3-D Simulation of Silicon Oxidation: Challenges, Progress and Results

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Abstract— **We report a new algorithm for solving the moving boundary problem of oxidation of silicon in 3D structures. The algorithm solves many of the boundary and mesh quality problems that makes 3D oxidation simulations challenging. Using this algorithm, we demonstrate that complicated 3D oxidation steps can be performed and results can be obtained in a reasonable amount of time.**

Keywords— Oxidation, moving boundary, LOCOS, trench oxidation

I. INTRODUCTION

Many modern device geometries (FinFETs, state of the art bulk and SOI CMOS devices) require simulation in three dimensions (3D), either simply because the device cannot be simulated in 2D due to its operation, or because the 3D effects are too large to ignore. Even though 3D implantation and diffusion simulations have been well established for some time, 3D oxidation simulations lagged behind.

It can be argued that for cutting edge CMOS devices there is not much need for performing 3D oxidation simulation, since they tend to use shallow trench isolation (STI) instead of local oxidation of silicon (LOCOS) for isolation and in such devices the gate oxide has been replaced by high-k dielectrics. However, for power and memory devices, the device engineers still wish to accurately model the topology of their 3D structure, as well as the stress-buildup due to the oxidation. The oxidation processes used in power devices are especially challenging for simulation, since the grown oxides tend to be several hundred nm thick and the surfaces tend to be non-planar.

Previous attempts [1,2,3] in solving the 3D oxidation simulation problem remained somewhat limited in scope and could not handle the thick oxides required to manufacture power devices. Maintaining interface and mesh quality becomes critical as the oxide thickness increases, so a new algorithm had to be devised.

II. 3D OXIDATION WITH MOVINGMESH ALGORITHM

To support such 3D oxidation processes, we developed a new algorithm in Sentaurus Process called MovingMesh. The algorithm uses a body-fitted tetrahedral bulk mesh, and material interfaces are represented explicitly as triangulated surfaces, each of which conforms to the neighboring bulk mesh. Mesh motion is done in the Lagrangian description meaning that the mesh vertices move together with the material. Interface surface meshes and bulk volume meshes conform and move together. Our design was motivated by the need for accurate segregation, accurate dopant profile, and dose conservation. We wanted the MovingMesh framework to support high fidelity simulation. An example of lower-fidelity design is the Eulerian description in which the bulk meshes are stationary, and the interface meshes move through the bulk without conforming to the bulk meshes. Another non-conservative design is to use level sets to represent moving interfaces and regenerate the bulk meshes all over again every time step.

Our design choice increases the difficulty in maintaining the quality of tetrahedrons in the bulk meshes, the quality of triangles in the interface meshes, and the quality of the underlying geometry, especially during long oxidation processes dictated by power device design. After a number of time steps, a reasonable-shaped tetrahedral or triangular element can become a very poor element that harms the solvers and limits the time step to practically zero. Furthermore, the underlying geometry can become so rough that no reasonable quality mesh can be generated. After many years of research, we developed a set of tools that solved these problems, so that the simulation can run to completion with accurate, conservative, and trustworthy result.

III. EXAMPLES

A. 3D LOCOS Corner

One of the classic 3D oxidation examples is the LOCOS oxidation of a mask corner. Fig. 1 shows results for oxidation of 120nm nitride hard mask corner at 950C under 6.5l/min O_2 and 6l/min H_2 flow. The oxidation time is 25min, 1h 45min, 3.5h and 10h and the grown oxide thickness is 100nm, 300nm, 500nm and 1µm, respectively. As expected, at the mask corner the oxide is thicker since the oxidant can enter under the nitride mask from two directions. Therefore the nitride mask lifts up in the corner substantially more than predicted by 2D bird's beak simulations.

Fig 2 shows the same process, but using an opposite mask polarity, such that the inside corner of the mask is oxidized. Notice that due to the stress at the mask corner, created by the nitride layer pushing down from both sides, the oxide is thinner as compared to the sides of the mask.

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B. *Snow-plow effect*

Phosphorus preferably segregates into the silicon side at the silicon/oxide interface. During the oxidation process, the moving silicon/oxide front pushes the phosphorus profile in the silicon that is consumed by oxidation deeper into the substrate, creating a pile-up on the silicon side of the silicon/oxide interface. This is called the snow-plow effect.

In a convex 2D trench corner, this effect is stronger at the corner, since phosphorus is pushed from both top and side. In a 3D convex trench the pile-up at the corner expected to be even bigger than the 2D case. This affects the doping distribution in a 3D device significantly and will result in device characteristics that cannot be predicted by using 2D oxidation results.

Fig. 3 shows results for wet oxidation of a 3D trench corner at 1150C, for 5, 11, 25 and 50 minutes respectively. The initial wafer is uniformly phosphorus doped at 5e16cm-3. The grown oxide is shown only as an outline for clarity and its thickness is 200nm, 300nm, 500nm and 700nm, respectively. The 3D snow-plow effect is clearly visible.

There is also an inverse effect for a dopant that prefers to segregate into the oxide, like boron. In this case, boron piles up on the oxide side of a bottom corner of a trench. This effect is shown in Fig. 4, under the same oxidation conditions as before. The silicon region under the oxide is not shown for clarity.

C. *Vertical pillar MOS transistor*

As discussed previously, one of the challenges of performing 3D oxidation is to maintain surface and mesh quality. This is not only important for the oxidation step itself, but is also required to ensure success of the subsequent etch, deposition, mask and other structure modification steps. Moreover, the surface must be sufficiently smooth such that no artifacts in device simulation occur.

We demonstrate the superiority of our approach using a challenging 3D vertical pillar MOS transistor example. The process involves two 3D oxidation steps (a 30nm LOCOS corner and a 5nm gate oxide), as well as several mask, etch and deposition steps. In Fig. 5, the structure is shown before and after LOCOS, before and after gate oxidation and at the end of the process flow.

IV. CONCLUSION

A new MovingMesh algorithm was developed to address moving boundary problems such as 3D oxidation. Since the algorithm is capable of maintaining mesh and boundary quality even after large changes in the structure, fairly thick oxidation processes, such as those for power devices, can be simulated in 3D using Sentaurus Process.

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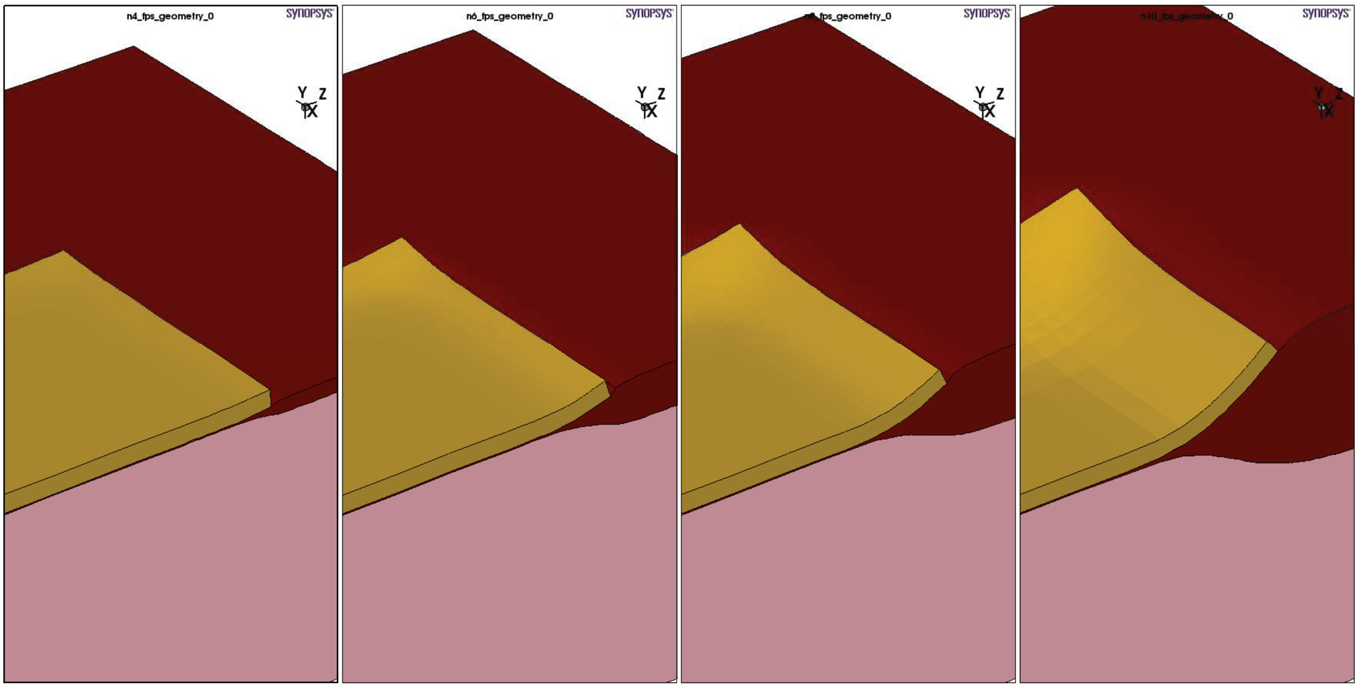

Figure 1: 3D LOCOS corner with 100nm, 300nm, 500nm and 1μm oxide thickness

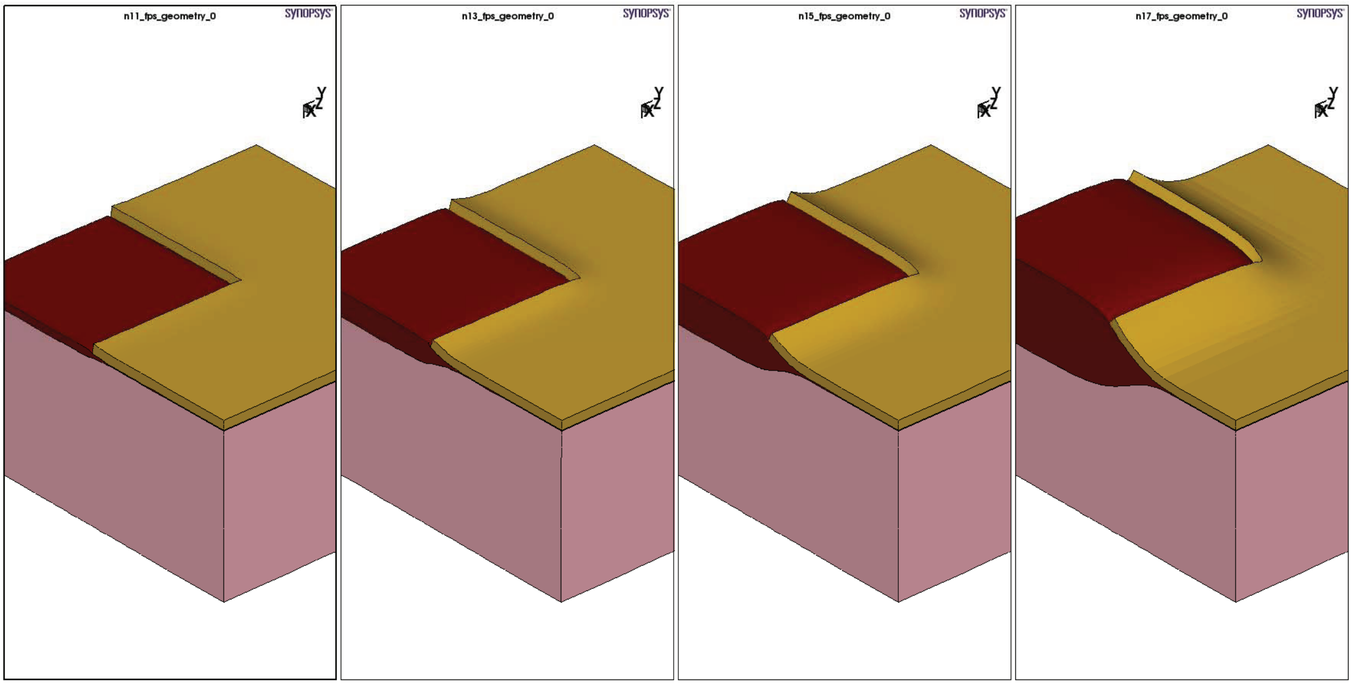

Figure 2: 3D inverse LOCOS corner with 100nm, 300nm, 500nm and 1µm oxide thickness

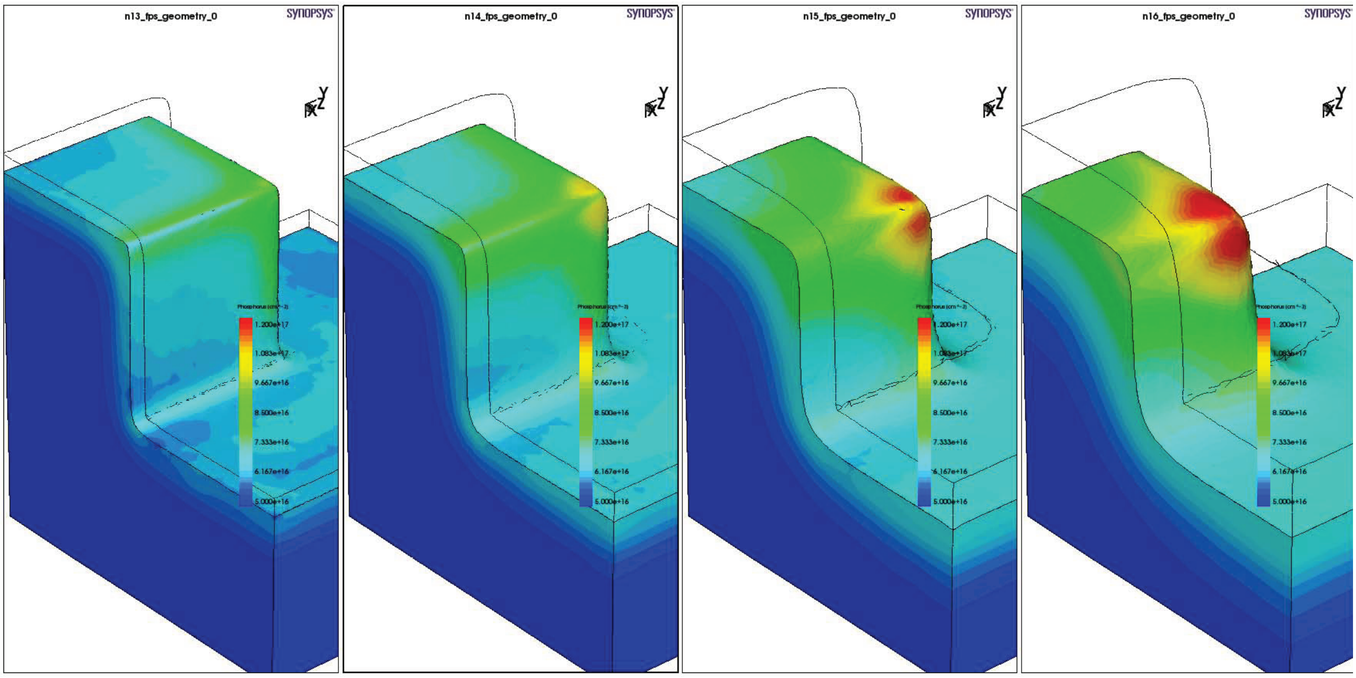

Figure 3: Phosphorus snow-plow effect at an oxidized 3D trench corner

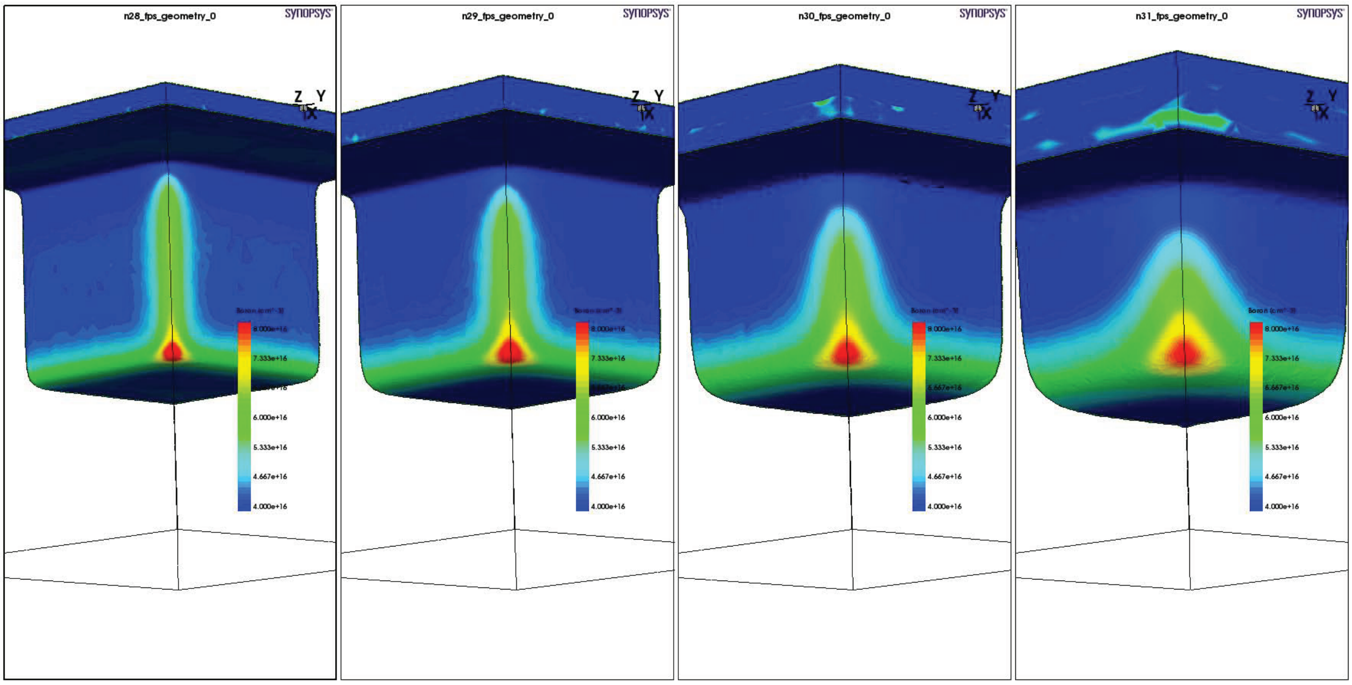

Figure 4: Boron pile-up in the oxide at an oxidized 3D bottom trench corner

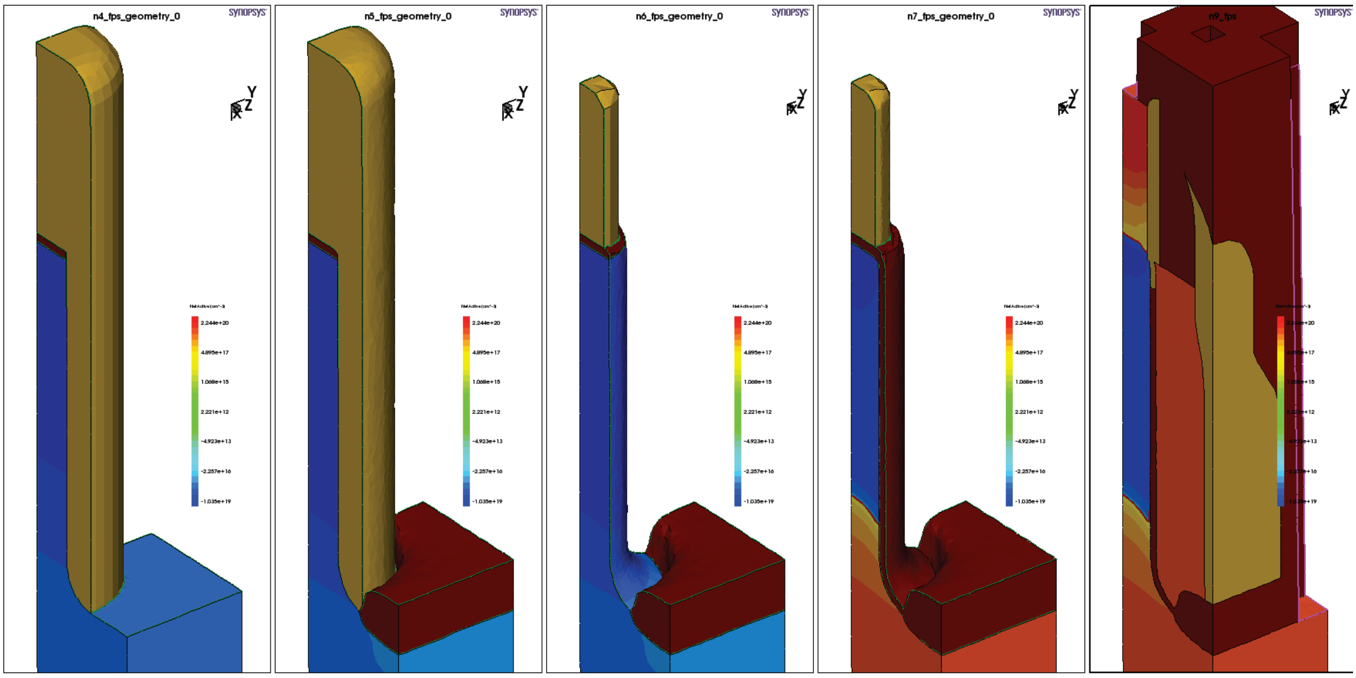

Figure 5: Vertical pillar MOS transistor before and after LOCOS, before and after gate oxidation and final structure