A Novel Approach to Three-Dimensional Semiconductor Process Simulation: Application to Thermal Oxidation

Vasily Suvorov, Andreas Hoessinger and Zoran Djurić
Silvaco Technology Center, Compass Point, St Ives, Cambridgeshire, PE27 5JL, UK.

INTRODUCTION

One of the major issues in three-dimensional semiconductor processes simulation is the problem of moving interfaces. The standard approach involves very complex and often unstable mesh generation algorithms. Alternatively, we applied the level set method on fixed Cartesian meshes [1], where the meshing algorithms are not needed, and all differential equations can be solved by the standard finite-difference methods.

However, there are two problems associated with this methodology: approximating of general-type boundary conditions near the interface and handling of a big scale ratio of sizes in complex structures. In the last decades a considerable progress has been achieved in resolving both issues (e.g. [2], [3], [4]). In our development we use our original in-house numerical method, the method described in [3] and the concept of Adaptive Mesh Refinement (AMR) [4]. The above principles are cornerstones of a software package Victory, Silvaco's three-dimensional process simulation framework. In this work we demonstrate Victory's capability to simulate numerically the most demanding process, namely thermal oxidation.

MODELLING OF THERMAL OXIDATION

Three different processes occur simultaneously during the thermal oxidation: diffusion of oxygen, a chemical reaction at oxide/silicon interface and a volume expansion of the newly formed oxide. The aim of the modelling and simulation is to explain and predict the resulting shape of oxide and mechanical stresses developed in a structure during the process. Our physical model assumes Newtonian viscous constitutive model for oxide and nitride (valid for relatively high temperatures).

The mathematical model comprises three different sets of equations: i) equation for level-set function to track moving interfaces; ii) diffusion equation to describe oxidant behaviour; iii) the system for incompressible Navier-Stockes equations for creeping flow. The first set also constitutes a core of the etching/deposition module.

For illustration purposes we have modeled three typical oxidation process steps: locos, polysilicon oxidation and trench oxidation. Figures 4 and 5 demonstrate two different types of 3D bird's beak effects obtained by rather long time oxidation which is the numerically most critical application.

Moreover Fig. 6 shows iso-surfaces of compressive (blue) and tensile (red) mechanical stresses near the silicon surface obtained during trench oxidation. The stresses resulting from locos and reoxidation will be presented in a full version of the paper.

CONCLUSION

The state-of-the-art finite-difference methods for the simulation of thermal oxidation is presented which can handle arbitrary complex geometries. This enables us to design a new generation process modelling tool that avoids meshing/re-meshing procedures.

REFERENCES

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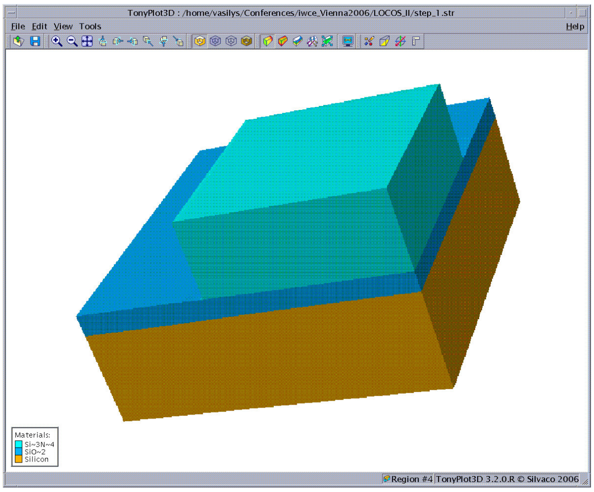

Fig. 1. Input structure for the locos process built by Victory's etching/deposition module

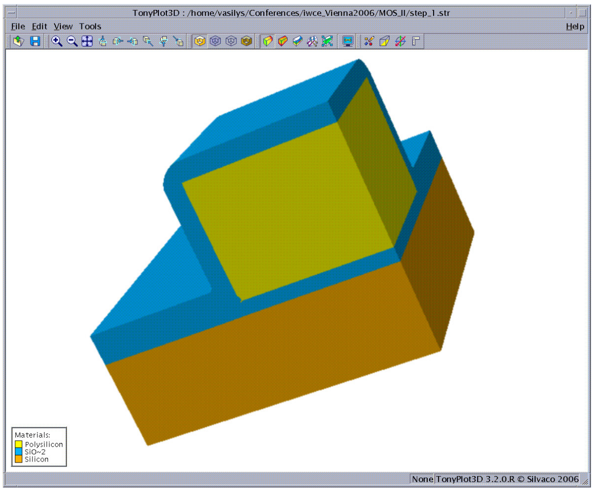

Fig. 2. Input structure for reoxidation of two oxidizable regions

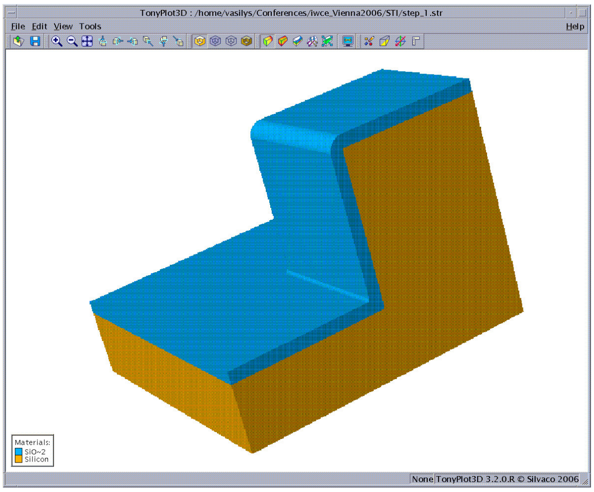

Fig. 3. Input structure for trench oxidation generated by the etching/deposition module

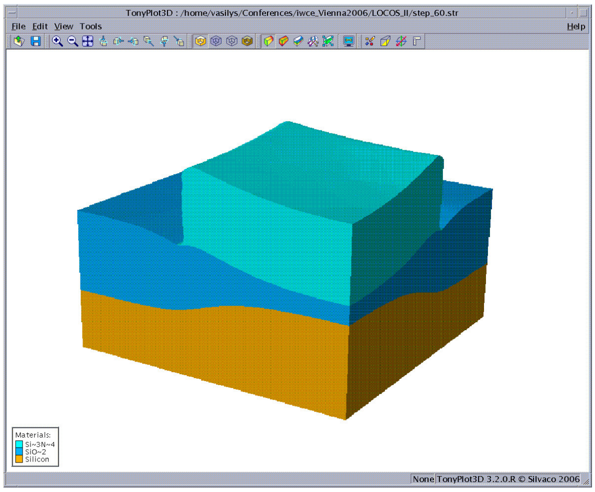

Fig. 4. Locos structure after 10 min wet oxidation at T=1000^{o}C

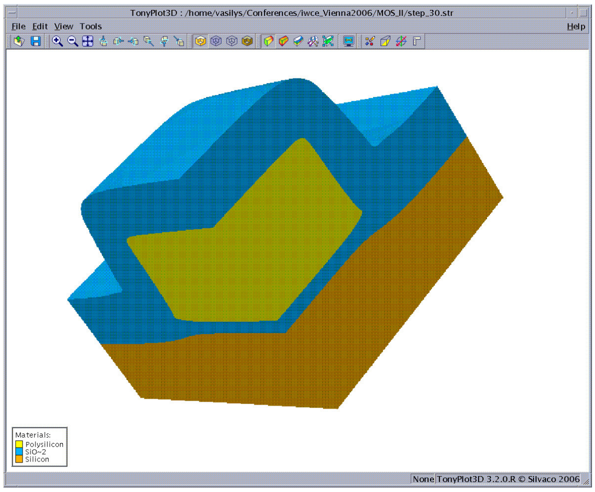

Fig. 5. Shape of the device after 5 min reoxidation of the polysilicon and the silicon substrate

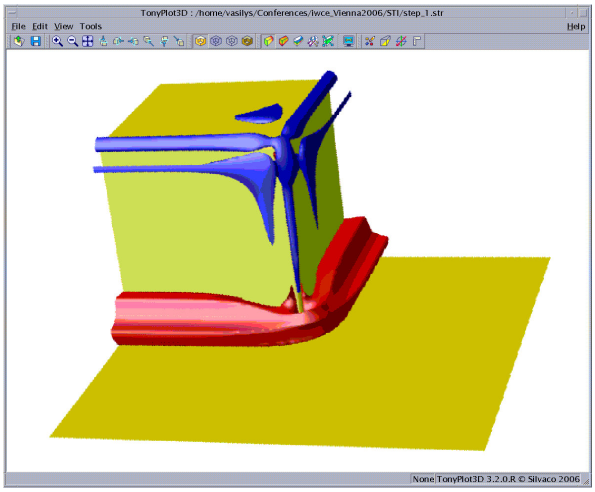

Fig. 6. Iso-surfaces of compressive pressure P = -5400 MPa (blue) and tensile one P = 13200 MPa (red) in oxide. Yellow surface is the oxide/silicon interface in the trench