Quasi Steady State Approximation of Interstitial Diffusion During Oxidation of Silicon

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ABSTRACT

To calculate the two dimensional dopant profiles near oxidizing boundaries it is vital to have accurate interstitial profiles. The quasi steady state approximation for the interstitials is described and the time to achieve quasi steady state is estimated. The approximation is compared to a numerical solution to examine its accuracy.

It is well established that oxidation of silicon injects silicon interstitials into the bulk. This excess of interstitials drastically effects the diffusivity of dopants in silicon. To accurately predict two dimensional impurity profiles, the two dimensional nature of the interstitials must be accurately solved.

Several authors [1,2] have proposed solutions for the interstitials under steady state conditions. The interstitials obey the following relationship:

$$\frac{\partial C_I}{\partial t} = \nabla(D_I \nabla C_I) - K_r(C_I - C_I^*)$$

Subject to the following boundary condition at the oxidizing interface:

$$D_I \frac{\partial C_I}{\partial y} - K_I(C_I - C_I^*) = g_I(x,t)$$

where C_I is the interstitial concentration, D_I is the interstitial diffusivity, K_r is the bulk recombination constant, K_I is the surface recombination velocity, and g_I is the generation as a function of lateral distance and time. The solutions of Hamasaki to these equations assumed a perfect sink at the pad oxide, and the solutions of Shin and Kim assumed the vertical profile was an exponential. A new solution has been calculated which assumes a finite surface recombination velocity and solves for the vertical behavior of the interstitials. The solution assumes only that a quasi steady state exists and that symmetry conditions may be applied to the left and right mask edge. A picture of the solution is shown in figure 1. The values plotted are contours of the excess interstitial concentration normalized by the maximum excess interstitial concentration. The maximum excess occurs under the center of the oxidizing stripe, which is at the right hand side of figure 1. The wafer is being oxidized between 10.0 and 60.0 microns and there is a pad oxide between 0.0 and 10.0 microns. The figure shows the sharp curvature of the interstitial profile near the edge of the oxidizing stripe, which is due to the high surface recombination velocity.

The onset of quasi steady state is also estimated. These estimates provide realistic values at which the quasi steady state approximation is valid. Hu [3] found one dimensional solutions of the interstitial concentration at the surface of an oxidizing interface as a function of time. The quasi steady state solution depends on the maximum surface concentration reaching a value that depends on only the generation rate, the diffusivity, the bulk recombination, and the surface recombination. The surface concentration eventually reaches

$$g_I(t)/\sqrt{D_I * K_r + K_I}$$

at the middle of the oxidizing stripe. By calculating how long it would take Hu's solution of the surface concentration to reach 99% of the expression above, an estimate can be obtained of the time to reach quasi steady state. Figure 2 shows the time to reach steady state as a function of the bulk recombination time.

Both the times have been scaled by K_I^2/D_I. It takes much longer to come to quasi steady state in the case when the bulk recombination is weak. Unfortunately, this is the typical case. For a diffusion length of 25.0 microns, a diffusivity of $5.0 * 10^{-7} cm^2/s$ and a surface recombination velocity of $1.0 * 10^{-4} cm/s$, the time to reach steady state is 165 minutes. By using a two dimensional simulator such as SUPREM IV, the solution values after each time step can be examined to determine the onset of quasi steady state. It can be seen from this plot that the agreement between the estimated time to quasi steady state and the occurrence of the steady state as calculated from SUPREM IV is very good.

In summary, a two dimensional quasi steady state solution was calculated using a finite surface recombination velocity. The time to reach the onset of quasi steady state is estimated and compared to numerical simulation results.

References

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2. Y-S. Shin and C-K. Kim, "The Effect of Si-SiO_2 Interface on the Excess Point Defect Distribution in Silicon," in *Semiconductor Processing, ASTM 850*, p. 283, 1984.
3. S.M. Hu, "Kinetics of Interstitial Supersaturation and Enhanced Diffusion in Short-Time/Low Temperature Oxidation of Silicon," *Journal of Applied Physics* , vol. 57, p. 45279, 1985.

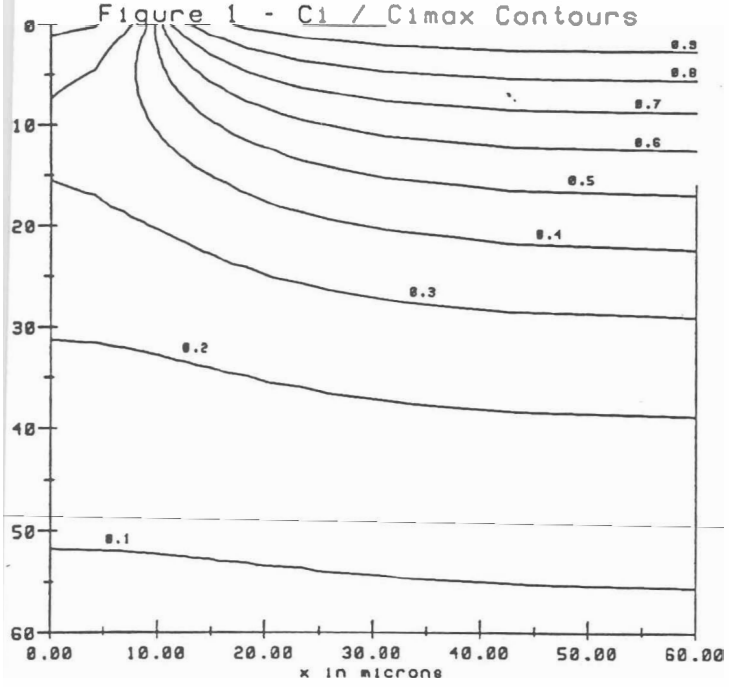

Figure 1 - Interstitial Contours from the Quasi Steady State Approximation under a Oxidizing Surface

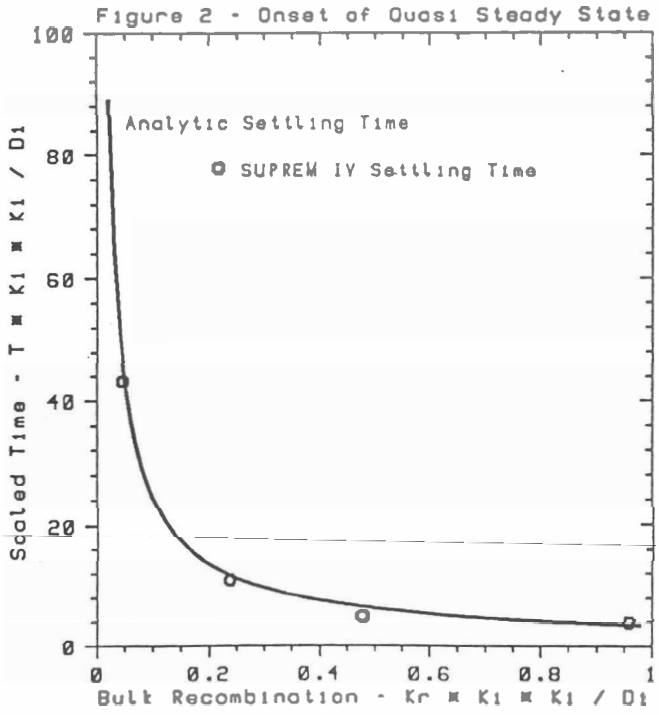

Figure 2 - Time to reach the onset of quasi steady state from analytic estimates and numerical solution values