SPATIAL VARIATIONS IN POINT DEFECT CONCENTRATIONS AND THEIR IMPACT ON SUBMICRON DEVICE STRUCTURES

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We have developed a model for the spatial extent of point defect interactions in silicon based on fundamental physical interactions. The model is able to consistently account for the broad range of experimental results, including experiments which had previously given effective interstitial diffusivities which ranged over more than five orders of magnitude. This model predicts strong nonuniformities in point defect concentrations in submicron structures that are not expected based on standard analyses, but which lead to critical changes in these structures, such as reverse short channel effects.

INTRODUCTION

Integrated circuit fabrication processes such as oxidation, ion implantation, and high concentration diffusion perturb point defect concentrations, both locally and in nearby regions. These and other processes depend critically on point defect concentrations and concentration gradients. Therefore, in order to accurately model the fabrication of submicron integrated circuit structures, it is essential to correctly consider the spatial variations in point defect concentrations. One of the major barriers to such modeling is the lack of consensus on appropriate point defect models and parameters. For example, when experiments are conducted to determine interstitial diffusivity, the resulting calculations vary over 3-6 orders of magnitude [1-6].

In this work, we show that by using a more complete model for bulk and interface interactions, it is possible to consistently account for the broad range of experimental measurements, which had previously given rise to such a large spectrum of point defect parameter values. We then apply this model, which was characterized primarily with experimental data at relatively long times and high temperatures, to interactions in submicron device structures for processes with much lower thermal budgets. Specifically, we examine transient enhanced diffusion leading to reverse short channel effects and diffusion in thin SOI layers. In both cases, the model effectively predicts the experimentally observed behavior, which deviates substantially from that expected using standard models.

MODEL AND COMPARISON TO EXPERIMENTS

Because similar experiments used to extract point defect parameters generally give consistent results, we conclude that the observed discrepancies in interstitial diffusivity values stem not from unreliability of the experimental results, but rather from the fact that the models used to extract them from the experimental measurements ignore important interactions. First, Frenkel pair recombination, and thus the effect of vacancy diffusion on interstitial profiles, were neglected in many of the calculations. Even more critically, standard modeling greatly oversimplifies the interactions of point defects with films and interfaces by using a constant effective recombination velocity. Extending our previous models of oxidation enhanced diffusion [7] to the nonoxidizing system [8], we conclude that interstitials (excess silicon) segregate strongly from silicon to SiO_2 layers, where they diffuse very slowly. Because the gradient in the excess silicon concentration in the oxide controls the flux from the interface into the oxide, this behaves similarly to an effective recombination rate that decreases with time. The resulting model is given by point defect continuity equations in the silicon:

$$\frac{\partial C_{\mathrm{I}}^{\mathrm{Si}}}{\partial t} = \nabla \cdot D_{\mathrm{I}}^{\mathrm{Si}} \nabla C_{\mathrm{I}}^{\mathrm{Si}} - k_r (C_{\mathrm{I}}^{\mathrm{Si}} C_{\mathrm{V}}^{\mathrm{Si}} - C_{\mathrm{I}}^{\mathrm{Si}*} C_{\mathrm{V}}^{\mathrm{Si}*}), \tag{1}$$

$$\frac{\partial C_{\mathrm{V}}^{\mathrm{Si}}}{\partial t} = \nabla \cdot D_{\mathrm{V}}^{\mathrm{Si}} \nabla C_{\mathrm{V}}^{\mathrm{Si}} - k_r (C_{\mathrm{I}}^{\mathrm{Si}} C_{\mathrm{V}}^{\mathrm{Si}} - C_{\mathrm{I}}^{\mathrm{Si}*} C_{\mathrm{V}}^{\mathrm{Si}*}); \tag{2}$$

and for excess silicon in the oxide:

$$\frac{\partial C_{\mathrm{I}}^{\mathrm{SiO_2}}}{\partial t} = \nabla \cdot D_{\mathrm{I}}^{\mathrm{SiO_2}} \nabla C_{\mathrm{I}}^{\mathrm{SiO_2}}; \tag{3}$$

along with boundary conditions at the Si/SiO_2 interface:

$$\hat{n}_{\mathrm{Si/SiO_2}} \cdot D_{\mathrm{I}}^{\mathrm{Si}} \nabla C_{\mathrm{I}}^{\mathrm{Si}} \Big|_{\mathrm{Si/SiO_2}} = \hat{n}_{\mathrm{Si/SiO_2}} \cdot D_{\mathrm{I}}^{\mathrm{SiO_2}} \nabla C_{\mathrm{I}}^{\mathrm{SiO_2}} \Big|_{\mathrm{Si/SiO_2}} + \sigma_{\mathrm{I}} (C_{\mathrm{I}}^{\mathrm{Si}} - C_{\mathrm{I}}^{\mathrm{Si}*}), \tag{4}$$

$$\hat{n}_{\mathrm{Si/SiO_2}} \cdot D_{\mathrm{V}}^{\mathrm{Si}} \nabla C_{\mathrm{V}}^{\mathrm{Si}} \Big|_{\mathrm{Si/SiO_2}} = \sigma_{\mathrm{V}} (C_{\mathrm{V}}^{\mathrm{Si}} - C_{\mathrm{V}}^{\mathrm{Si}*}), \tag{5}$$

where segregation of interstitials across the interface is assumed to be fast so that

$$m_{\mathrm{Si/SiO_2}} = \left(C_{\mathrm{I}}^{\mathrm{SiO_2}} / C_{\mathrm{I}}^{\mathrm{Si}} \right)_{\mathrm{Si/SiO_2}}. \tag{6}$$

We have tested our model by comparing its predictions to experimental results. We find that using point defect concentrations and diffusivities derived from metal diffusion experiments [5, 9, 10] the model can consistently account for the full range of observations, reproducing experiments which require effective diffusivity values up to five orders of magnitude smaller [2, 3, 11] when less complete models are used. Figures 1 and 2 show examples of the match of the model to some of the experimental data. The simulations were performed with a version of SUPREM IV [12] modified to include interstitial segregation to and diffusion in SiO_2 films. The values of the activated parameters used in all the simulations are listed in Table 1. (Note that σ_{V} is neglected and the effects of surface regrowth of both interstitials and vacancies are included in $\sigma_{\mathrm{I}}^{\mathrm{eff}}$.)

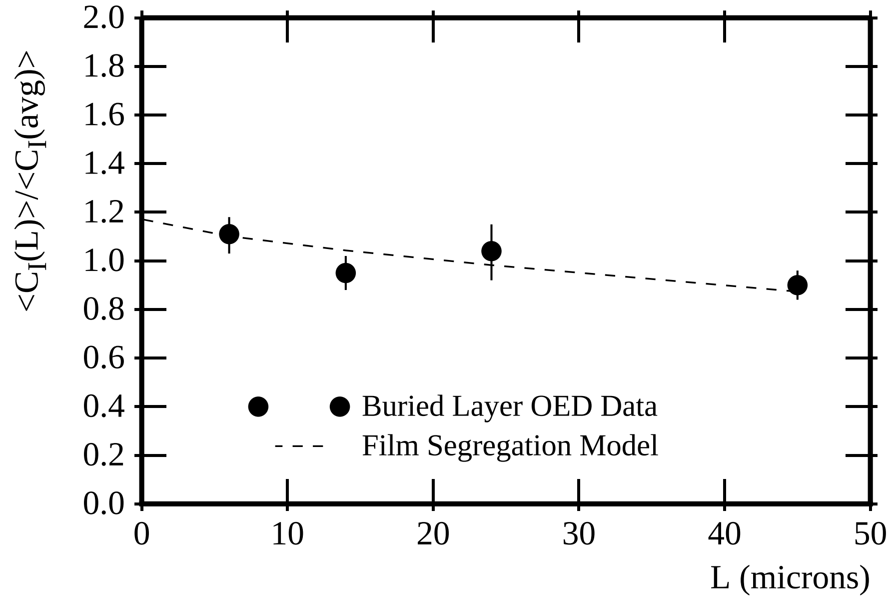

Figure 1: *Comparison of model for spatial extent of point defect interactions to relative diffusivity enhancement of phosphorus buried layers as a function of depth for a 1 h oxidation at 1100*°C *in dry* O_2 *(Agarwal and Dunham [11]).*

APPLICATION TO SUBMICRON STRUCTURES

Most of the data typically used for characterizing the spatial extent of point defect concentrations is for larger thermal budgets than are used in for submicron devices. However recent observations of reverse short channel effects and diffusion in SOI structures provide the opportunity for model verification in the submicron domain. Extrapolating the model described above, which was quantified at relatively high temperatures and long times, to submicron structures, we find that interface interactions (e.g., segregation to films) play a dominant role. This leads to strong variations in lateral and vertical point defect distributions that would not be predicted with previous models of point defect diffusion, but have profound effects on the resulting device structures.

As an example, the model predicts that the channel doping profile of submicron MOS devices depends strongly on the channel length for source/drain processing that results in interstitial injection, such as ion implantation and oxidation. Figure 3 illustrates simulated doping and interstitial profiles in the channel region of short and long channel devices following a 40 minute 700°C anneal of a phosphorus LDD implantation. As above, the simulations were performed with a modified version of SUPREM IV. Because the dose is below the amorphization threshold, in modeling transient enhanced diffusion we were able to assume that the initial damage profile could be approximated by an excess interstitial profile equal to the phosphorus implant profile.

Film segregation to the gate oxide leads to the large gradient in the interstitial

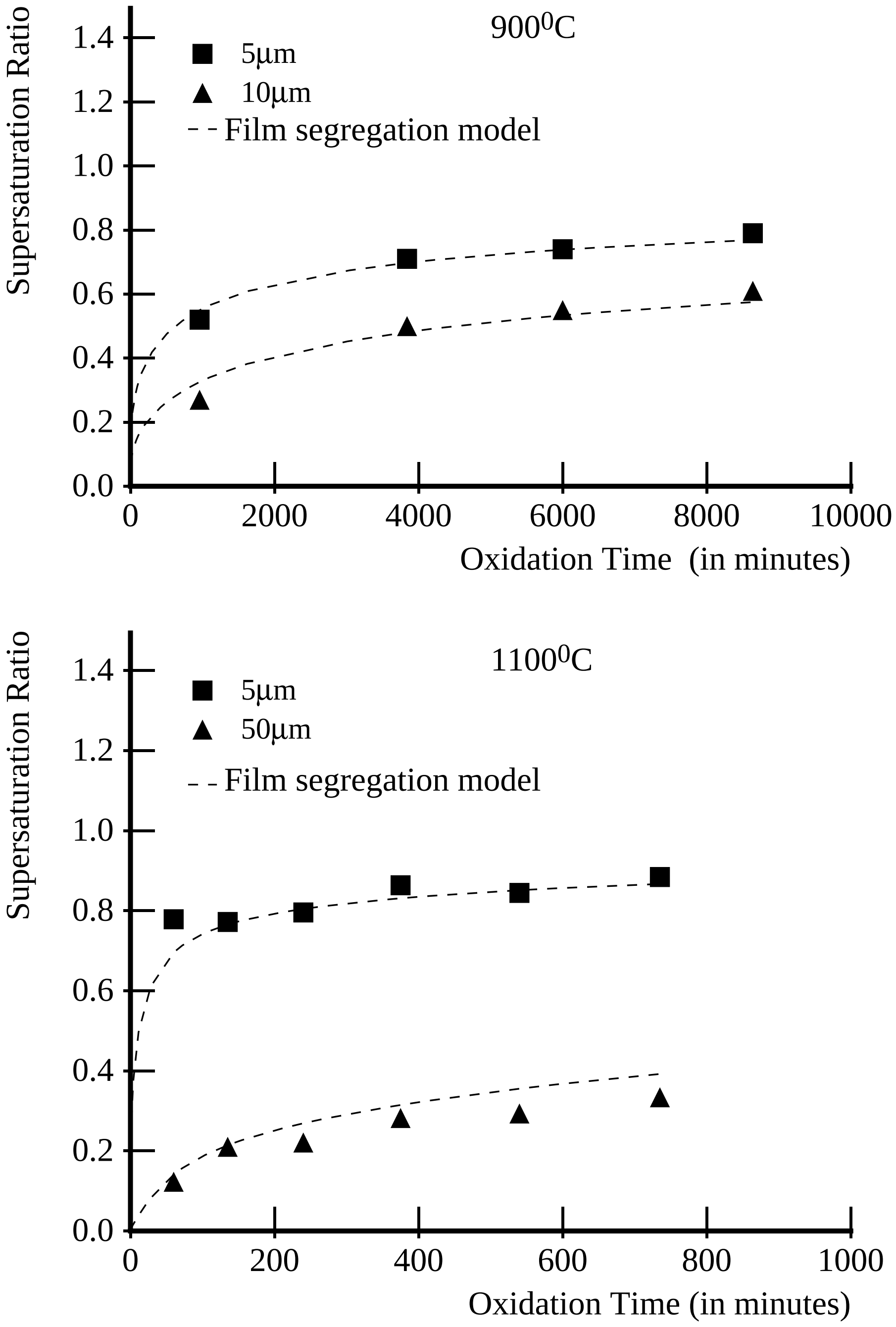

Figure 2: *Comparison of model to relative diffusivity enhancement versus time for boron near the center of nitride/oxide stripes serving as oxidation barriers during local oxidation at (a) 900°C and (b) 1100 °C. Data from Griffin et al. [2].*

Table 1: *Parameters used in the simulations. Those parameters marked with references are from previously published results as indicated. The other parameters values were determined based on optimizing the fit to experimental data which had previously resulted in contradictory values for point defect parameters in silicon [2, 3, 11].*

Parameter	Pre-Exponential Term	Activation Energy (eV)
$C_{\mathrm{V}}^{\mathrm{Si}*}$ [5]	$1.4\times10^{23}\,\mathrm{cm}^{-3}$	2.0
$D_{\mathrm{V}}^{\mathrm{Si}}$ [5]	$3.0\times10^{-2}\,\mathrm{cm}^2/\mathrm{sec}$	1.8
$C_{\mathrm{I}}^{\mathrm{Si}*}$ [5]	$2.9\times10^{24}\,\mathrm{cm}^{-3}$	3.18
$D_{\mathrm{I}}^{\mathrm{Si}}$ [5]	$51\ \mathrm{cm}^2/\mathrm{sec}$	1.77
k_r [13, 14]	$3.16\times10^{-6}\,\mathrm{cm}^3$	2.44
$D_{\mathrm{I}}^{\mathrm{SiO_2}}$ [15]	$13.0\ \mathrm{cm}^2/\mathrm{s}$	4.5
$\sigma_{\mathrm{I}}^{\mathrm{eff}}$	$4.2\times10^{4}\,\mathrm{cm}/\mathrm{sec}$	1.90
$\mathrm{m_I}$	1.24	-2.11

concentration, which due to coupled diffusion results in a flux of boron towards the surface and an increased threshold voltage. At the same time, the interstitial supersaturation deeper in the channel broadens the channel doping profile, reducing the body coefficient as observed experimentally [16, 17]. The resulting change in threshold voltage due to the nonuniform point defect concentrations ($\sim 0.2\,\mathrm{V}$) matches that observed experimentally under similar conditions [17].

Rafferty *et al.* [16, 17] were able to model experimentally-observed threshold voltage and body coefficient changes with channel length, but required an effective interface recombination velocity much too high to be consistent with longer time experiments [2, 3]. In contrast, the model described in this work can account consistently for both short and long time data because the segregation of excess interstitials to the SiO_2 films results in an effective interface recombination velocity which decreases with time. In addition, because the threshold voltage shifts are due primarily to point defect gradients, they occur even when the channel doping is nearly flat near the surface as observed by Jacobs *et al.* [18].

For thin SOI structures, interface interactions can lead to strong effects even in one dimensional structures, where they are easier to observe directly. The model described here predicts that during oxidation of SOI structures, the interstitial supersaturation will vary strongly with depth due to segregation of excess interstitials to the buried oxide layer. Exactly this behavior has been observed by Crowder *et al.* [19] using measurements of asymmetric boron diffusion profiles. As shown in Fig. 4, the

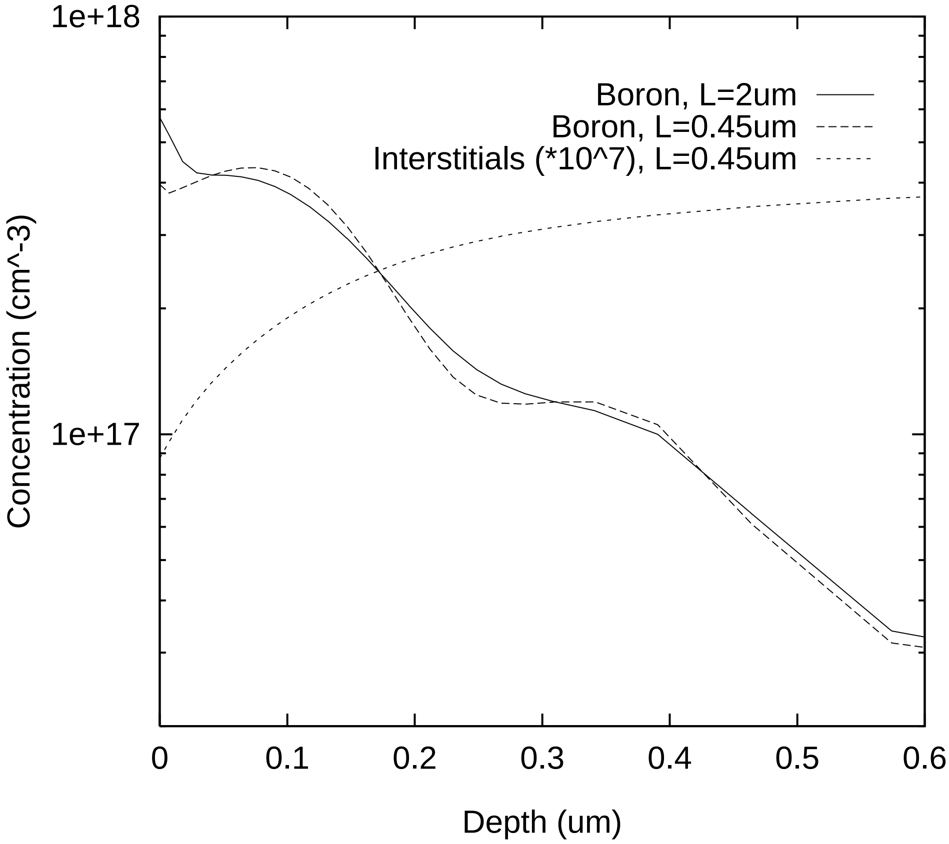

Figure 3: *Simulated boron doping profiles in the center of short (0.45*μm*) and long (2*μm*) channel devices following annealing of LDD implants. Also shown is the interstitial supersaturation as a function of depth at the center of the channel of the short channel device.*

resulting profiles match closely to the predictions of the model described in this work. As with the reverse short channel effects, the data can also be matched using the standard model, but only if interface recombination is assumed to be very fast, which is inconsistent with results at longer times/higher temperatures.

CONCLUSIONS

In summary, we have developed a model for the spatial extent of point defect interactions in silicon based on fundamental physical interactions which is able to account for the broad range of experimental results in a consistent manner, including data which had originally been used to extract point defect parameters differing by many orders of magnitude. This model predicts strong nonuniformity in point defect concentrations in submicron structures that are not expected based on standard analyses, but which lead to critical changes in these structures that have been observed experimentally. The critical element of the model is the preferential segregation of in-

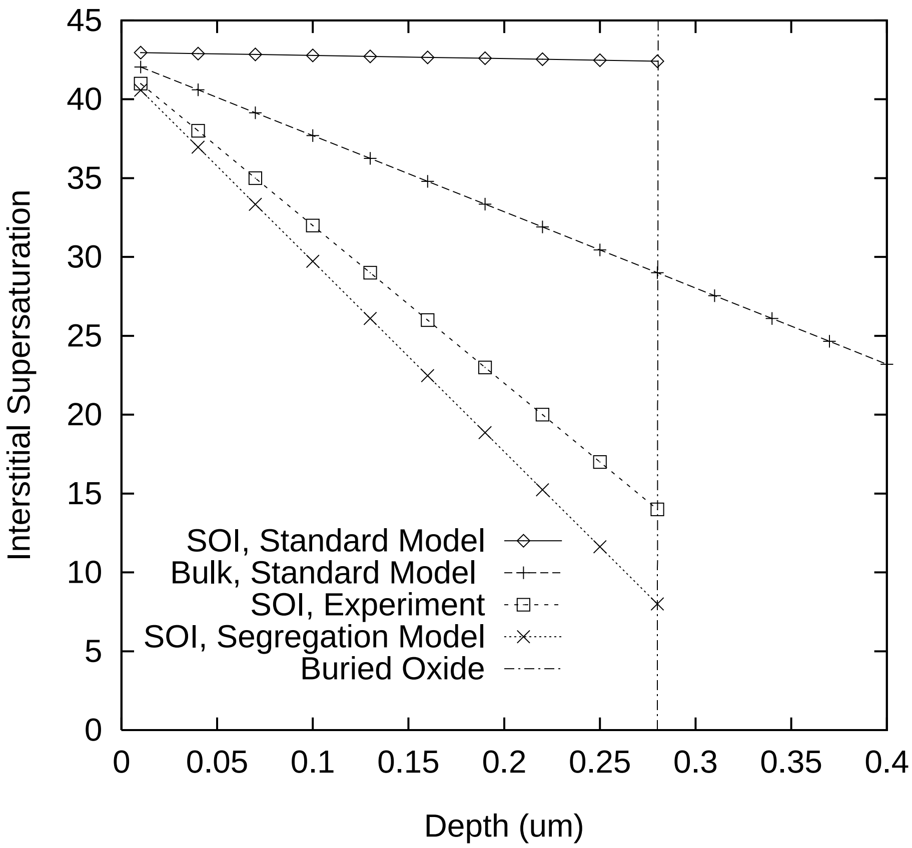

Figure 4: *Interstitial supersaturation versus depth during oxidation of bulk and SOI samples. Shown is variation with depth required to match asymmetry in experimental boron profiles in thin SOI silicon, as well as model predictions for both standard model and film segregation model. Note that using parameters extrapolated from longer times and higher temperatures, the film segregation model effectively predicts the interstitial distribution with depth. Experimental and standard model results are from Crowder et al. [19].*

terstitials (excess silicon) to oxide films, which behaves like an effective recombination velocity that decreases with time.

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KEYWORDS

Page 1: Interstitials, vacancies, point defect parameters, interstitial diffusivity, spatial extent

Page 2: Recombination, segregation

Page 3: Reverse short channel effects, transient enhanced diffusion

Page 4: Lateral diffusion

Page 5: Equilibrium concentrations, SOI