Void Shape Evolution of Silicon: Level-Set Approach

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Introduction: The void shape evolution of silicon is a process where trenches etched on silicon are transformed into different shaped empty spaces in silicon when the sample is thermally annealed at high temperatures (~1100° C) in a non-oxidizing atmosphere [1-2]. The arrangement of the initial trenches leads to different final geometrical outputs where, in some cases, coalescence between neighboring trenches occurs. The objective of this work is to represent these topological transformations with the highest possible accuracy through simulations.

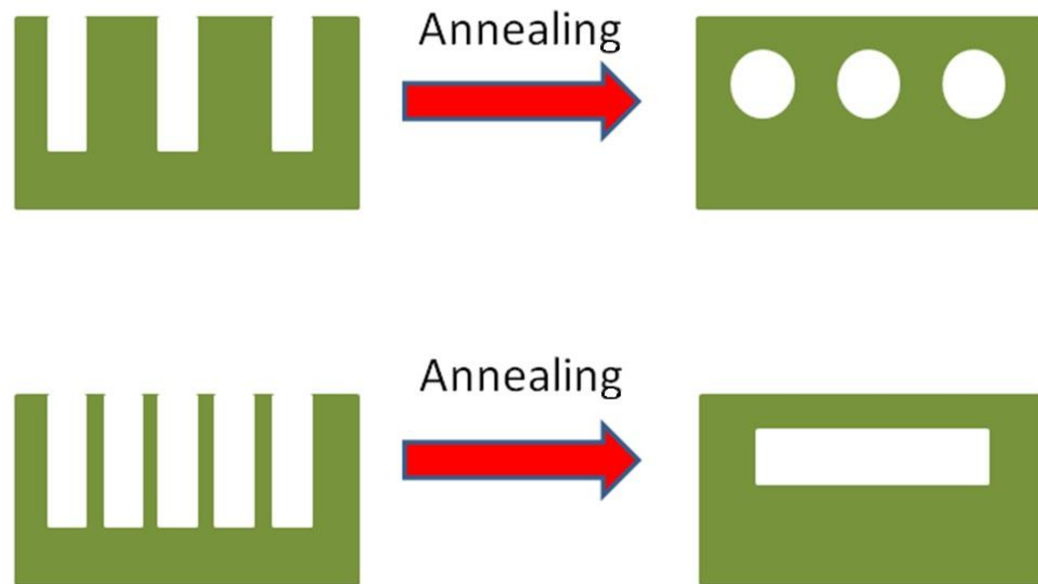

Figure 1. Void shape evolution scheme

Computational Methods: The model was built around the surface diffusion (custom PDE) equation [3], which describes the velocity of the surface depending on atomic parameters of the solid, multiplied by a concentrating interface function, δ:

$$u_{i,S} = \frac{D_S(p,T)\Omega^2 X_S \gamma}{k_B T} \Delta_S(\kappa) n_i \delta(\phi)$$

Level-Set method was used for computing the evolution of the surface by employing the surface diffusion velocity as the advection velocity of the Level-Set interface, which also yields the normal, n_i, and the curvature, κ, as derivatives of the Level-Set function, ϕ:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \gamma\nabla\cdot\left(\varepsilon\nabla\phi - \phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)$$

$$\mathbf{n} = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi = 0,5}$$

$$\kappa = -\nabla\cdot\mathbf{n}\big|_{\phi = 0,5}$$

Stabilization parameters, ε and γ, are calibrated in each simulation and a linear discretization is chosen so as to use bigger geometries.

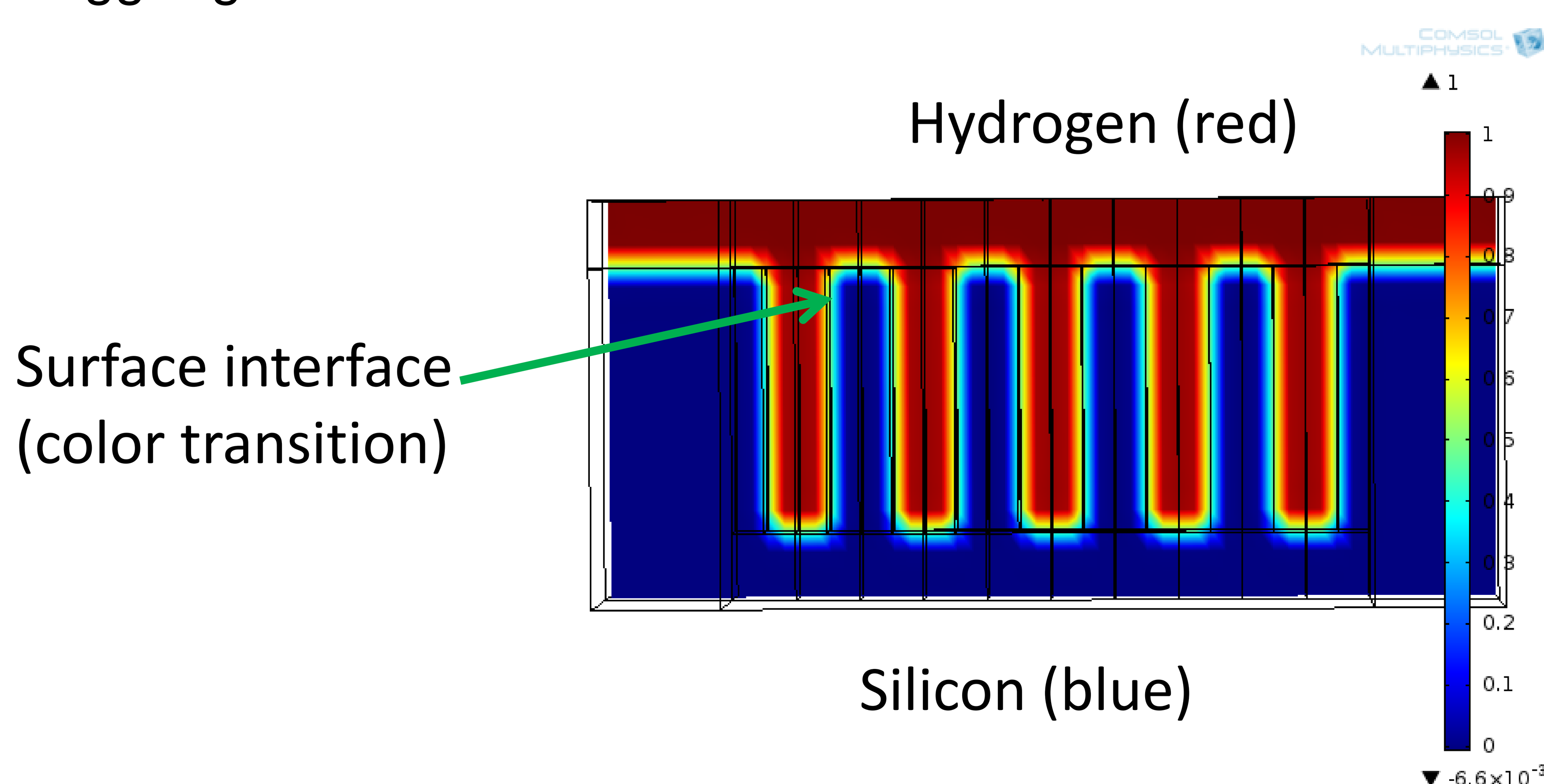

Figure 2. Initial geometry example

Results: The following figures consistently represent an evolution similar to those in literature while being able to simulate the coalescence (not possible before with the ALE method):

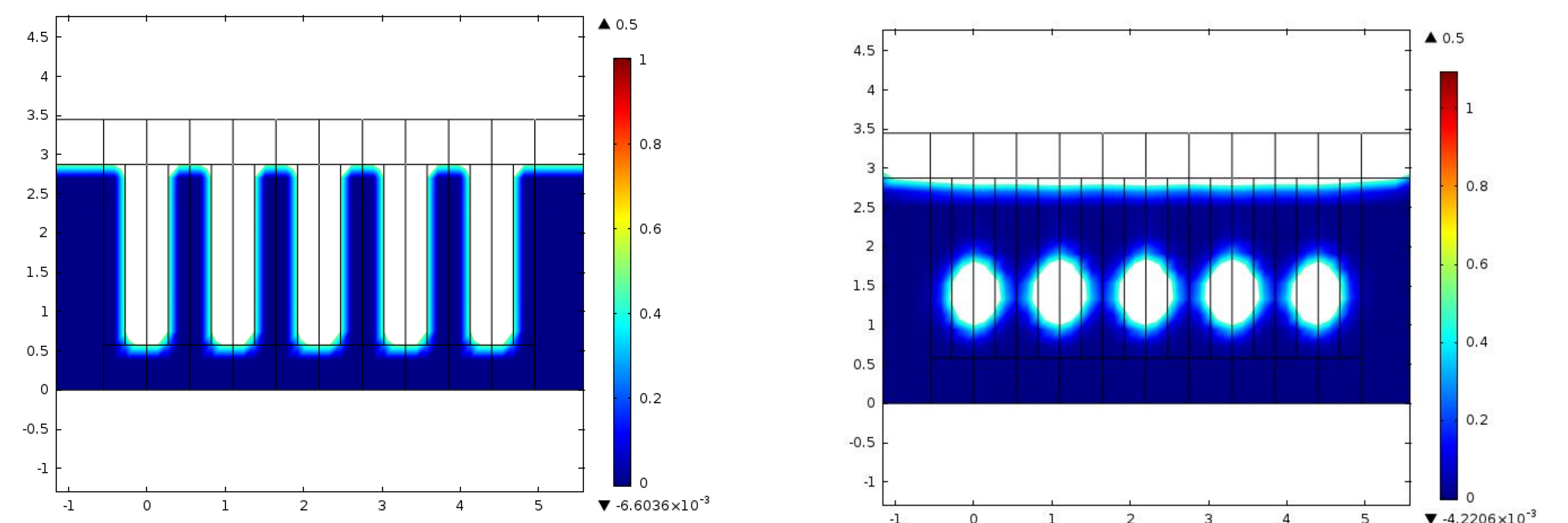

Figure 3. Initial (left) and final (right) geometries: no coalescence

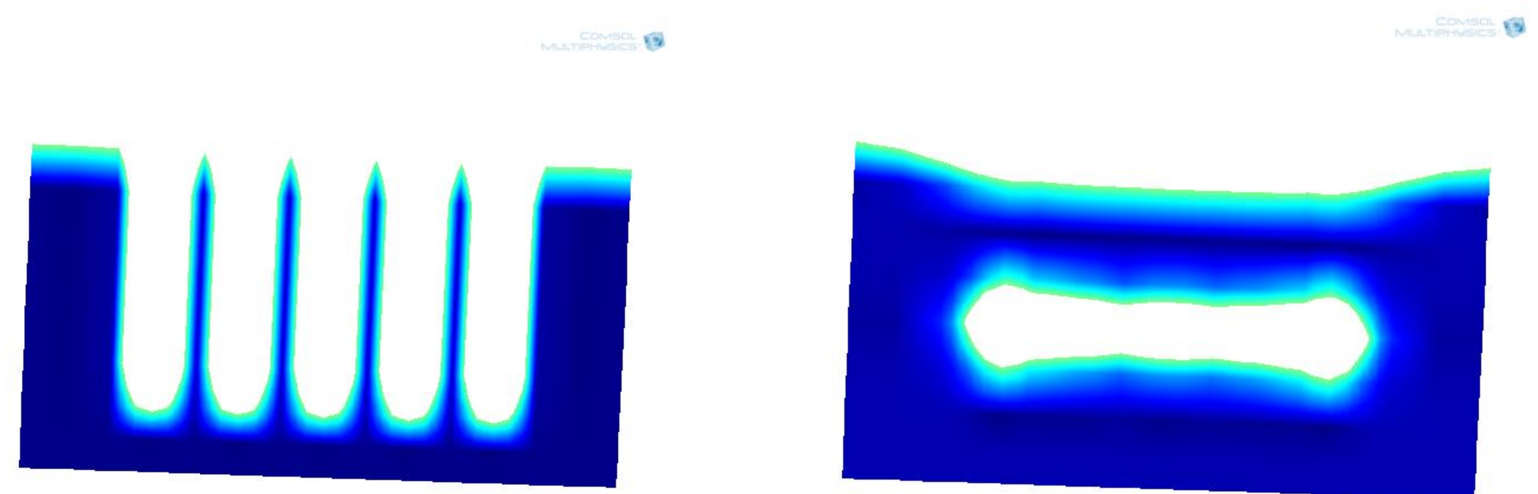

Figure 4. Initial (left) and final (right) geometries: with coalescence

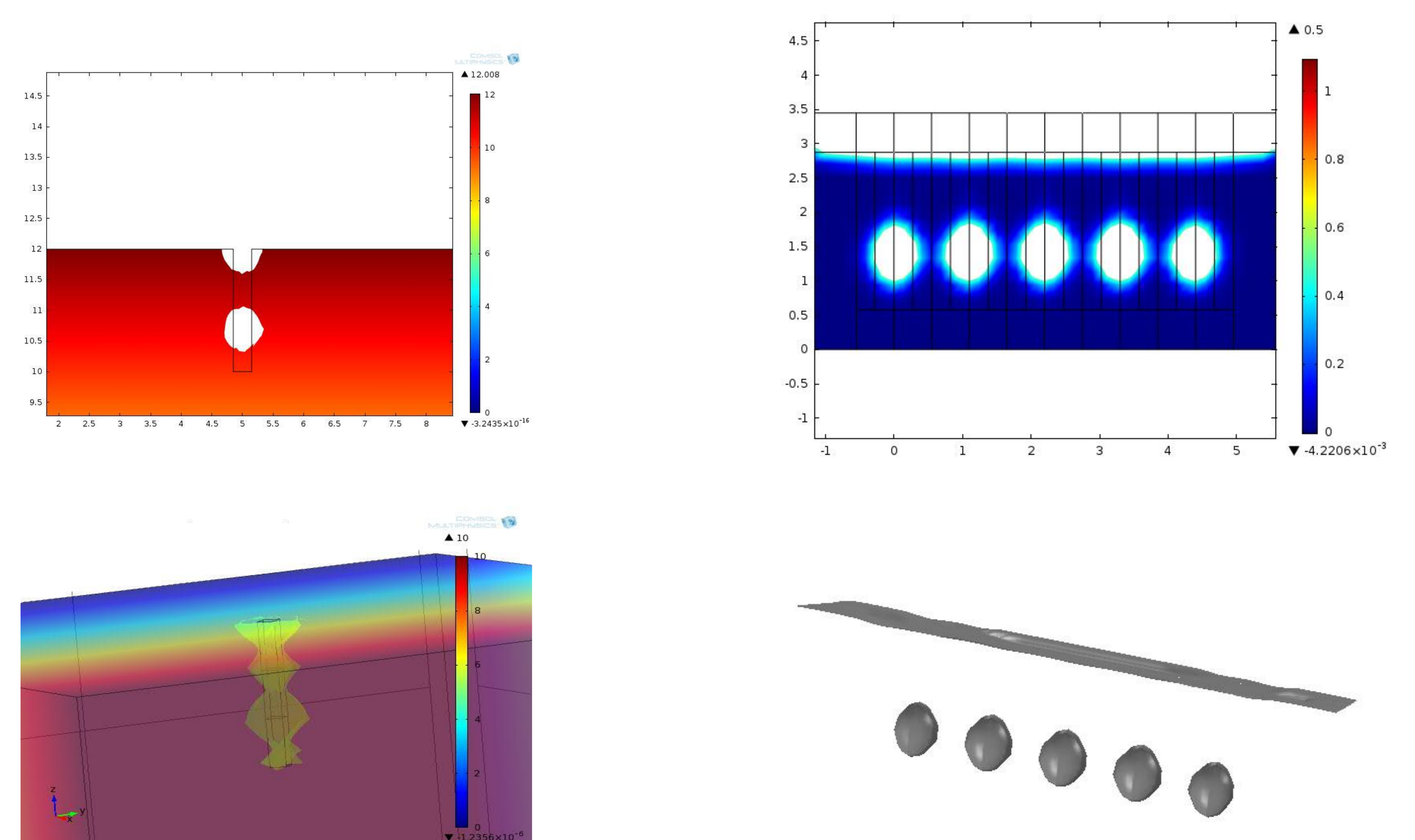

Figure 5. Cross-section and 3D view with moving mesh (left) compared to level-set (right)

Conclusions: Level-Set proved to be more useful than Moving Mesh for this kind of simulations. Coalescence was successfully simulated, and the results were similar to those in the literature. The next step is to choose consistent stabilization parameters to cover a wide range of simulations in shorter times. The successful prediction of void structures can be useful to build SON (Silicon-On-Nothing) devices, micro-cooling channels or pressure sensors with a more cost-effective technique.

References:

1. T. Sato et al., Fabrication of Silicon-on-Nothing Structure by Substrate Engineering Using the Empty-Space-in-Silicon Formation Technique, Japanese Journal of Applied Physics, vol. 43, pp. 12-18, (2004)
2. I. Mizushima et al., Empty-space-in-silicon technique for fabricating a silicon-on-nothing structure, Appl. Phys. Lett., 77, 3290, (2000)
3. W. W. Mullins, Theory of Thermal Grooving, J. Appl. Phys. , 28, 333 (1957)

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