

# Simulation of Denuded Zone Formation in CZ Silicon

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## Abstract

In ULSI device processing technology, internal gettering (IG) of metallic contaminants is an important issue. The structure of IG wafers consists of the bulk microdefect region and a defect-free subsurface region, termed as “denuded zone” (DZ). In our work, we present a detailed analysis of the coupled diffusion-oxygen precipitation problem encountered in the simulation of the denuded zone formation.

## 1. Introduction

In ULSI device processing technology, internal gettering (IG) of metallic contaminants is considered to be an important issue. A well-controlled IG process can lead to a significant improvement in yield and device performance. In general, the structure of IG wafers consists of the bulk microdefect region and a defect-free subsurface region, termed as “denuded zone” (DZ).

In a controlled IG process, two important factors need to be kept in mind. (i) Only a certain amount of bulk microdefects should be nucleated for gettering of metallic contaminants because excessive precipitation would lead to a reduction in dissolved oxygen concentration and loss in resistance against wafer warpage and (ii) a well-defined DZ must be created to minimize the growth of residual microdefects near the wafer surface. A typical controlled IG cycle consists of three annealing steps. The first step, termed as “denudation”, is to deplete the oxygen from the subsurface region via out-diffusion. The second and third steps are necessary to nucleate and grow the microdefects to the size that is thermodynamically stable.

Defects engineering, including the modeling of the IG process, becomes increasingly important in the development of ULSI device fabrication processes. The experimental determination of DZ, oxygen precipitate sizes and microdefect densities is toilsome. The theoretical prediction and the use of computer models can help to interpret the results from precipitation experiments. It also saves total process development time and cost.

In several models for oxygen precipitation and DZ-formation proposed [1], [2], it is assumed that oxygen precipitation in silicon occurs through homogenous nucleation

despite the fact that more and more evidence points towards a heterogenous mechanism [3]. In homogenous models, steady-state equations [2] have been commonly used to describe the precipitation behaviour. On the other hand, these models cannot explain the dissolution of preexisting precipitates and do not take into account the size distribution of precipitates.

In our work based on the model of Schrems *et al.*[4] for oxygen precipitation we present a detailed analysis of the coupled diffusion-precipitation problem encountered in the simulation of the denuded zone formation. Oxygen precipitates are described by a size distribution function  $f(n)$ , i.e. by the number of precipitates per  $cm^3$  containing  $n$  oxygen atoms as a function of  $n$ . Growth and dissolution is described by chemical rate equations for the smallest precipitates ( $n \leq 20$ ) in combination with a single Fokker-Planck equation for all larger precipitate sizes. These equations are coupled with the diffusion equation for interstitial oxygen. In this work the model is applied for studying oxygen precipitation not only in the bulk, but also as a function of the depth perpendicular to the wafer surface.

## 2. Model

A detailed description of the model for bulk oxygen precipitation can be found elsewhere[4]. The model describes the growth and dissolution of oxygen precipitates statistically. It combines chemical rate equations (RE) for an accurate description of the smallest clusters with an approximating Fokker-Planck equation (FPE) for describing all larger precipitate sizes. The coefficients in the resulting system of differential equations are related to the growth and dissolution rates of the oxygen precipitates containing the Gibbs free energy of an individual oxygen precipitate. Assuming spherical precipitates composed of  $SiO_2$ , the Gibbs free energy  $G(n, t)$  of a precipitate with  $n$  oxygen atoms is modelled as the sum of volume energy  $G_O$  and interfacial energy  $G^{if}$ ,

$$G_O = -nkT \ln \left( \frac{C_O}{C_O^{eq}} \right) \quad G^{if} = 4\pi r^2 \alpha \left( 1 + \left( \frac{\zeta_1}{n} \right)^{1/3} + \left( \frac{\zeta_2}{n} \right)^{2/3} \right) \quad (1)$$

$C_O$  and  $C_O^{eq}$  denote the concentration of interstitial oxygen atoms and their solubility.  $G^{if}$  is proportional to the square of the precipitate radius  $r$  and to the unit surface energy  $\alpha = 0.31 Jm^{-2}$  [3] corrected by a factor containing free parameters  $\zeta_1$  and  $\zeta_2$  [5]. The values  $\zeta_1 = 0.22$  and  $\zeta_2 = 0.33$  have been used.

The model for bulk oxygen precipitation has been extended for DZ simulation by taking oxygen diffusion into account and by treating the precipitation process as a function of the distance from the wafer surface. The differential equation for interstitial oxygen ( $C_O$ ) contains a diffusion and a precipitation ( $C_{O,OP}$ ) term,

$$\frac{\partial}{\partial t} C_O = D_O \frac{\partial^2}{\partial x^2} C_O - \frac{\partial}{\partial t} C_{O,OP} \quad C_{O,OP} = \int n \cdot f(n) dn. \quad (2)$$

$D_O$  denotes the effective diffusivity. This equation is solved together with the RE/FPE for the oxygen precipitates by PROMIS [6]. As initial value  $C_O(t=0) = 9.5 \cdot 10^{17} cm^{-3}$ , as boundary condition  $C_O(x=0) = C_O^{eq}$  is assumed. In order to avoid troubles due to the large range of  $n$  ( $1 \dots 10^{11}$ ) a transformation  $\rho(n)$  has been applied.  $\rho$  equals  $n$  for the smallest precipitates, and  $\rho(n)$  is a cubic function for larger  $n$ , carefully selected to avoid both large nonlinearities and an excessive range of  $n$ .

### 3. Results and Discussion

Since the small nuclei have an ultimate importance for the following precipitation the numerical simulations take into account the thermal history of samples including cooling down in crystal growth approximately described by an exponential decrease of temperature from  $1400^{\circ}\text{C}$  to  $450^{\circ}\text{C}$  in 1h. Figures 1–3 show the size distribution function after each step of a typical HI-LO-HI anneal used for denuded zone formation ( $1100^{\circ}\text{C}/16\text{h} + 650^{\circ}\text{C}/16\text{h} + 1000^{\circ}\text{C}/16\text{h}$ ). The logarithm of the size distribution is shown as a function of  $\log(n)$  and  $x$ . In the first step (Fig. 1), due to the high temperature mainly outdiffusion occurs while only small precipitates emerge. In the second step (Fig. 2), due to the low temperature almost no diffusion occurs while important precipitation (nucleation) takes place. It can be seen that less precipitation occurs near the surface because of the lower interstitial oxygen concentration than in the bulk. The precipitates in the bulk may grow in the third step (Fig. 3) because the radius of the larger ones is larger than the critical radius at the higher temperature of this step. In contrast, the radius of all precipitates at the surface is smaller than the critical radius. Therefore they tend to dissolve.

Figures 4 and 5 show the interstitial oxygen concentration depicted as a function of depth after each step of two different IG annealing cycles. The shape of the interstitial oxygen profile can be explained by out-diffusion of the oxygen from the subsurface region during the first HI anneal at  $1100^{\circ}\text{C}$  and by precipitation of oxygen in the bulk at successive anneals. The final interstitial oxygen distribution is in good agreement with the experimental data of Isomae et al. [8]. The experimental data could only be explained by assuming the value by Takano and Maki [9] for long range diffusion coefficient  $D_O$  and the value by Craven[7] for oxygen solubility  $C_O^{eq}$ .

### 4. Conclusion

The effect of the IG anneal cycles on the oxygen precipitation and DZ formation in CZ-silicon was studied. Extensions of the recently developed model of Schrems et al. were discussed. The results imply that long range out-diffusion has to be assumed and crystal growth condition and thermal history of the wafer play a significant role with respect to DZ formation.

### References

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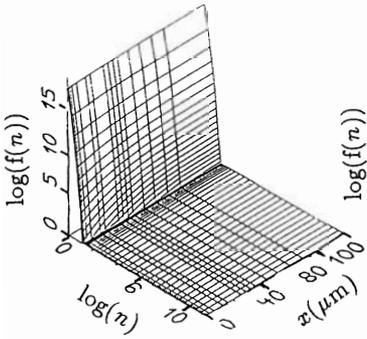


Figure 1: Size distribution function as a function of  $\log(n)$  and  $x$  after 1100°C/16h anneal.

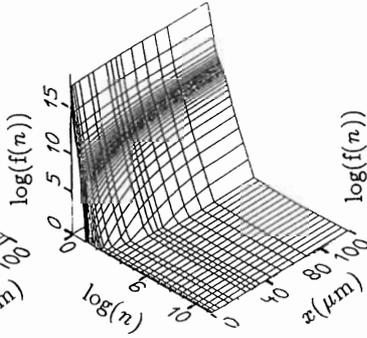


Figure 2: Size distribution function as a function of  $\log(n)$  and  $x$  after 1100°C/16h + 650°C/16h anneal.

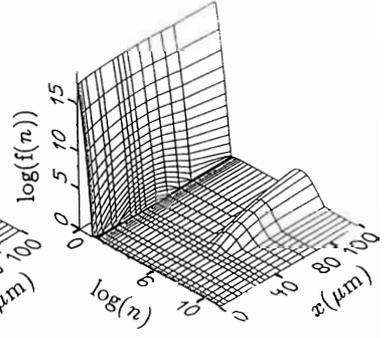


Figure 3: Size distribution function as a function of  $\log(n)$  and  $x$  after 1100°C/16h + 650°C/16h + 1000°C/16h anneal.

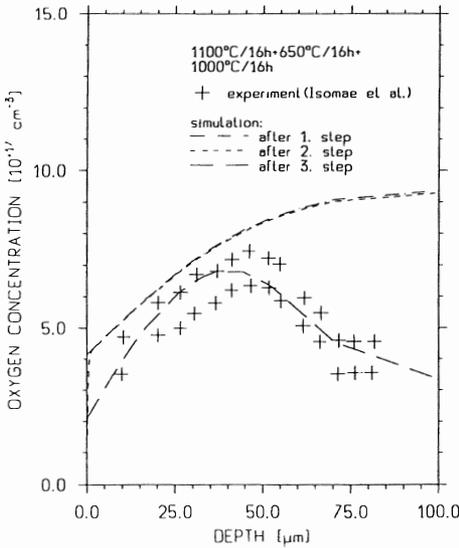


Figure 4: Depth profile of interstitial oxygen concentration in the wafer subjected to three-step annealing (1100°C/16h+650°C/16h+1000°C/16h)

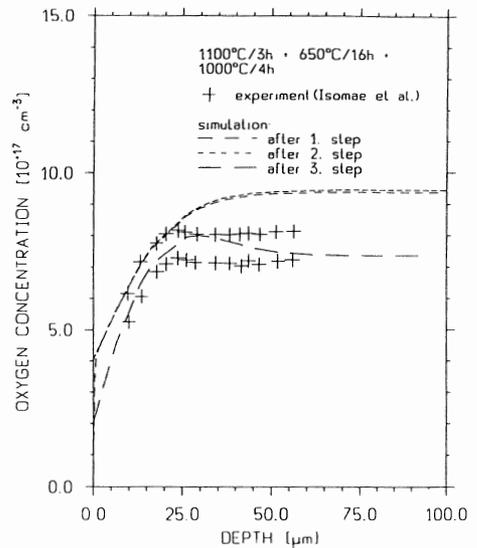


Figure 5: Depth profile of interstitial oxygen concentration in the wafer subjected to three-step annealing (1100°C/3h+650°C/16h+ 1000°C/4h)