Consistent Quantitative Model for the Spatial Extent of Point Defect Interactions in Silicon

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Abstract

The silicon point defect properties which control the spatial extent of their interactions (e.g., interstitial diffusivity) have been calculated by many researchers. However, large discrepancies exist in the reported values of these parameters, and it is essential to have a consistent set of parameters for use in process simulation. To meet this need, we present here a model which includes important interactions which have been ignored in previous analyses, specifically bulk recombination of interstitials with vacancies and segregation of interstitials to surface oxide films. We assess the effectiveness of the model in predicting the spatial extent of point defect interactions by comparing simulation results with a wide range of experimental data. Although this same experimental data previously gave large differences in calculated parameter values, we obtain a single set of model parameters which can account for the full range of data in a consistent manner.

1 Introduction

Integrated circuit fabrication processes such as diffusion, film growth and extended defect kinetics interact through changes in point defect concentrations. Because of the rapid diffusivity of point defects at processing temperatures, these interactions can occur over distances of microns [?, ?, ?, ?, ?], affecting device structures not only locally, but also in neighboring regions. The spatial extent of these interactions becomes even more important as both device dimensions and tolerances continue to shrink. However, large discrepancies exist in reported values of fundamental point defect parameters, such as interstitial diffusivity, which control the spatial extent of interactions [?, ?]. These discrepancies can be understood by recognizing that in many cases, point defect parameter values have been determined using models which neglect important phenomena, and thus the parameters represent effective rather than true values. In this work, we show that by using a more complete model of point defect interactions, it is possible to provide a consistent explanation for a wide range of experimental observations that had previously appeared contradictory.

To begin, Section 2 discusses some of the experiments that have been used to calculate the silicon interstitial diffusivity, and provides some motivation for the physical model developed in this work. Section 3 develops the model, which includes bulk recombination and segregation of interstitials to surface films such as oxides. Section 4 discusses parameter choices, and in Section 5, the simulations are compared with a large range of experimental data, yielding a single consistent set of parameters.

2 Background and Motivation

Despite the huge discrepancies in calculated parameter values, similar experiments generally give consistent and repeatable values for the effective silicon interstitial diffusivity. The resulting trends are summarized in Table 1. Experiments which measure enhanced diffusion or stacking fault growth at the wafer frontside during backside oxidation [?, ?, ?, ?, ?] or the lateral extent of oxidation enhanced diffusion (OED) [?, ?, ?, ?, ?], generally yield slow effective diffusivity values ($\approx 10^{-9}$ cm^2/sec at 1100°C). Intermediate effective diffusivity values ($> 10^{-8}$ cm^2/sec at 1100°C) have been calculated from OED of buried layers [?, ?], while metal diffusion experiments [?, ?, ?, ?, ?] give a higher effective diffusivity ($\approx 10^{-6}$ cm^2/sec at 1100°C).

Griffin *et al.* [?] explained these differences by assuming that trap species present in Czochralski and float-zone silicon, but absent from epitaxial silicon, slow down the propagating diffusion front of interstitials, thus resulting in a reduced effective diffusion coefficient. The fast diffusion noted in the metal diffusion experiment is explained by assuming that the gettering or metal indiffusion process causes a much higher supersaturation of interstitials which rapidly fill the traps and allow unimpeded diffusion. One of the problems of the trapping model is that, to date, no plausible trap candidate, which is present in floatzone and

Czochralski material but absent in epitaxial material, has been suggested.

The repeatability of experimental measurements suggests that the analyses of the experiments rather than the experiments themselves are the source the discrepancies in calculated interstitial diffusivity values. Models used in calculating interstitial diffusivity typically oversimplify the system, using an effective diffusivity ($D_{\rm I}^{\rm eff}$) to account for all bulk interactions and a constant effective regrowth velocity ($\sigma_{\rm I}^{\rm eff}$) to account for all interface effects:

$$\frac{\partial C_{\rm I}}{\partial t} = \bigtriangledown \cdot D_{\rm I}^{\rm eff} \bigtriangledown C_{\rm I}, \tag{1}$$

$$\hat{n} \cdot D_{\rm I}^{\rm eff} \bigtriangledown C_{\rm I} = \sigma_{\rm I}^{\rm eff}(C_{\rm I} - C_{\rm I}^{*}), \tag{2}$$

where $C_{\rm I}$ is the interstitial concentration in silicon and $\hat{n}$ is the interface normal. However, under many conditions, additional interactions such as Frenkel pair recombination can be expected to play an important role.

An observation that can be made from Table 1 is that the best predictor of whether high or low diffusivity values will be calculated is whether interstitial concentration is monitored near an interface or within the bulk. When defects are monitored near interfaces, such as in lateral OED or backside OED experiments, low values of effective diffusivity are calculated, while calculations from experiments which monitor defect concentrations in the bulk, such as buried layer or metal diffusion experiments, result in much higher diffusivity values. The fact that low effective interstitial diffusivity values are calculated only for surface markers suggests that a more complete model for interactions with films and interfaces in needed. Further support for this position comes from Rogers *et al.* [?], who examined the growth/shrinkage of stacking faults beneath thermally grown oxides and CVD nitrides during backside oxidation and found that a model based on a time-dependent interface regrowth velocity produced a better fit to their data than a static model. In the following section, we develop an improved model for point defect redistribution which, in addition to Frenkel pair recombination, includes segregation to surface films as the basis for a time-dependent effective regrowth velocity.

3 Model Development

Figure 1 illustrates some of the point defect interactions occurring in silicon during VLSI fabrication processes. The salient point defect interactions considered in this work, that have previously been largely ignored, are bulk recombination and interactions with films beyond a non-constant regrowth velocity, specifically, segregation of interstitials to surface films. Bulk recombination with vacancies slow down the diffusion front of interstitials, giving a slower calculated effective value for diffusivity, while segregation of interstitials to films results in an effective regrowth velocity which decreases with time, again appearing as a slower effective diffusivity when monitoring concentrations near substrate/film interfaces [?]. Both of these effects would reduce the supersaturation observed at short times for backside oxidation and lateral OED experiments and cause the calculated effective diffusivity to be much reduced in such experiments.

To include the effect of interstitials being slowed by bulk recombination with vacancies, we solve the continuity equations for both defects in the bulk, including Frenkel pair recombination:

$$\frac{\partial C_{\mathrm{I}}}{\partial t} = \nabla \cdot D_{\mathrm{I}} \nabla C_{\mathrm{I}} - k_r (C_{\mathrm{I}} C_{\mathrm{V}} - C_{\mathrm{I}}^* C_{\mathrm{V}}^*) \tag{3}$$

$$\frac{\partial C_{\mathrm{V}}}{\partial t} = \nabla \cdot D_{\mathrm{V}} \nabla C_{\mathrm{V}} - k_r (C_{\mathrm{I}} C_{\mathrm{V}} - C_{\mathrm{I}}^* C_{\mathrm{V}}^*), \tag{4}$$

where k_r is the recombination rate and C_{I}^* and C_{V}^* represent equilibrium values.

The boundary conditions for this system correspond to point defect fluxes at oxidizing and nonoxidizing oxide films. At oxidizing $\mathrm{Si/SiO_2}$ interfaces, rapid interstitial generation and recombination effectively controls the interstitial supersaturation [?, ?, ?, ?] at a value that is known from standard OED experiments or from available data at the oxidizing interface. At non-oxidizing $\mathrm{SiO_2}$ film interfaces, standard models assume a constant interface regrowth velocity which is proportional to the excess point defect concentration:

$$\hat{n} \cdot D_{\mathrm{I}} \nabla C_{\mathrm{I}} = \sigma_{\mathrm{I}} (C_{\mathrm{I}} - C_{\mathrm{I}}^*), \tag{5}$$

$$\hat{n} \cdot D_{\mathrm{V}} \nabla C_{\mathrm{V}} = \sigma_{\mathrm{V}} (C_{\mathrm{V}} - C_{\mathrm{V}}^*). \tag{6}$$

We now turn our attention to the fact that in using a simple constant regrowth velocity in Equation (5), we have oversimplified the boundary condition for interstitials at the non-oxidizing $\mathrm{Si/SiO_2}$ interfaces. In previous work, Dunham [?] has argued in favor of the extension of models, for enhanced diffusion during oxidation of silicon [?, ?] and nitridation of $\mathrm{SiO_2}$ [?], to nonoxidizing oxide films. This extension leads naturally to the conclusion that interstitials (excess silicon) segregate strongly to oxide films from the silicon and diffuse within that film. Verification of this model comes from the observation by Celler and Trimble [?] of complete dissolution of a thin silicon layer in an $\mathrm{SiO_2}$ film. This conclusion is further supported by observation of retarded diffusion of phosphorus and enhanced diffusion of antimony during inert ambient annealing [?, ?] and the fact that a nitrided oxide manifests a much higher effective regrowth velocity than a nitride-capped oxide [?, ?].

In the model proposed in this work, interstitials (excess silicon) are assumed to segregate rapidly between the silicon and oxide, so that at the interface,

$$C_{\mathrm{I}}^{\mathrm{SiO_2}} = m_{\mathrm{I}} C_{\mathrm{I}}, \tag{7}$$

where m_{I} is the segregation coefficient. Note that the actual model implemented includes a finite segregation velocity, but that this value is chosen large enough to maintain the relation in Equation (7). Figure 2 shows a schematic of the effect of the segregation mechanism on interstitial concentrations near a non-oxidizing $\mathrm{Si/SiO_2}$ interface.

The continuity equations in the silicon are given by Equations (3) and (4), but we must now also include a continuity equation for interstitials within the oxide, given by

$$\frac{\partial C_{\mathrm{I}}^{\mathrm{SiO_2}}}{\partial t} = \nabla \cdot D_{\mathrm{I}}^{\mathrm{SiO_2}} \nabla C_{\mathrm{I}}^{\mathrm{SiO_2}}. \tag{8}$$

The boundary condition for interstitials at the Si/SiO_2 interface is modified to include the segregation of interstitials to the oxide film, giving

$$\hat{n} \cdot D_{\mathrm{I}}^{\mathrm{Si}} \bigtriangledown C_{\mathrm{I}} = \hat{n} \cdot D_{\mathrm{I}}^{\mathrm{SiO_2}} \bigtriangledown C_{\mathrm{I}}^{\mathrm{SiO_2}} + \sigma_{\mathrm{I}}(C_{\mathrm{I}} - C_{\mathrm{I}}^{*}). \tag{9}$$

The SiO_2/Si_3N_4 interface is modeled as a reflecting boundary for excess silicon [?] owing to experimental observations showing Si_3N_4 as a good diffusion barrier [?, ?].

The segregation process acts in many ways like an effective regrowth velocity which decreases with time. When there is a supersaturation of interstitials in the substrate, interstitials near the interface segregate to the oxide setting up a diffusion gradient within the SiO_2. Initially this results in a large flux of silicon into the oxide as the concentration gradient in the oxide is very large. As time goes on, the region of the oxide near the interface starts to "fill up" with excess silicon, reducing the concentration gradient and thus the flux into the oxide. This behavior can be confused with a slow interstitial diffusivity because of the resulting delay in the rise of interstitial supersaturation near an Si/SiO_2 interface. The effects of film segregation are particularly pronounced in lateral OED experiments, because the lateral diffusion occurs primarily in the near surface regions.

We use the SUPREM IV process simulator [?] to solve the coupled point defect equations given by Equations (3), (4), (6), (7), (8) and (9). The version of SUPREM IV that we use has been modified to allow segregation of point defects to films, as well as diffusion of point defects in materials other than silicon. The solution to this coupled system of equations yields the interstitial supersaturation which we then compare to experimental data, both our own and that obtained from sources in the literature.

4 Model Parameters

Based on the model presented in the previous section, the parameters which control the spatial extent of point defect interactions are the point defect diffusivities (D_{I}, D_{V}) and equilibrium concentrations in silicon (C_{I}^{*}, C_{V}^{*}), the Frenkel pair recombination rate (k_r), the regrowth velocities (σ_{I}, σ_{V}), the interstitial segregation coefficient (m_{I}) and the diffusivity of excess silicon in SiO_2 ($D_{\mathrm{I}}^{\mathrm{SiO_2}}$). However, the spatial extent of point defect interactions is just one aspect of the common Si/SiO_2 system, and many of these parameters have been calculated based on other experimental results as summarized in Table 2.

For the point defect diffusivity and equilibrium concentrations, we use values obtained by Bracht *et al.* [?] from metal diffusion experiments. Such experiments provide the best measure of these properties because they are based on measurements of metal distributions in the bulk, thereby eliminating interface effects, and include Frenkel pair recombination in the analysis. As we will show in the next section, the resulting high interstitial diffusivity becomes consistent with other experiments when bulk and surface-film interactions which slow the diffusion front are included. Although Bracht *et al.* base their analysis on experiments utilizing zinc, other recent work based on gold and platinum diffusion gives very similar parameter values [?, ?]. These parameters also agree well with self-diffusion measurements [?, ?].

If we assume that the bulk recombination coefficient k_r is diffusion-limited, then

$$k_r = 4\pi a(D_{\mathrm{I}} + D_{\mathrm{V}}) \approx 4\pi a D_{\mathrm{I}}. \qquad (10)$$

Using a fast interstitial diffusivity as obtained from metal diffusion experiments [?], leads to diffusion-limited value of k_r of approximately $10^{-11}\,\mathrm{cm}^2/\mathrm{sec}$ at 1100°C. However, we find that a lower value for bulk recombination obtained from OED/ORD experiments [?, ?] ($k_r = 3.5\times 10^{-15}\ \mathrm{cm}^{-3}\ \mathrm{sec}^{-1}$ at 1100°C) is sufficient to keep bulk recombination near local equilibrium ($C_{\mathrm{I}}C_{\mathrm{V}} \cong C_{\mathrm{I}}^*C_{\mathrm{V}}^*$) for the experimental conditions we consider in this work. Thus, we use the lower value to speed up the simulation times, as the simulation results are independent of k_r within this range.

The interstitial diffusivity in the SiO_2 ($D_{\mathrm{I}}^{\mathrm{SiO_2}}$) is calculated from experiments involving the migration of dopants due to temperature gradients within SiO_2 [?]. Extrapolating from Celler *et al.*'s data, which was fit to an Arrhenius relationship,

$$D_{\mathrm{I}}^{\mathrm{SiO_2}} = 13\,\mathrm{cm}^2\ \mathrm{sec}^{-1}\exp(-4.5\mathrm{eV}/\mathrm{kT}), \qquad (11)$$

we obtain a diffusion coefficient for interstitials within the oxide to be approximately $4\times 10^{-16}\mathrm{cm}^2/\mathrm{sec}$ at 1100°C, many orders of magnitude smaller than in silicon. Because of the very slow diffusivity, interactions with the substrate primarily affect only the near-interface region of the oxide, particularly at lower temperatures. For example, after a one hour anneal at 900°C, the expected diffusion depth ($2\sqrt{Dt}$) is only about 10 Å.

The remaining model parameters, which are not established based on other experimental measurements, are the interface regrowth velocities (σ_{I}, σ_{V}) and the segregation coefficient (m_{I}). Since bulk recombination is rapid enough to maintain $C_{\mathrm{I}}C_{\mathrm{V}}$ near the equilibrium product for the experimental conditions considered in this work, changes in the interface regrowth velocity for both interstitials and vacancies have nearly the same effect on interstitial supersaturation (as confirmed by simulation [?]). Thus it is very difficult to separate out the two factors and we can reduce the number of parameters by considering them together. Using the continuity equations for point defects together with their boundary conditions (Equations (3), (4), (5) and (6)) and including the condition for fast recombination ($C_{\mathrm{I}}C_{\mathrm{V}} \approx C_{\mathrm{I}}^*C_{\mathrm{V}}^*$) we obtain an effective interstitial regrowth velocity, $\sigma_{\mathrm{I}}^{\mathrm{eff}}$, which includes the effects of both interstitials and vacancies:

$$\sigma_{\mathrm{I}}^{\mathrm{eff}} = \sigma_{\mathrm{I}} + \sigma_{\mathrm{V}}(\frac{C_{\mathrm{V}}^*}{C_{\mathrm{I}}}). \qquad (12)$$

We use a constant value for $\sigma_{\mathrm{I}}^{\mathrm{eff}}$ in this work although it decreases slightly with increasing interstitial supersaturation. Since the experiments we consider have an interstitial supersaturation ($C_{\mathrm{I}} > C_{\mathrm{I}}^*$), the importance of vacancy regrowth is reduced. We thus set σ_{V} to zero in our simulations and allow σ_{I} to determine the effective extent of interface regrowth.

The final set of model conditions is the boundary condition at oxidizing interfaces. Since interactions at the interface and in the oxide effectively set the interstitial concentration at the oxidizing interface [?], fast interface generation and regrowth are used to fix the interstitial concentration. The value of interstitial supersaturation at the oxidizing Si/SiO_2 interface is determined either from oxidation kinetics along with the known dependence of interstitial supersaturation on oxidation rate [?], or from experimental data at the oxidizing interface, when available [?].

5 Comparison to Experimental Data

The numerical simulations, conducted using a modified version of SUPREM IV, yield the calculated interstitial supersaturation for each set of experimental conditions. We compare the model predictions to various data, both our own and that obtained from the literature, all using the diffusion of phosphorus or boron marker layers as an indicator of point defect concentrations. In comparing interstitial supersaturation with dopant diffusivity enhancement, we assumed the fractional interstitial components of diffusion to be $f_{\mathrm{I}} = 1.0$ for phosphorus [?] and $f_{\mathrm{I}} = 0.8$ for boron [?]. To minimize the impact of errors in values for interstitial supersaturation near oxidizing interfaces, normalized values for dopant diffusivity or interstitial concentration are used when possible in the comparisons.

The experimental results used came from four sources. The first set of data was obtained from the frontside oxidation of membranes with a buried phosphorus marker layer (Agarwal and Dunham [?]). The second set was from the backside oxidation of membrane structures with a buried phosphorus marker layer (Agarwal [?]), while the third set of data came from the backside oxidation of membranes with a frontside phosphorus marker layer (Ahn *et al.* [?]). Finally, the last set of data was obtained from the lateral OED of a boron marker layer beneath nonoxidizing stripes (Griffin *et al.* [?]). The comparison of the model to the experimental data is shown in Figures 3 through 6. The data in each graph is shown by symbols. Dashed lines represent the best fit of the simulations to the full set of data, where the parameters $\sigma_{\mathrm{I}}^{\mathrm{eff}}$ and m_{I} were optimized using the Levenberg-Marquardt optimization software PROFILE [?].

Figure 3 is a comparison of experiment and simulation for the frontside oxidation of a buried phosphorus marker layer, in membranes that are 6, 14, 24 and 45μm thick, after a 60 min oxidation at 1100°C in a dry oxygen ambient [?]. The value plotted on the y-axis is the ratio of the time-averaged interstitial concentration at each membrane thickness to the time-averaged interstitial concentration averaged over all membrane thicknesses, while the x-axis is the membrane thickness. Note that for these experiments the nonoxidizing interface at the backside is located too far away (500μm) to significantly influence the interstitial concentrations near the buried layers, so that the simulations are nearly independent of the two fitting parameters, both of which are associated with the nonoxidizing interface. Instead, the variation of interstitial concentration with depth depends primarily on the interstitial diffusivity and the relative equilibrium concentrations of interstitials and vacancies. The excellent match to the experimental results further supports the use of the point defect parameters from Bracht *et al.*. The simulations are also consistent with earlier buried layer experiments of Griffin *et al.* [?, ?], which were able only to provide an upper bound for the variation of interstitial concentration with depth.

Figure 4 shows the fits to data obtained from the backside oxidation of silicon membrane structures while monitoring buried phosphorus marker layers at a depth of 45μm from the nonoxidizing front oxide interface [?]. The results shown are for floatzone silicon substrates at the end of a 4 h and 20 h oxidation at 1100°C, respectively. The membrane thicknesses (distance from marker layer to backside) are 100, 141, 265 and 512μm for the 4 h experiment and 100, 156, 284, 519μm for the 20 h experiment. Again, the fit is quite good, especially for the 4 h oxidation.

Figure 5 is a plot of interstitial supersaturation as determined from phosphorus diffusivity enhancement for backside oxidation experiments by Ahn *et al.* [?] using floatzone silicon etched to form 20, 55, 104 and 530μm membranes. The oxidation was in a dry oxygen ambient at 1100°C for times ranging from 60 min (1 h) to 3360 min (56 h). The simulation results shown use a rapid interstitial diffusivity, but include Frenkel pair recombination and interface segregation as described above. Although the parameter values are optimized to fit a much broader range of data, the model presented in this work provides a similar match to the experimental results as the model originally used to analyze this data set (Equations (1) and (2) with a much smaller effective diffusivity on the order of 10^{-9}cm^2/sec). Note that the superior fit shown in the original presentation of this data [?] used a different effective diffusivity and interface regrowth rate for each membrane thickness.

Finally, Figure 6 shows the normalized excess interstitial supersaturation ratio between the center of inert stripes and the wide oxidizing regions where the maximum diffusivity enhancement occurred,

$$\text{Supersaturation Ratio} = \frac{\dfrac{\left\langle C_{\mathrm{I}}^{\text{inert}} \right\rangle}{C_{\mathrm{I}}^{*}} - 1}{\dfrac{\left\langle C_{\mathrm{I}}^{\text{oxidizing}} \right\rangle}{C_{\mathrm{I}}^{*}} - 1}, \tag{13}$$

where the $\langle\rangle$ represent time-averaged values. Both data and simulation results are shown versus oxidation time at 900, 1000 and 1100°C, for two different stripe widths in each case. The data points are derived from reported values of the lateral decay length calculated based on a range of stripe widths used by Griffin [?, ?]. As can be seen, the model does an excellent job of accounting for both the time dependence and stripe width dependence of the experimental data.

Since the data includes results at 900, 1000 and 1100°C, we are able to extract activated model parameters as listed in Table 3. These activated parameters as well as those in Table 2 were used for all the simulation results shown. In comparing interstitial diffusion, D_{I}, and interface regrowth, σ_{I}, the activation energy for interface regrowth is slightly larger than that for interstitial diffusion, which suggests a small additional energy barrier for the interface regrowth reaction in excess of the bulk migration energy. The ratio of σ_{I} to D_{I} is about 275 at 1100°C, which is about a factor of 2 to 4 smaller than previous reports [?, ?, ?, ?, ?], as expected, since these earlier analyses neglect interface segregation, thereby increasing their calculated interface regrowth rate.

The negative activation energy for the segregation coefficient is expected from the definition of m_{I} (Equation (7)), since C_{I}^{*} has an activation energy of 3.18 eV while the equilibrium value for $C_{\mathrm{I}}^{\mathrm{SiO_2}}$ has a much smaller activation energy, as evidenced by the large solubility of silicon in SiO_2 at high temperatures [?]. Thus, segregation of excess silicon to SiO_2 becomes stronger as the temperature is lowered. The resulting segregation coefficient at 1100°C is 6.9×10^{7}, giving an equilibrium solubility of excess silicon in SiO_2 in contact with silicon ($m_{\mathrm{I}}C_{\mathrm{I}}^{*}$) of about $4 \times 10^{20}\mathrm{cm}^{-3}$, or a little less than 2% of the silicon concentration in stoichiometric SiO_2. Extrapolating to 1405°C, we get a solubility of about $2 \times 10^{21}\mathrm{cm}^{-3}$ or about 10% of the silicon concentration in stoichiometric SiO_2, consistent with the lower limit of 3% calculated by Celler and Trimble [?] based on silicon dissolution in SiO_2 at this temperature.

6 Conclusions

As illustrated in Figures 3 through 6, the model developed in this work is able to match a broad range of experimental data over a range of temperatures, from which widely disparate interstitial diffusivity values had previously been calculated. In contrast to previous work, a single consistent set of point defect parameters are extracted. The model is consistent with the full range of experiments utilized to quantify the spatial extent of point defect interactions in silicon, including metal diffusion and gettering, the depth dependence of enhanced diffusion of buried layers, the lateral spread of oxidation enhanced diffusion, and enhanced diffusion during backside oxidation of membrane structures. The model provides a fundamental basis for predicting the spatial extent of point defect interactions in VLSI structures.

The model is able to account for the full set of data because it includes point defect interactions in the bulk and with surface films which had previously been largely ignored: bulk Frenkel pair recombination and segregation of excess silicon to films. The role of film segregation is particularly important as low effective diffusivity values are generally observed only when measuring interstitial supersaturations near nonreacting film interfaces, (see Table 1), while bulk measurements of interstitial supersaturation, such as in the buried layer experiments and metal diffusion experiments respond much more rapidly in time. Considering segregation, the interstitial concentration near the film interface cannot increase until the concentration in the film increases also. For strong preferential segregation to the film, as calculated in this work and also observed previously for oxides [?, ?], the rise in interstitial concentration is substantially delayed, accounting for the slow calculated effective interstitial diffusivities in previous work.

7 Acknowledgements

This work was supported by SEMATECH/SRC. We would like to thank Profs. Dmitri Antoniadis and Rafael Reif for facilitating use of the MIT Microsystems Technology Laboratory, Prof. Mark Law for some of the modifications to SUPREM IV required to implement the simulations performed in this work, and Dr. Peter Griffin for providing the raw data from experimental measurements of lateral OED.

Figure 1: *Schematic showing bulk and surface interactions which control the spatial extent of point defect interactions in silicon.*

Figure 2: *Close-up view at the non-oxidizing* Si/SiO_2 *interface showing the effect of segregation. The interstitial segregation coefficient* (m_I) *determines the ratio of the concentrations on either side of the interface.*

Figure 3: *Normalized diffusivity enhancement versus depth for phosphorus buried layers during a 60 min oxidation at 1100°*C *in a dry oxygen ambient. Data from Agarwal and Dunham.*

Figure 4: *Comparison of simulated versus measured diffusivity enhancement as a function of distance from the backside for phosphorus buried layers after backside oxidation at 1100°*C *in a dry oxygen ambient for (a) 4 hours and (b) 20 hours. Data from Agarwal [*?*].*

Figure 5: *Time-averaged phosphorus diffusion enhancement versus time during backside oxidation for a range of membrane thicknesses. Data from Ahn [*?*] utilizing 20*μm, *55*μm, *104*μm *and 530*μm *membranes at 1100°*C *in dry oxygen ambient as a function of oxidation time ranging from 60 min (1h) to 3360 min (56 h). The dashed line shows the interstitial supersaturation values obtained from a SUPREM IV simulation including both bulk recombination and film segregation.*

Figure 6: *Comparison of simulation and data for time-averaged interstitial supersaturation ratio (Equation (13)) at the center of nonoxidizing stripes of given widths at 900, 1000 and 1100°*C*, plotted versus oxidation time. Data from Griffin [*?, ?*]. The ratio is normalized to the time-averaged excess supersaturation in the wide oxidizing stripe regions where maximum OED occurs.*

Table 1: *Summary of previous calculations of effective interstitial diffusivity.*

Type of Experiment	Diffusion Through	Marker Location	Injection Level	Effective Diffusivity	References
Backside Oxidation	Cz, FZ	Interface	Low	Low	[?, ?, ?, ?, ?]
Lateral Extent of OED	Cz, FZ	Interface	Low	Low	[?, ?, ?, ?, ?]
Buried Layer	Epitaxial	Bulk	Low	High	[?, ?]
Metal Diffusion	Cz, FZ	Bulk	High	High	[?, ?, ?, ?, ?]

Table 2: *Parameters established based on previous experiments and used in the simulations.*

Parameter	Pre-Exponent	Activation Energy (eV)	Experimental Source	Reference
C_{V}^{*} (cm^{-3})	1.4×10^{23}	2.0	Metal Diffusion	[?]
D_{V} (cm^2/s)	3.0×10^{-2}	1.8	Metal Diffusion	[?]
C_{I}^{*} (cm^{-3})	2.9×10^{24}	3.18	Metal Diffusion	[?]
D_{I} (cm^2/s)	51	1.77	Metal Diffusion	[?]
k_r (cm^3)	3.16×10^{-6}	2.44	OED/ORD	[?, ?]
$D_{\mathrm{I}}^{\mathrm{SiO_2}}$ (cm^2/s)	13.0	4.5	Thermo-migration	[?]

Table 3: *Optimized model parameters based on simulations including bulk-recombination and segregation of interstitials to surface films.*

Parameter Calculated	Pre-Exponent	Activation Energy (eV)
σ_{I} (cm/sec)	4.2×10^{4}	1.90
$\mathrm{m_I}$	1.24	-2.11