Theoretical Simulations of Silicon-on-Nothing (SON) Structures

C. Grau[1], B. Bergmann[1], C.Breitkopf[1], F. Hoffmann[2], L.Brencher[2]
[1]Technische Universität Dresden, Dresden, Helmholtzstraße 14, 01062, Germany.
[2]Infineon Technologies GmbH, Dresden, Königsbrücker Strasse 180, 01099, Germany.

Introduction: Semiconductor industry is currently playing a very important role worldwide. Most devices used nowadays are built around semiconductor technology. Novel techniques for manufacturing silicon devices in a more cost-effective manner are constantly investigated for savings of economic resources.

One of those novel techniques is introduced: Silicon-On-Nothing. This process consists of an initial cylindrical trench which has a shape evolution under certain conditions: high temperature (1100 °C), low pressure (10 Torr) and a non-oxidizing atmosphere such as hydrogen (1). These conditions enable a, mainly, surface diffusion phenomenon whose final result is an empty space (usually spherical) below a silicon layer which has several applications (micro sensors, transistors, optical devices, etc.) and, moreover, it incurs in fewer costs than traditional etching processes.

The variation of temperature, pressure and geometry leads to different morphological evolutions (2). The objective of this research project is the control and prediction of the final structures while obtaining the limitations of current theories and further possible implementations.

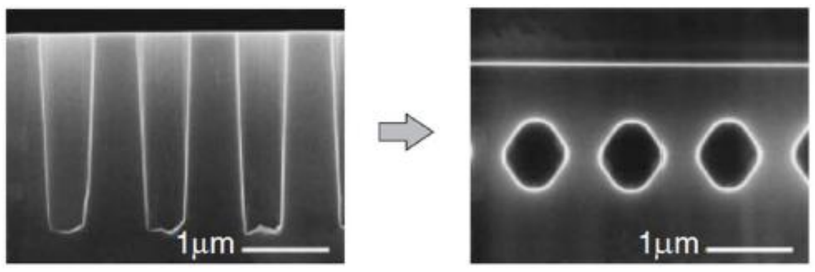


Figure 1. SON experimental literature example (1)

Computational Methods: For the computation of this problem, we have used, as a base, the theory developed by Mullins (3) and its implementation made by Sudoh (4). They use the difference of chemical potential as the driving force for the surface diffusion. The definition of a superficial chemical potential (μ) is given by the curvature of the surface: $\mu = \Omega\gamma K$, where Ω is the atomic volume, γ is the surface energy density and K is the curvature as the sum of the two main curvatures of the surface. The curvature is calculated by:

$$K = \vec{\nabla}\vec{n}$$

where $\vec{n}$ is the normal vector in every surface point. For convergence reasons, some Dirichlet boundary conditions are added to the boundary PDE equation. Those boundary conditions are attached to the initial trench and they define the sinusoidal perturbation of the surface and curvature with a characteristic wavelength, λ, based on the Rayleigh's instabilities (5). Figure 2 shows these definitions where the suffix "e" means extreme values of the waveform and the suffix "c" means the center of it.

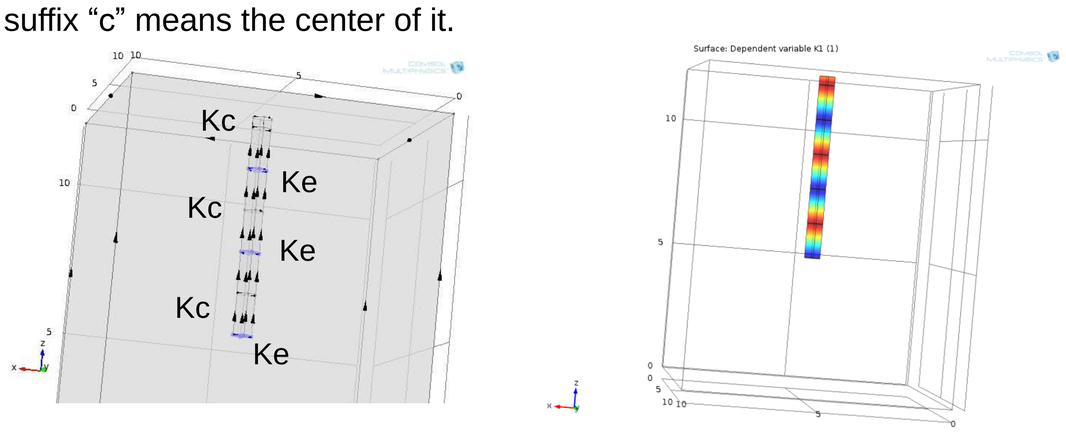


Figure 2. Curvature definition and color variation using "Extremely Coarse" mesh

When the curvature is computed, the normal velocity of the surface is calculated using Mullins' three-dimensional equation (3). It is defined using a boundary PDE:

$$v_n = \frac{D_S \Omega^2 X_S \gamma}{k_B T} \Delta K$$

where D_S is the surface diffusion coefficient, X_S is the surface atomic density, k_B is the Boltzmann constant and T is the temperature.

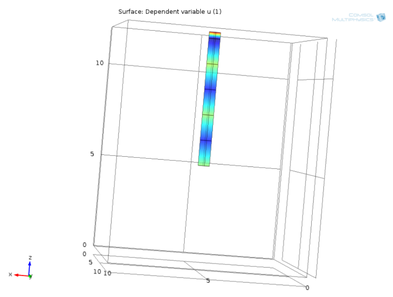
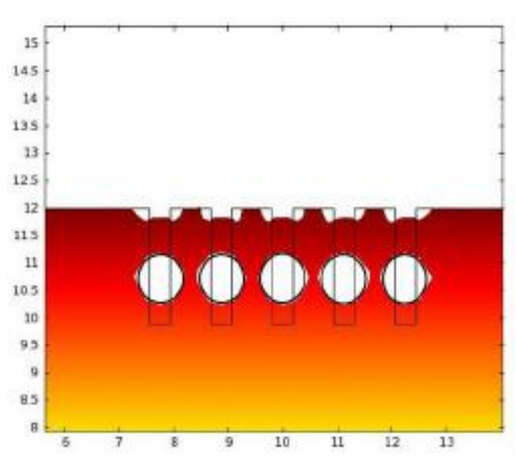


Figure 3. Normal velocity color variation using "Extremely Coarse" mesh

Results: Using the "Moving Mesh" interface, it is possible to reproduce the movement with a "extremely coarse" mesh as a smaller mesh results in a no convergence problem because of inverted mesh elements. Figure 4 and 5 show some of the results.



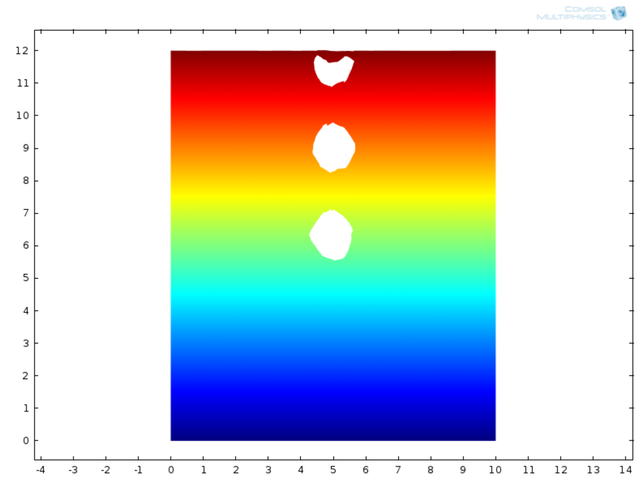


Figure 4. Simulation of Figure 1

Figure 5. Example with more than one final empty space

The **relative error observed** within the results varies between **0-14%** for the creation of one empty space in silicon which it is a good precision starting point.

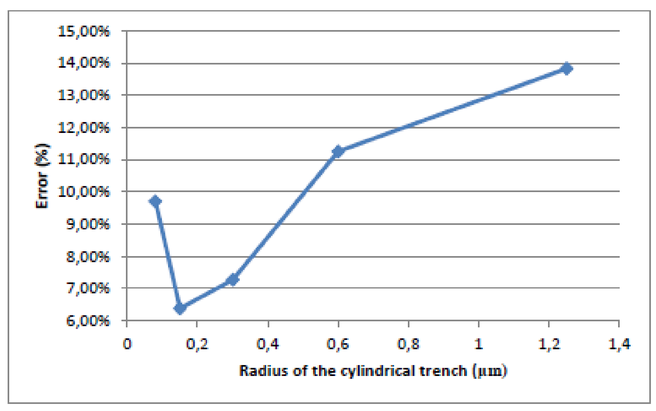


Figure 5. Relative error of the final diameter

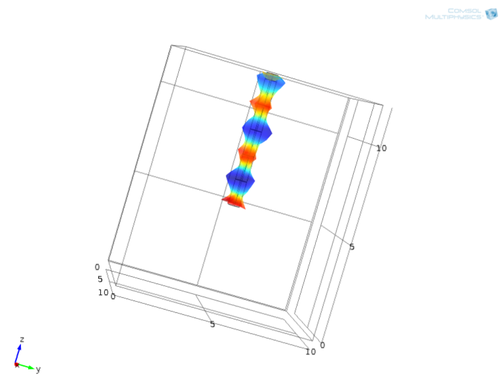


Figure 6. 3D view of the Figure 5

Looking at the figure 6, "Moving mesh" does not allow the surfaces to stop when intersecting themselves which provokes a distortion on the morphology of the result. This makes a cut-in plane (Figure 4 and 5) a satisfactory solution to see what really happened during the SON process.

Conclusions: Using the tools provided by COMSOL Multiphysics, it is possible to make a preliminary estimation of the final shape of the Silicon-on-nothing process. The results indicate that a margin of error of about 0-14% (compared to literature examples) is achieved so that it remains within respectable limits. Further developments on the mesh modeling and the implementation of additional physics will be able to present more accurate results.

This model also presents a good starting point for further developments on the control and prediction of different microstructures which are useful in a wide range of processes.

References:

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