Mechanical Stress Modeling for Silicon Fabrication Processes

Hernan A. Rueda[1], Stephen Cea[2] and Mark E. Law[1]
1 Department of Electrical and Computer Engineering, University of Florida
Gainesville, FL 32608-6200 USA
har@tec.ufl.edu law@tec.ufl.edu
2 Intel Corporation, Technology CAD Department, RA1-305, 5200 NE Elam Young Pkwy.
Hillsboro, OR 97124

Abstract-Two finite element methods are implemented to investigate localized mechanical stress fields generated during multiple stages of silicon IC fabrication. The boundary loading method (BL) uses the oxide interface stresses as a boundary condition for the substrate solution. In the fully integrated method (FI), the strains in substrate are calculated along with the oxide stress computation. Both of the methods can be used to couple stresses generated by oxidation volume expansion to strains present from other sources such as thermal expansion, dopants, and intrinsic film stresses. They are then evaluated on computational intensiveness and in stress solution variation. It is found that the BL method computes nearly the same oxide solution as the FI method and the oxide solution corresponds very well in the oxide and surface films for a LOCOS process.

I. INTRODUCTION

Large localized mechanical stresses can result from various stages of the IC fabrication process [1]. To relieve these stresses, the silicon substrate will yield and generate dislocations [2]. Dislocations generally degrade device performance, especially when present in critical regions for device operation [3]. Also the strain itself can affect device behavior by altering device parameters such as the energy bandgap [4] and carrier mobility. Therefore, it is important to build a better understanding of which are the critical stages in the process sequence that lead to larger stress magnitudes and in what regions these stresses are localized to.

The finite element method has been used extensively to analyze stress problems for many different applications [5-9]. Two different finite-element based methods have been developed to integrate oxidation volume expansion generated stress to other multiple sources of strain present in silicon process technology. The strain sources integrated with the oxidation-induced stresses include boron dopant-induced strain, thermal and intrinsic film induced strain. The two methods are then evaluated by computational intensiveness and in solution variation.

II. STRESS INTEGRATION METHODS

A. Boundary Loading Method

The boundary loading method (BL) is separated into two steps (Fig. 1). In the first step, the nonlinear viscoelastic oxide flow is computed with silicon acting as a rigid body and the surface films modeled as viscoelastic materials [8]. This assumption allows for a more efficient technique for solving the oxide growth, since only the surface films are iterated over in the nonlinear stress dependent oxidation solution.

The forces generated from the oxide growth acting on the silicon interface are saved and then used to drive the second step. These forces are input as boundary loading forces for calculation of the substrate stress. Therefore the second step becomes a boundary value problem. Silicon is modeled as an isotropic elastic material. Strain may be exerted from dopants and defects in the silicon substrate and also is included as a stress source in the second step of this method.

B. Fully-Integrated Method

The second method developed (FI) is similar to the finite element method implemented by Senez [9]. In this method, the stresses in the silicon are solved for during the oxide flow calculation from multiple sources simultaneously (Fig. 2). This technique becomes very computationally intensive because the silicon elements are also assembled into the nonlinear oxidation equation. This usually results in an order of magnitude more elements included to adequately define the substrate and reduce the effect of the reflecting boundaries on the solution. Therefore, the FI method's Newton iteration involves a much larger matrix than the BL method and results in much slower performance overall.

As in the previously described method, the surface films are modeled as viscoelastic bodies and the silicon substrate is modeled as an isotropic elastic material. The boundary condition at the oxidant reaction interface is similar to the polysilicon boundary condition: the silicon flows and is consumed. Additionally, strain from dopants and defects may be exerted in the silicon substrate and also is included as a stress source in this method.

III. STRAIN SOURCES INCLUDED

Other strain sources can be integrated with the oxidation-induced strains using either of the previously described methods. Deposited films exert stress in the substrate due to

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an intrinsic or thermal expansion mismatch stress [1]. The highest magnitude stress due to these mechanisms generally lies at the film edges or in nonplanar regions. The intrinsic stress is included as a biaxial stress oriented tangentially along the interface on which it is grown or deposited. The thermal expansion stress is oriented as a hydrostatic stress.

Boron dopant-induced strain has also been included as a stress source in the substrate. Each implanted boron atom is assumed to settle substitutionally. Due to its smaller atomic radius, each boron atom exerts a local tensile strain of 0.014 angstroms per percentage of boron in the crystal lattice [10]. This strain is oriented as a hydrostatic strain.

IV. COMPARISON AND RESULTS

After running a matrix of LOCOS simulations, it is found that both methods agree very well in the computed oxide growth shapes. The Bird's Beak heights and lengths differ only slightly. Therefore, the rigid body assumption does not affect the outcome for the oxide growth very much. To compare the stress fields generated between the two methods, the maximum and tensile and compressive hydrostatic pressure was analyzed. It is found that the fully-integrated method computes higher compressive stress magnitudes for the substrate.

The boundary loading method is much less computationally intensive (Table 1) and therefore can be implemented for both two- and three- dimensional stress computation (Fig. 3-5). For application in three dimensions, the fully-integrated method needs to be optimized.

V. CONCLUSION

Strain calculations have been extended to integrate contributions from multiple sources simultaneously (Fig. 6). Two separate methods have been developed to handle this. The two methods analyzed agree qualitatively on the nature of the stress (tensile or compressive) solution. However they do differ on the magnitude of compressive stresses produced, especially at the Bird's Beak. Experiments and further analysis are needed to verify and calibrate either system. The fully-integrated method for computing stresses also needs to be optimized for three-dimensional application.

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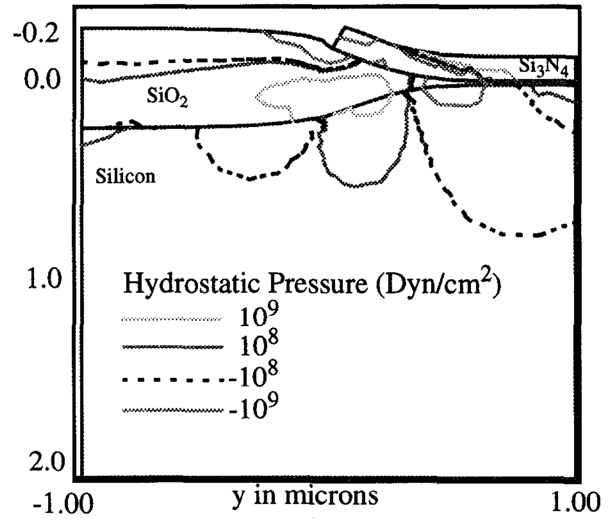

Figure 1. 2D Stress field solution computed by the boundary loading method for an 80 min 1000C wet LOCOS process with 10 nm pad oxide and 150 nm nitride thickness.

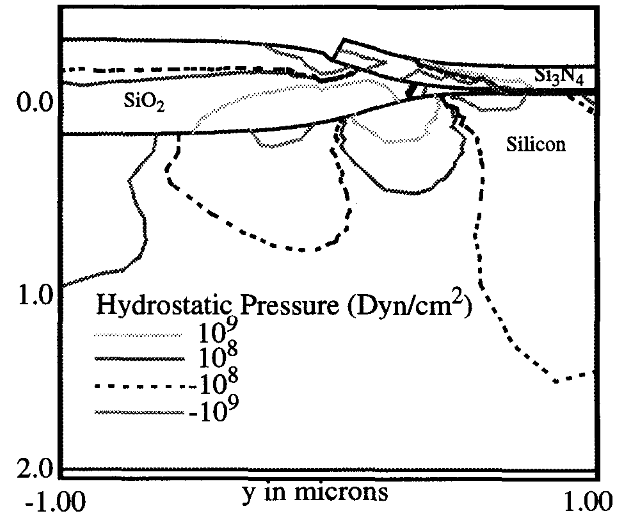

Figure 2. 2D Stress field solution computed by the fully integrated method for an 80 min 1000C wet LOCOS process with 10 nm pad oxide and 150 nm nitride thickness.

TABLE I-Comparison of each method for the 2D LOCOS process.

Method	CPU Time (sec)	Bird's Beak Height (um)	Max. Comp. Pressure (D/cm^2)	Max. Tensile Pressure (D/cm^2)
BL	501	0.335	1.5e9	-1.8e9
FI	1136	0.316	4.0e9	-1.6e9

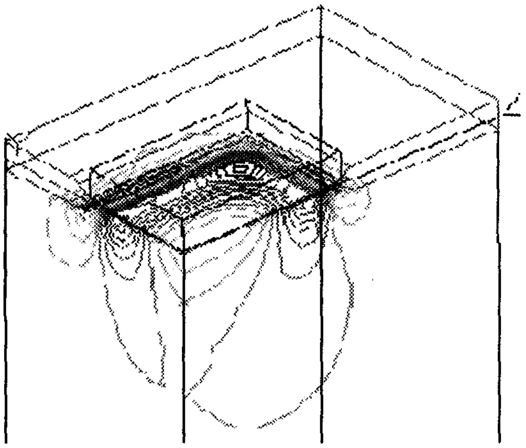

Figure 3. Three-D Substrate Stress distribution computed by the Boundary Loading Method for 1000° C 15 min LOCOS corner structure with 10nm pad ox and 150nm nitride thickness.

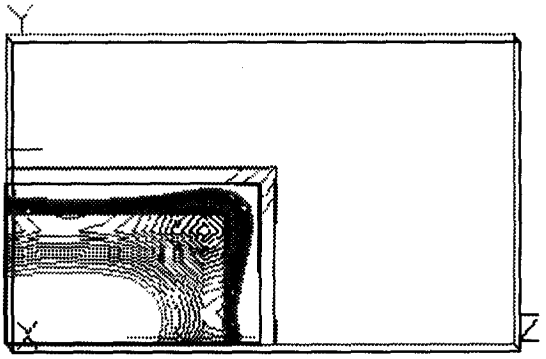

Figure 4. Isolines indicate the tensile stresses computed in the substrate are at a maximum just under the nitride corner.

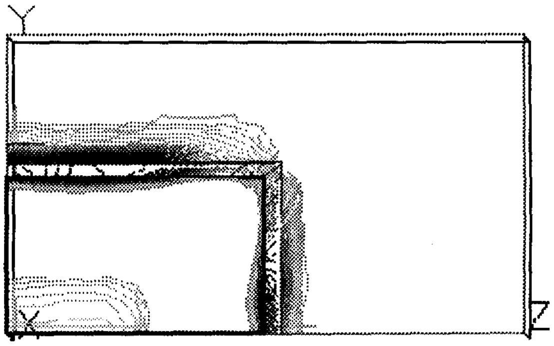

Figure 4. Compressive stresses computed in the substrate are at a minimum just under the nitride corner due to the lifting of the nitride mask by the increased height of the bird's beak.

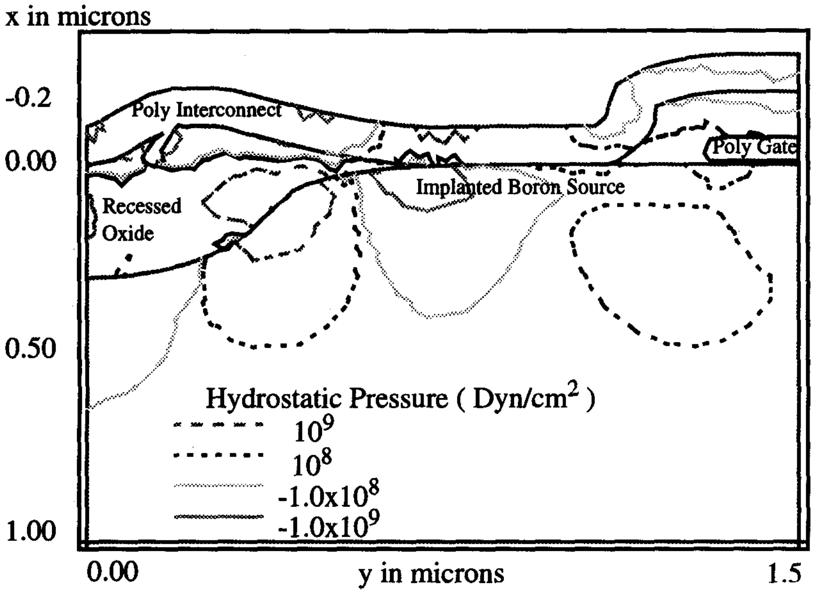

Figure 6. Example of integrating various strain sources' stress contributions for a MOS device process computed by the fully-integrated method. The stresses due to the recess oxidation dominate the region. The compressive region due to the poly gate edge is split by the tensile strain of boron doped source region.