3D Simulation of Oxidation Induced Stress Using Cartesian Meshes with Adaptive Refinement

The formation of isolation trenches is one of the key process steps used in power device fabrication. Also the intensive scaling of modern semiconductor devices requires significant stress engineering to enhance carrier mobilities and avoid extended defect formation. Simulation results from complex 3D trench and lateral isolation structures are presented together with the inbuilt oxidation induced mechanical stress in the grown oxides. Fast transition of compressive to tensile stresses has been obtained for concave-convex surfaces with internal hydrostatic pressures ranging from 0.04 to –0.04 N/μm^2 .

A previous publication [1] introduced a new simulation framework (VICTORY PROCESS, Silvaco's 3D TCAD tool) based on using Cartesian meshes with adaptive refinement. Unlike unstructured tetrahedral meshes, this approach makes use of the level set method on fixed Cartesian meshes and does not involve re-meshing algorithms that represent a major obstacle in modelling 3D processes. VICTORY PROCESS also uses finite difference numerical schemes to solve the oxidation modelling equations. The implementation of general-type boundary conditions at arbitrary implicit interfaces and the approximation of the equations at the interface between fine and coarse Cartesian meshes are major milestones. Novel, in-house finite-difference schemes were developed and successfully implemented in a commercial simulation framework to overcome these issues. This paper demonstrates the capability and versatility of the Cartesian framework to simulate and analyse oxidation-induced stress.

To quantify the accuracy of the novel numerical schemes, the stress distribution produced by 3D VICTORY PROCESS was compared with results from ATHENA (Silvaco's 2D TCAD tool based on SUPREM IV) as seen in Figure 1. Both tools used an incompressible viscous model for oxide and nitride to simulate the LOCOS (Local Oxidation of Silicon) process. Figure 1 shows the mean of the diagonal stress components (pressure); p = -0.5*(Sxx+Syy). Good quantitative agreement between the two simulators has been obtained. As expected, the simulation reveals compressive pressure on the concave oxide/silicon interface and tensile pressure on the convex interface [2].

An important issue in stress engineering is to model the stress behavior when an interface changes its curvature in complex 3D corners. To investigate this question, a 3D LOCOS structure incorporating a 90º bend was simulated (Fig. 2), while maintaining the rheological material model and the process conditions from previous example. A cutplane parallel to the substrate, that captures the changes of the curvature of the silicon/oxide interface (concave - convex - concave) after oxidation, is shown in Fig. 2. Figure 3 shows the extracted 1D pressure contour along the interface. As a result of the curvature changes, the high compressive pressure rapidly decays and reverses to a peak of tensile pressure near the mask corner illustrated by the trough near 0.5μm. Figure 4 shows the oxidation of a vertical trench isolation structure. After 75 minutes

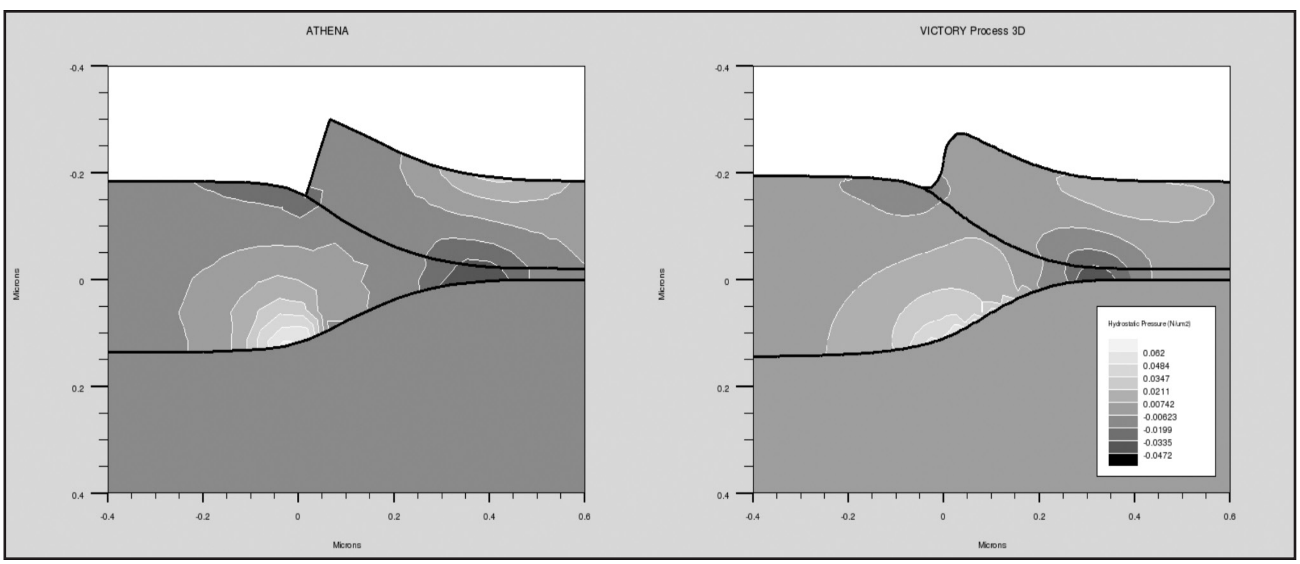

Fig. 1. Distribution of pressure resulted from simulation of LOCOS process (wet oxide, T = 1000C, time = 30 min). Left panel- ATHENA (2D SUPREM IV), right panel - VICTORY PROCESS (3D).

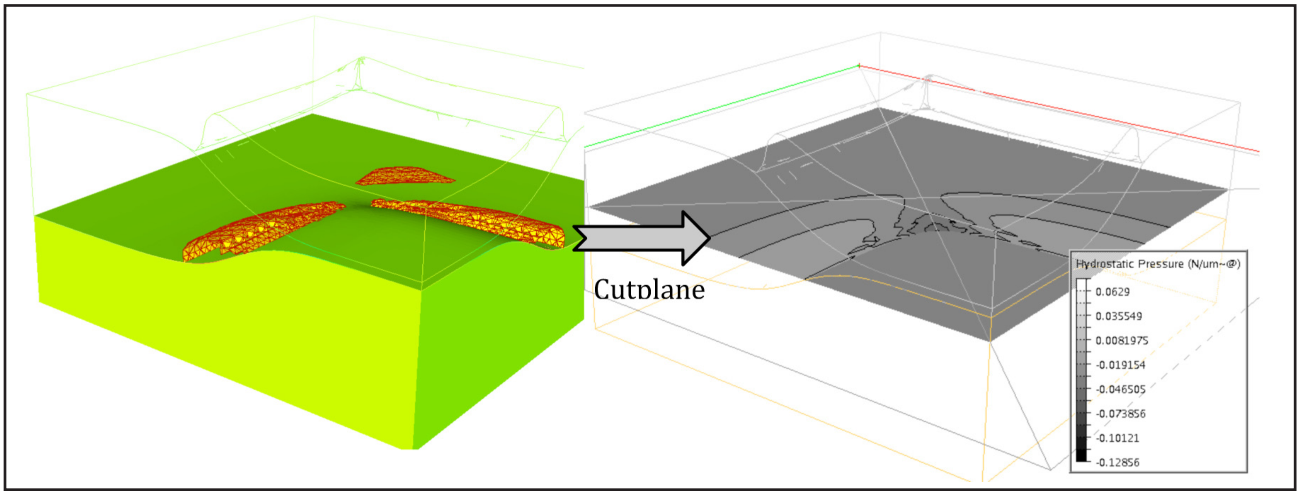

Fig. 2. 3D LOCOS modeling. Left panel shows 3D isosurfaces of 0.03N/μm² pressure contours and the cutplane extracted from that shows a 2D contour map of the pressure around the oxide/silicon corner.

wet oxidation at 1000ºC the data show the accumulation of compressive stress at the bottom Si/SiO2 edges while the tensile stresses are located in the upper Si/SiO2 edges and a complex mix at the edge corners.

In conclusion, this paper presents true 3D calculations of oxidation induced stress behaviour in complex 3D lateral and vertical trench isolation structures using quantified-state-of-the-art finite difference numerical methods and Cartesian meshes.

References

[1] V.Suvorov, A.Hossinger, Z.Djuric and N. Ljepojevic, A novel approach to three-dimensional semiconductor process simulation: Application to thermal oxidation, J. Comput. Electron. 5 291 (2006).

[2] Dah-Bin Kao, James P. McVittie, William D. and Krishna C. Saraswat, Two-dimensional thermal oxidation of silicon - II. Modeling stress effects in Wet Oxides. IEEE Transactions on Electron De-

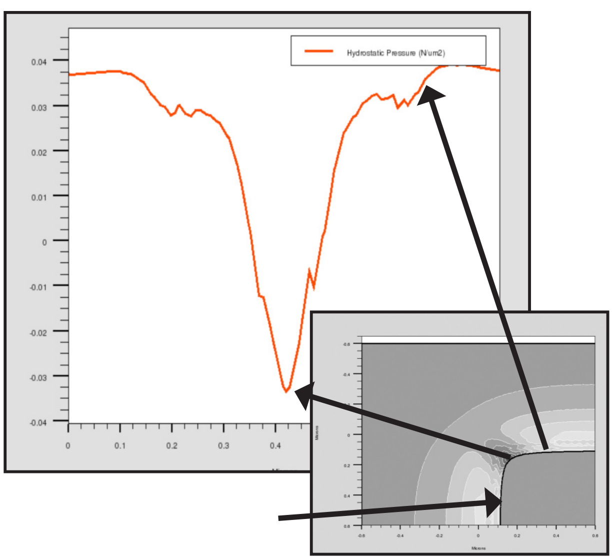

Fig. 3. Pressure distribution along the oxide/silicon interface. The compressive pressure in concave regions near the structure edges decays to tensile values towards the centre due to compensating curvatures.

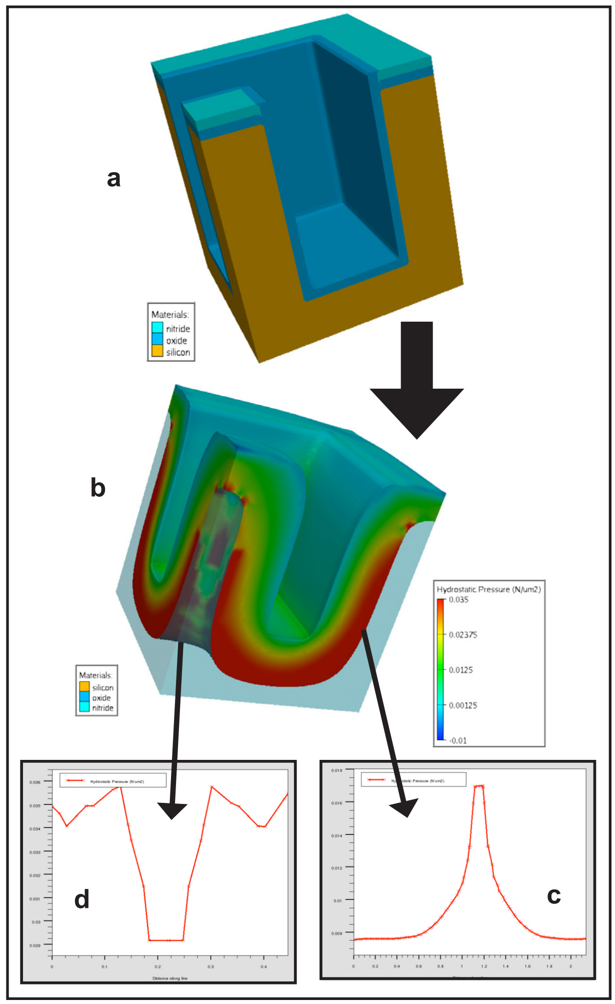

Fig. 4. 3D trench oxidation modeling. (a) shows the initial trench corner structure with thin oxide and nitride layer on the surface. (b) shows the structure evolution after 75 minutes of wet oxidation at 1000ºC. (c) shows the hydrostatic pressure contours along the outside bottom corner along the Si/SiO2 interface. (d) shows the hydrostatic pressure contours along the inside bottom corner along the Si/SiO2interface. Once again the fast transition between the tensile and compressive strain can be seen as the complex curvatures meet in the bottom edge corners.