very similar in its form to the established equation without pressure effects.\(^8\) In Eq. (15), the quantities dependent on the pressure are denoted with subscript \(p\), and they correspond exactly to the terms without the pressure effects.\(^8\) The diffusivity term in the parentheses in Eq. (15) can be named as \(D_{AXc}(P)\) and further related with the diffusivity without the pressure effect \(D_{AXc}(P=0)\), by using Eqs. (6) and (12):
\[ D_{AX}(P) = \sum c_{AX} K_{AX}(P) G_{X} C_{AX}^{-1}(P) \]

\[ = D_{AX}(P=0) \exp \left( -\frac{\Delta H_{AX}^{f}(P)}{kT} \right) \]  

(16)

\[ D_{AX}(P=0) = \sum D_{AX}(P=0) G_{X}, \]  

(17)

where

\[ D_{AX}(P=0) = d_{AX} K_{AX}(P=0) C_{AX}^{-1}(P=0) \]

\[ = d_{AX} C_{AX}^{i}(P=0) C_{A}(P=0) \]

\[ = d_{AX} C_{AX}^{i}(P=0) C_{A}(P=0) \]  

(18)

The approximation in Eq. (18) is valid only when the unpaired dopant concentration under inert intrinsic doping conditions \( C_{A}(P=0) \) is about the same as the total concentration of dopant atoms \( C_{A}(P=0) \), since the pair assessment had not been considered in measurements of the inert diffusivities in the literature. For boron and phosphorus, the values of \( (K_{AX}(P=0) C_{X}(P=0))^{-1} \) are found to be much larger than unity for both interstitial and vacancy mechanisms, so Eq. (18) is meaningful. This means that we can use the measured diffusivities as values of \( D_{AX}(P=0) \) in the diffusion equations. Substituting Eqs. (16) and (17) into Eq. (15), we finally get an expression for the total diffusive flux of dopant atoms as follows:

\[ -J_{AX} = \sum_{X} (D_{AX}(P=0) G_{X}) \exp \left( -\frac{\Delta H_{AX}^{f}(P)}{kT} \right) C_{A}(P) \]

\[ \times \frac{C_{X}}{C_{X}(P)} \exp \left( -\frac{\Delta H_{AX}^{f}(P)}{kT} \right) C_{A}(P) n_{i} \]

\[ \times \frac{C_{A}(P) C_{X}(P) n}{C_{X}(P) n_{i}} \]

\[ = \sum_{X} D_{AX}(P=0) \exp \left( -\frac{\Delta H_{AX}^{f}(P)}{kT} \right) C_{A}(P) \frac{C_{X}}{C_{X}(P)} \exp \left( -\frac{\Delta H_{AX}^{f}(P)}{kT} \right) C_{A}(P) n_{i} \]

\[ \times \frac{C_{A}(P) C_{X}(P) n}{C_{X}(P) n_{i}} \]

\[ = \sum_{X} D_{AX}(P=0) \frac{C_{X}}{C_{X}(P)} \exp \left( -\frac{\Delta H_{AX}^{f}(P)}{kT} \right) C_{A}(P) \frac{C_{X}}{C_{X}(P)} \exp \left( -\frac{\Delta H_{AX}^{f}(P)}{kT} \right) C_{A}(P) n_{i} \]

(19)

Thus, the final equation incorporates the pressure effects on the unpaired dopant and equilibrium point defect concentrations, which are calculable from the formation energy dependence and the pairing theory. The dopant diffusivity component \( D_{AX}(P) \) under the pressure \( P \) is associated with the known diffusivity \( D_{AX}(P=0) \) in the absence of pressure and the formation enthalpy of the pair \( \Delta H_{AX}^{f}(P) \). The relationship of Eq. (16) is consistent with the theoretical expression of the activation enthalpy of diffusion \( Q_{AX} \) as the sum of the migration enthalpy \( H_{AX}^{m} \) and the formation enthalpy \( H_{AX}^{f} \) of the pair, assuming that the migration enthalpy does not change significantly due to the pressure:

\[ \Delta Q_{AX} = Q_{AX}(P) - Q_{AX}(P=0) \]

\[ = H_{AX}^{m} + H_{AX}^{f} - (H_{AX}^{m}(P=0) + H_{AX}^{f}(P=0)) \]

\[ = H_{AX}^{f} - H_{AX}^{f}(P=0) \]

\[ - H_{AX}^{f}(P=0) \]

\[ = \Delta H_{AX}^{f}(P) \]

(20)

The change in defect formation enthalpy \( \Delta H_{AX}^{f}(P) \) is equal to the interaction energy of dislocations and point defects if the pressure is due to the dislocation loops. Rewriting Eq. (16) for each type of defects, we have

\[ D_{AX}(P) = D_{AX}(P=0) \exp \left( -\frac{P \Delta V_{AX}}{kT} \right) \]

\[ D_{AV}(P) = D_{AV}(P=0) \exp \left( -\frac{P \Delta V_{AV}}{kT} \right) \]

(21)

In a compressive medium, therefore, diffusivity of dopant-interstitial pairs decreases while that of dopant-vacancy pairs increases. The diffusivities change in the opposite direction under tensile stress, as argued by Cowern, et al.

III. BORON SEGREGATION AROUND DISLOCATION LOOP LAYER

The above model was exercised first by simulating boron redistribution around dislocation loops. Sadana et al. observed that boron is segregated during annealing into the region of dislocation loops created by high-dose arsenic implantation. New systematic experiments were performed in this work to monitor the temperature and time dependence of the boron pileup. We used an isoconcentration boron layer in (100) silicon wafers created by long time diffusion high-temperature diffusion in Chocalski silicon and implanted silicon in two steps with doses large enough to create dislocation loops \( 2\times10^{15} \text{ cm}^{-2} \) at 150 keV plus \( 6\times10^{14} \text{ cm}^{-2} \) at 80 keV). After the subsequent annealing in Na at different temperatures from 600 to 1000 °C the boron profiles were measured by secondary-ion mass spectrometry (SIMS). The loop distribution was measured by plan-view transmission electron microscopy (PTEM), as shown in Fig. 2. The depth location of the dislocation loop layer was also revealed by cross-section TEM (XTEM) in Fig. 3, which is on the same sample as the PTEm picture in Fig. 2 shows. The results show that the boron pileup occurs with very little change in profile shape from 15 min to 2 h.

Simulations were performed with the above diffusion model in the process simulator FLOOPS where the point-defect-based model for loop evolution was also implemented. Initial distributions of point defects were assumed to follow a Pearson-IV function with peak concentrations of about 1 \( \times 10^{16} \text{ cm}^{-3} \), which is a reasonable value considering the reduction in defect supersaturation during the rapid process of loop formation. The assumption roughly approximates the point defect distribution at the initial stage of an-
nealing near the original amorphous/crystalline interface where the dislocation loops are nucleated. There is still great uncertainty in the initial damage conditions resulting from ion implantation, and the simulations performed are dependent on this initial condition. The initial loop size distribution was based on the PTEM measurements of a sample as shown in Fig. 2. The simulated distribution of loops at 240 min agrees with the data extracted from the PTEM picture.

Figure 4 shows the calculated pressure field surrounding a layer of dislocation loops centered at 0.17 \(\mu m\) below the surface of the wafer. The pressure was computed by integrating the pressure components from each loop and averaging over the entire loop distribution. The abruptness in the transition from compression to tension around the layer boundary is reduced in the pressure \(P\) calculated by considering the distribution of loop size. The pressure field in Fig. 4 affects the equilibrium concentrations of interstitial and vacancy as shown in Fig. 5. The effective elastic volume expansions \(\Delta V_I\) and \(\Delta V_V\) in Eqs. (1) and (2) were calculated based on sphericity of interstitial and vacancy with radii, \(r_0 = 1.11 \ \text{\AA}\) and \(r_s = 2.47 \ \text{\AA}\), respectively. Dilatation factor for \(\Delta V_I\) used for the two-dimensional model was 0.5. Inside the loop layer, the compressive pressure tends to attract vacancies and to repulse interstitials, and the redistribution of point defects relieves the strain. The local variation of pressure...
Figure 6 shows good qualitative agreement between the simulations and the SIMS measurement of the piled-up boron profile at 900 °C, which stays almost unchanged from 15 to 120 min. The boron segregation occurred at the depth position of the dislocation loop layer observed by XTEM in Fig. 3. The profile shape is consistent with the similar observation of the redistribution of implanted boron in the post-amorphized silicon substrate. The simulations from 15 to 240 min show the boron pileup and segregation around the dislocation loop layer, qualitatively in accordance with the temporal behavior observed in the data. The pileup of boron was not observed under the annealing condition at 1000 °C, where the dislocation loops are dissolved quickly enough and the pressure is negligible. At 600 and 700 °C, there are dislocation loops in the samples, but the diffusivity of boron is not large enough to cause pileup. At 800 °C, the boron segregation occurred to a larger degree than in the case of the simulation at 900 °C, with the peak concentration at about $5 \times 10^{17}$ cm$^{-3}$. The pileup at 800 °C was also observed to stay almost unchanged from 60 to 360 min, which is the phenomenon consistent with the 900 °C case.

As shown in Eqs. (19), (21), and (22), the dopant diffusivity components vary with the pressure in different ways for the dopant-interstitial and the dopant-vacancy pair. Inside the dislocation loop layer where the compressive pressure tends to keep out dopant-interstitial pairs, the diffusion via interstitialcy mechanism decreases. On the contrary, vacancy-mediated diffusion is locally enhanced there, since more dopant-vacancy pairs as well as vacancies are attracted towards the loop layer center and the binding of the pair is reinforced. The extent of these variations depends on the effective volumes of boron-defect pairs $\Delta V_{BI}$ and $\Delta V_{BV}$. The value of $\Delta V_{BI}$ used in the simulation was estimated based on the volume of sphere with a radius equal to the sum of the radii of a boron atom and a Si self-interstitial. In case of $\Delta V_{BV}$, such estimation is not possible, since a dopant atom can be viewed as paired with more than one vacancy whenever they exist within or at the third-nearest neighbor sites in diamond structure. The assumed value of $\Delta V_{BV}$ was two times as large as $\Delta V_{BI}$. Equations (19), (21), and (22) suggest that $\Delta V_{BV}$ should be large enough in comparison to $\Delta V_{BI}$ in order for the boron redistribution to take place, for $D_{BV}(P=0)$ is about 25% of $D_{BI}(P=0)$.

In Fig. 7, the simulation shows the temporal variation in supersaturation of interstitial and vacancy at the depth position of loop layer center ($\sim 0.17 \mu m$) during the annealing at 900 °C. When there are dislocation loops causing the boron segregation (solid lines), most of the interstitials around the loop layer are captured very rapidly by the strong interaction with the dislocation loops through a diffusion-limited process. The efficient sink action of the loops diminishes the interstitial supersaturation $C_I/C^*_I$ much sooner than the case without the loops. On the other hand, vacancies remain supersaturated (solid line), since the rapid reduction of interstitials leads to the situation where vacancies do not find enough interstitials to recombine with. This result agrees qualitatively with Borucki's simulation in three dimensions.

Thus, the time dependence of the boron segregation shown in Fig. 6 can be explained in terms of our pressure-dependent model as follows. Under the supersaturation of vacancies, the segregation is initiated by the repulsion of boron-vacancy pairs due to the tensile stress just outside the loop layer boundary. The pile-up process continues with the enhanced diffusivity of boron-vacancy pairs and the flux of boron directed towards the center inside the loop layer of compression. Finally, in about 15 min, compensation of the pressure gradient and the boron concentration gradient is achieved to attain the steady state of the pileup. The simulations in Fig. 6 are obtained through the short time behavior of boron diffusion, and our pressure-dependent diffusion model is verified qualitatively with the agreement on time dependence.

The simulation in Fig. 6 shows less extended depletion of boron in deep regions than the data. The best explanation for this effect is inaccuracies in the starting defect profiles used in these simulations. As has been pointed out earlier, there is driving force of defects towards the loops during the growth and formation, which our model includes. A different
initial defect profile will produce different gradients of defects towards the loops, and create a different depletion depth near the loops. At this point, there is still controversy over the initial damage density resulting from implantation above the amorphous threshold. Additionally, if the dislocation loops are formed by directly capturing the boron atoms together with the Si self-interstitials, the stress around the loop layer will be relaxed by the smaller volume of boron atoms, and the pressure effects will decrease with time. Further experimental evidence through RTA will be required to confirm this possibility. More rigorous simulation requires further knowledge on the loop formation process and as-implanted point defect distributions near the amorphous/crystalline interface, as well as the solid phase epitaxial recrystallization.

IV. CONCLUSION

The atomistic model for pressure effects on dopant diffusion is derived by accounting for the variation of formation enthalpy of dopant-defect pairs due to hydrostatic pressure. The model leads to a physics based simulation of the boron segregation around the dislocation loops and the phosphorus retarded diffusion under compressive pressure. The diffusion phenomena induced by pressure can be further clarified by probing the time dependence of transient diffusion at the initial stage and by measurement of the stress distribution.

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