Feature-Scale Modeling and Characterization of Oxide APCVD

Thye-Lai Tung
Intel Corporation, Santa Clara, CA 95052, USA

Summary

A model based on quasi-static diffusion has been developed to model oxide deposition at the feature scale for O_2/SiH_4-based Atmospheric Pressure Chemical Vapor Deposition (APCVD). This program employs a unique boundary layer generation that empirically describes the behavior of the boundary layer in gas flow. The program has been optimized to fit experimental data. An unusual trend in the experimental data may be explained by transitional flow in narrow trenches.

Formulation

Flow transport always plays a critical role in bringing reactants to the wafers in a CVD system. Because of the short scattering lengths involved in APCVD, the transport at the feature scale may still be determined by scattering-dominated flow and diffusion. In a typical O_2/SiH_4-based APCVD, there is an oversupply of O_2 with respect to SiH_4 (silane). Hence the reaction process is controlled by SiH_4 (or an intermediate species). If we ignore the role of flow for the time being and look at diffusion, we note that a quasi-static single-species diffusion model can be used to describe the oxide deposition process. The specifications for such a system are given by

- $C = C_0$ at the free boundary, Γ_f
- $D\ \delta C/\delta n = k_s C$ at the reacting surface, Γ_s
- $\nabla^2 C = 0$ in the domain, Ω

where C is the concentration of the active species, C_0 the concentration at the free boundary, D the diffusion coefficient, and k_s the reaction rate. The characteristic length of the system is defined by D/k_s.

Next, we relate the flow dynamics to the free boundary of the simulation domain. In a moving-belt APCVD system that we consider in this paper, the gas flows over a wafer surface in different directions as the wafer moves. On an average sense, the flow has a zero net velocity. The flow introduces mixing that increases the apparent diffusivity. Further away from the surface, the increased flow enhances the apparent diffusivity. In our simplification, there is a stagnant layer above the surface that has a fixed diffusivity. For the region beyond the free boundary Γ_f, the diffusivity is so high that the concentration is kept constant there.

APCVD models have been presented before [1,2,3], but the formulation of the boundary layer has not been adequately treated in them. Typically the free boundary is assumed to be flat. The inadequacy of this assumption is illustrated in Fig. 1. A better approach is to make the boundary layer conformal. Moreover it should be thicker over a trench and thinner over a line, as one would typically expect from a gas-flow behavior. The equi-potential contour technique has all these desirable properties.

In this method, we treat the feature boundary as an electrode and set its potential Φ to be zero. Far above the surface, we constraint that $\partial\Phi/\partial y$ be a constant. The free boundary we seek is given by the equi-potential contour of a specific $\Phi=\Phi_f$. As shown in Fig. 2, the boundary layer is thinner over a line and thicker over a trench.

Calculations for both diffusion and potential contours are done with the boundary-integral equation method.

Characterization and Observation

The model has been fitted to experimental data for trenches of different widths on the two adjustable parameters: the characteristic length (D/k_s) and the equi-potential value Φ_f. The experimental and simulation data are shown in Fig. 3. Simulation matches especially well for wide trenches, but it deviates in narrow ones with large overhangs at the sidewalls and reduced bottom thicknesses. The simulation behavior follows our intuition in that, as the trench opening is more constricted, the worse the overhang and thinning should be. However the experimental data show a different systematic trend: as the trench width gets smaller, the overhang actually improves and the bottom thinning is less servere. The narrow-trench data can be fitted quite well if we double the diffusivity, as shown in Fig. 4. Among a few probable explanations, the one that should be considered seriously is that transitional flow [4] is the dominant mode of transport within the narrow trenches. The small scattering probability produces a higher apparent diffusivity.

Acknowledgments

The author would like to thank L. Uzelac from Intel Portland for supplying the experimental data and P. Leon for discussions on boundary layer issues.

References

[1] "Deposition Profile Simulation Using the Direct Simulation Monte Carlo Method," M. Ikegawa and J. Kobayashi, J. Electrochem. Soc., Vol 136, p. 2982.

[2] "Simulation of CVD Process by Boundary Integral Technique," H. J. Oh, S. W. Rhee, and I. S. Kang, J. Electrochem. Soc., vol 139, p. 1714.

[3] "Topography Simulation of APCVD," E. Suzuki, and K. Ueno,", Extended Abstract for the 52nd Autumn Meeting, 1991, Jap. Soc. Appl. Phy., p. 635 (in Japanese).

[4] "Silicon Processing for the VLSI Era," S. Wolf and R. Tauber, Lattice Press, 1986, p. 76.

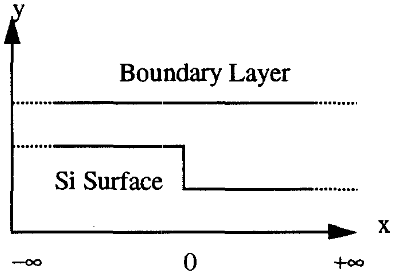

Fig. 1. Poor flat-layer approximation on a step: the right side is always thicker than the left even far away from x=0.

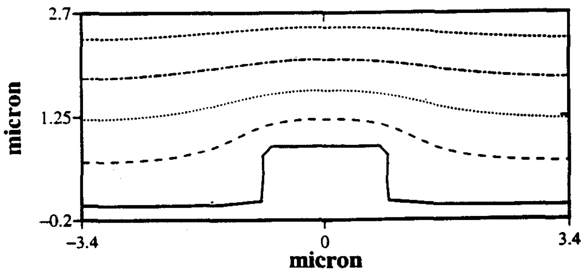

Fig. 2. Equi-potential contours for a line. The contours crowds over the line and spread out over the trenches.

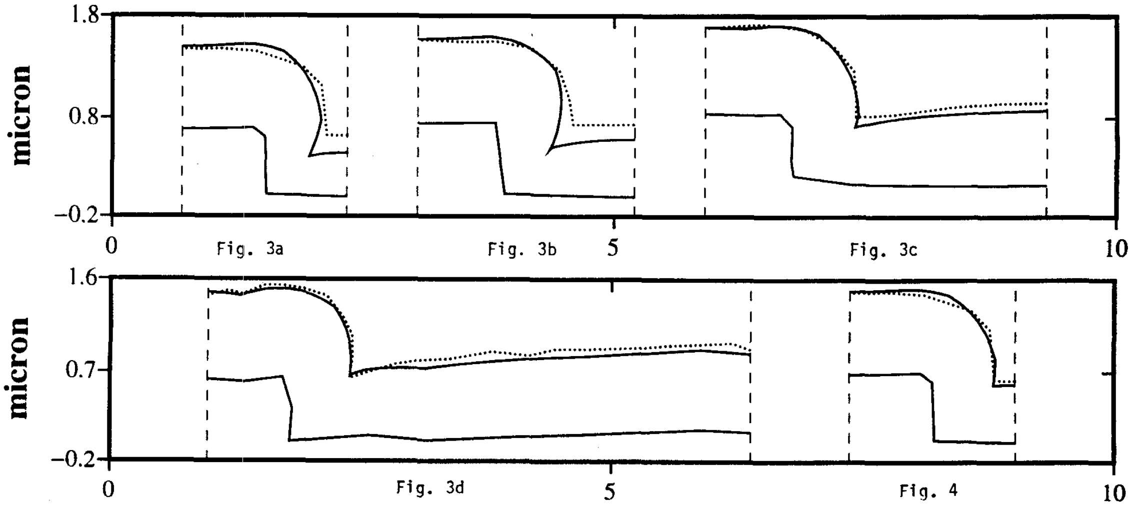

Fig. 3a-3d. Experimental data (dotted lines) and simulation results (solid lines) for trenches with different openings. Only half sides are shown.

Fig. 4. Doubling the diffusivity improves the simulation result for the narrow trench shown in Fig. 3a.