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Quantitative 2D Stress Dependent Oxidation with Viscoelastic Model

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Abstract

For the proper modelling of the stress in two-dimensional local oxidation, oxide and nitride have to be considered as viscoelastic materials. This paper presents an original calibration of the viscoelastic model. It is based on the effect of stresses on the grown oxide thickness.

Viscoelastic treatment of thermal oxidation has the valuable advantage to take into account the mechanical properties of IC manufacturing materials in a large temperature range. Various models [1,2] have been introduced in the past, but their calibration just includes the oxide properties and neglects nitride modelling, or the oxide is assumed purely viscous [3]. In this paper, a viscoelastic oxidation model is compared to Kao's results and field oxide thickness reduction experiments. A self-consistent method is exposed which allows the coupled adjustment of oxide and nitride properties. The entire model is then applied to practical cases.

1. Numerical aspect

The 2D-oxidation model is implemented in the multilayer process simulator IMPACT 4 [4]. The stress dependent oxide motion is solved with a Gauss method, combined to an algorithm for profile and wavefront reduction of the mechanical matrix [5]. The benefits of this algorithm is obvious, compared to CG [6], at high temperature kinetics where oxide behaves like an incompressible viscous material giving a near undefined expression to the strain-stress relation. Oxidation simulations at 800 ^{o}C and 1100 ^{o}C with respective oxide viscosity equal to 10^{16} and 10^{12} poises were treated by both solvers : the CPU time is reduced by a factor 3 at 800 ^{o}C and by a factor 10 at 1100 ^{o}C.

2. Calibration

The stress dependence of oxide diffusivity and reaction rate constant is introduced according to Kao and Sutardja [7,8]. The corresponding activation volumes are V_d and V_k. Non-Newtonian behavior are assumed for oxide and nitride. The Eyring's plasticity formula [8] is used and requires the determination of the low stress viscosity and plasticity activation volume, respectively V_o, V_{po} for oxide and V_n, V_{pn} for nitride.

The calibration of Kao's experiments starts at low temperature with arbitrary value of V_d. Concave structure with large radii provides the adjustment of V_0 while V_{po} is obtained for small radii. V_k is defined by comparison with the convexe structure results. The influence of diffusivity lowering on the oxide growth, V_d, is deduced through LOCOS thinning with large nitride mask aperture. V_d is modified and the previous procedure is repeated. Table 1 presents the best oxide parameters. The simulated concave structure is given in figure 1. Figure 2 shows the agreement with Kao's data at 900°C and 1000°C.

Since specific direct experiment for nitride does not exist, the modelling is achieved by simulations of the local oxide thinning phenomenon in structures with narrow nitride mask opening. They reveal that V_{pn} has rather no influence in oxide thickness reduction for thick nitride, V_n is the dominant parameter. On the contrary, V_{pn} can be deduced from thin nitride experiments where its effect is pronounced (see figure 3). Numerous iterations are necessary to define the nitride properties.

3. Application to practical cases:

Two real examples were chosen in literature to demonstrate the validity of the modelling. A LOCOS structure [9] was simulated, in steam ambient, at 1000°C to grow 0.47 µm thick field oxide. The oxide thickness variation with decreasing nitride mask opening is presented in figure 4 and is compared to experiment. Figure 5 corresponds to the growth of a ROI structure [10] in the case of a very small nitride length. For these examples, the set of parameters is : V_d $=75$ A^3, $V_k=15$ A^3, $V_0=2.10^{14}$poises, $V_{po}=425$ A^3, $V_n=5.10^{15}$ poises, $V_{pn} = 170$ A^3 and good agreement is obtained that validates the global approach.

4. Conclusions

A new method for the calibration of the viscoelastic oxidation model has been developped. Its procedure couples together the adjustment of Kao's experiments with the fitting of the oxide thinning phenomenon in the LOCOS structure. Consequently, the respective influence of oxide and nitride in the generation of stresses are more accurately modeled. The extension of the method to other IC materials is desirable to study advanced isolation structures.

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Temperature (°C)	VD (Å^3)	VK (Å^3)	V_0 (poises)	V_{np} (Å^3)
800	75	15	9.10^{15}	300
900			6.10^{15}	390
1000			2.10^{14}	425
1100			4.10^{13}	1000

Table 1: Best parameters for KAO's data.

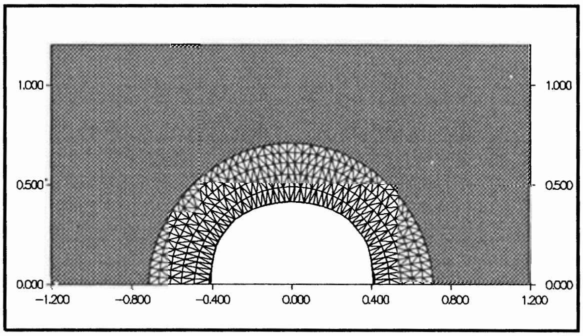

Figure 1 : Simulated concave structure.

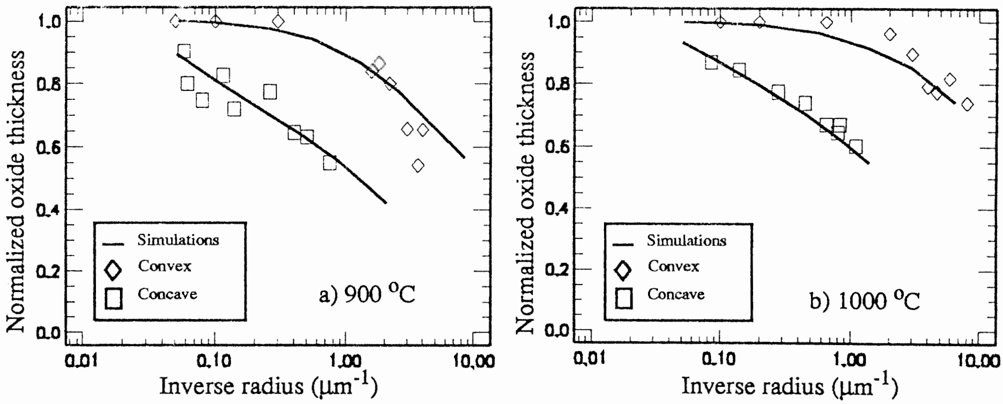

Figure 2 : Adjustment to KAO's data at a) 900 °C and b) 1000 °C.

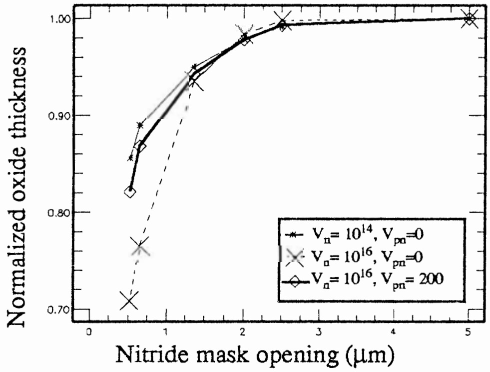

Figure 3 : Effect of nitride properties on the oxide thickness reduction in case of thin film (0.09 µm)

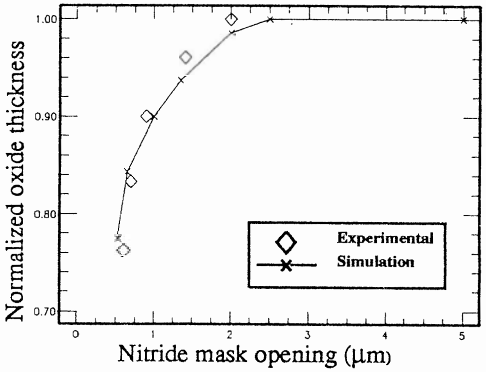

Figure 4 : Effect of nitride properties on the oxide thickness reduction in case of thin film (0.09 µm)

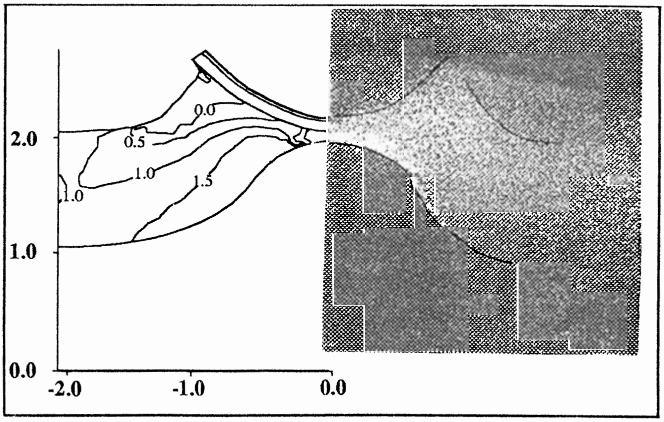

Figure 5 : Recessed oxide structure at 1000 °C with pad-SiO_2 (20 nm)/ Si_3N_4 (120 nm). The final field oxide is 1. µm. Simulated pressure distribution is given. Stress units are 100 MPa.