

An Improved Calibration Methodology for Modeling Advanced Isolation Technologies

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Abstract

An improved calibration methodology for simulating advanced isolation technologies using SUPREM-IV is presented. Based on the experimental determination of the material properties of silicon nitride, an improved parameter set for the stress dependent oxidation models is derived. The calculated substrate stress using this new parameter set is compared with micro-raman spectroscopy stress measurements to validate the calibration methodology.

Introduction

With the scaling of IC technologies to deep-submicron dimensions, the inter-device isolation becomes increasingly critical. Local Oxidation of Silicon (LOCOS) is still the dominant isolation technology due to its process simplicity and superior isolation characteristics. However, pushing the scalability limits of LOCOS technology has become virtually impossible without relying on accurate process simulators. Accurate simulations and design for manufacturability require knowledge of the material properties of the layers involved. Typically, these parameters are determined by fitting complete isolation structures after field oxidation using stress dependent oxidation models where SiO_2 and Si_3N_4 are treated as non-linear viscous and linear viscous materials, respectively. While the experimental boundary shapes correlate well with SUPREM-IV simulations over a wide temperature range, the absolute values of the model parameters are still uncertain. In this paper, we determine experimentally the viscosity of thin LPCVD silicon nitride films as a function of temperature and derive the other model parameters based on these experimental data. A comparison of the stress levels in the substrate with those obtained by micro-raman spectroscopy [1] is presented as well and is used to validate the calibration procedure.

Experimental results and calibration methodology

LPCVD silicon nitride films were deposited on silicon substrates at a temperature of 780 °C. After deposition, the film thickness was recorded. Subsequently, the wafers were annealed in argon and steam at 900, 1000 or 1100 °C for 60 minutes. The length of the anneal was chosen so that it would be of the order of the film relaxation time. The initial film thickness was about 140 nm. After the 900 °C, 1000 °C and 1100 °C anneals, a decrease in film thickness was observed (figure 1). The film stress, measured at room temperature using a wafer curvature measurement set-up, was found to increase with anneal temperature from 1070 MPa to 1180

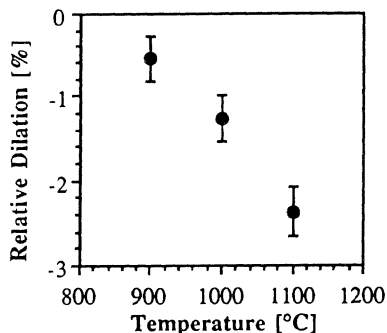


Figure 1: Relative change in Si₃N₄ thickness with anneal temperature

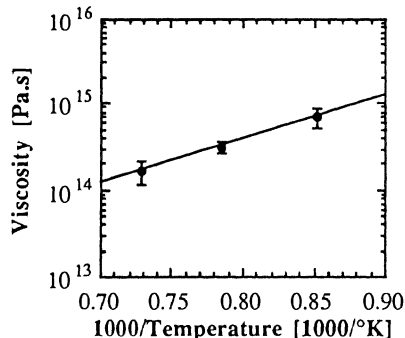


Figure 2: Arrhenius plot of the experimental Si₃N₄ viscosity

MPa. This increase is believed to be due to film densification [2]. The high stresses observed in as-deposited silicon nitride films are primarily due to non-equilibrium deposition conditions and to a lesser extent to the thermal mismatch between the film and the substrate [2]. A very similar behavior is observed for samples annealed in steam, indicating that the annealing ambient does not affect the densification or the viscous flow behavior. If we assume that film shrinkage occurs in an isotropic manner, the viscosity of the silicon nitride as a function of temperature can be approximated using a simple linear viscous model described by $-(\Delta d/\Delta t) = \sigma/\eta$, where $\Delta d/\Delta t$ is the magnitude of the film shrinkage rate, σ is the film stress and η is the nitride viscosity. The experimental results for the viscosity of silicon nitride estimated using this model are summarized in figure 2. The results fit an Arrhenius expression extremely well. It is worthwhile noting that the Si₃N₄ viscosity extracted by this method is independent of any fits to experimental LOCOS boundary shapes and forms the foundation for the calibration strategy to be discussed in the next section.

In SUPREM-IV, high temperature oxide deformation is described by a non-linear viscous flow model with stress dependent oxidation parameters. This appears to give excellent fits to oxide thinning data on convex and concave structures of different radii for temperatures between 900 °C and 1100 °C [3,4]. Silicon nitride is treated as a purely viscous material, an approximation we will show to be valid. The viscosity, oxidant diffusivity and reaction rate have the following stress dependency:

$$\eta = \eta_0 \frac{\tau V_c/kT}{\sinh \tau V_c/kT} \quad (1), \quad D = D_0 e^{-PV_d/kT} \quad (2), \quad k_s = k_{s0} e^{-\sigma_n V_r/kT} \quad (3),$$

where τ is the shear stress, P the hydrostatic pressure and σ_n the normal stress. V_c , V_d and V_r are the activation volumes for critical stress, stress-dependent diffusion, and stress-dependent reaction rate respectively. This leaves us with a set of five fitting parameters to model any isolation boundary shape: η_0 the low stress viscosity, which must be specified for both nitride and oxide and the three activation volumes V_c , V_d and V_r . These five parameters form a quintuplet and cannot be chosen independently. The quintuplet is not unique in that identical boundary shape solutions can be obtained when η_0 is multiplied and V_c , V_d and V_r are divided by a constant. In the previous section, we have experimentally determined the viscosity of silicon nitride and will scale the default SUPREM-IV quintuplet according to the ratio of the original fitted values [5] and the experimental values of the Si₃N₄ viscosity. In order to verify the quintuplet scalability, simple LOCOS structures with 10 nm pad-oxide and 100 nm silicon nitride were simulated using the two parameter sets which are presented in table 1. It is clear from figure 3 that there is no significant difference in the boundary shapes when the model parameters are scaled appropriately. When analyzing the simulated stress

levels in the substrate however, there is a distinct difference between the two quintuplets (figure 4). The ratio between the stress components, calculated with the two different quintuplets is approximately equal to the nitride viscosity scale factor, irrespective of the stress component and the temperature.

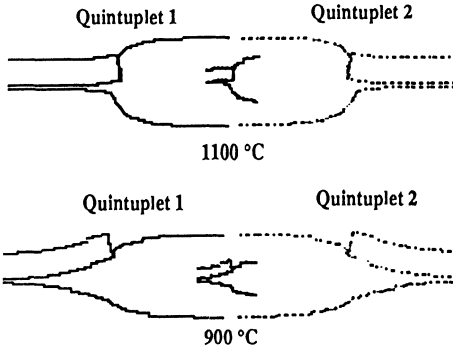


Figure 3: SUPREM-IV boundary shapes for the two quintuplets

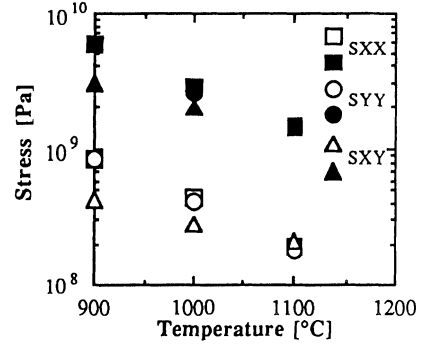


Figure 4: Plot of maximum magnitude of the different stress components along Si-SiO₂ interface as a function of temperature (Open: Quintuplet 1, Solid: Quintuplet 2).

Quintuplet	Parameter	900 °C	1000 °C	1100 °C
1 (default)	$\eta_{\text{nitride}}[\text{Pa.s}]$	1.15E14	4.7E13	2.3E13
	$\eta_{\text{oxide}}[\text{Pa.s}]$	2.5E14	2.8E13	4.5E12
	$V_c [\text{\AA}^3]$	300	522	1000
	$V_d [\text{\AA}^3]$	65	65	65
	$V_r [\text{\AA}^3]$	12.5	12.5	12.5
2 (scaled)	$\eta_{\text{nitride}}[\text{Pa.s}]$	7.1E14	3.12E14	1.67E14
	$\eta_{\text{oxide}}[\text{Pa.s}]$	1.67E15	1.87E14	3.01E13
	$V_c [\text{\AA}^3]$	44.8	78	149
	$V_d [\text{\AA}^3]$	9.7	9.7	9.7
	$V_r [\text{\AA}^3]$	1.9	1.9	1.9

TABLE I: Overview of the two parameter sets used in the simulations.

the average stress σ_{XX} over a depth of 0.3 μm away from the bird's beak region from the SUPREM-IV simulations yielded an average stress σ_{XX} of 0.02 GPa when using quintuplet 1 to simulate the structure and 0.14 GPa when using the experimentally derived quintuplet. Clearly, the parameter set derived from the experimental nitride viscosity gives the best agreement and it can probably be improved by a more careful interpretation of the micro-raman results.

Micro-Raman spectroscopy is one of the few techniques that allows the direct measurement of stress levels in the silicon substrate with small enough resolution so that an estimate of the stresses can be made [1,6]. In order to compare our results with those obtained by micro-raman, the same LOCOS structures De Wolf et al. [1] used in their experiments were simulated. Micro-raman spectroscopy measures the average stress over a depth of about 0.3 μm [6]. On wide Si₃N₄ lines (> 4 μm) away from the bird's beak, a tensile stress σ_{XX} of 0.52 GPa was estimated from the raman shift measurements for this particular LOCOS structure[1]. Calculating

Conclusion

We have shown that the fitting parameters for the oxidation models in SUPREM form a quintuplet that can be scaled and yield identical boundary shapes of LOCOS structures for many different parameter sets. The calculated stresses in the substrate however do not remain constant but scale as well. This has serious implications when designing new isolation structures. Based on the scalability information and the experimentally extracted nitride viscosity, we designed a strategy that allows for an improved calibration of SUPREM-IV.

References

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