Void Shape Evolution of Silicon Simulation in COMSOL Multiphysics®

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Introduction: The void shape evolution of silicon consists of the morphological change of a trench etched in silicon due to the minimization of the surface energy. This minimization is carried out by a redistribution and diffusion of the atoms belonging to the interface.

The importance of this process resides in the ability to create voids of different shape under a silicon layer (Silicon-On-Nothing or SON) from simple trenches which are arranged in a predefined pattern. The transformation is carried out through an annealing process at low pressure (~10 Torr), high temperature (~1100 ° C) and non-oxidizing atmosphere (hydrogen) [1, 2].

The aim of this work is to have an accurate prediction of the final geometry as a basis for the development of more complex semiconductor devices.

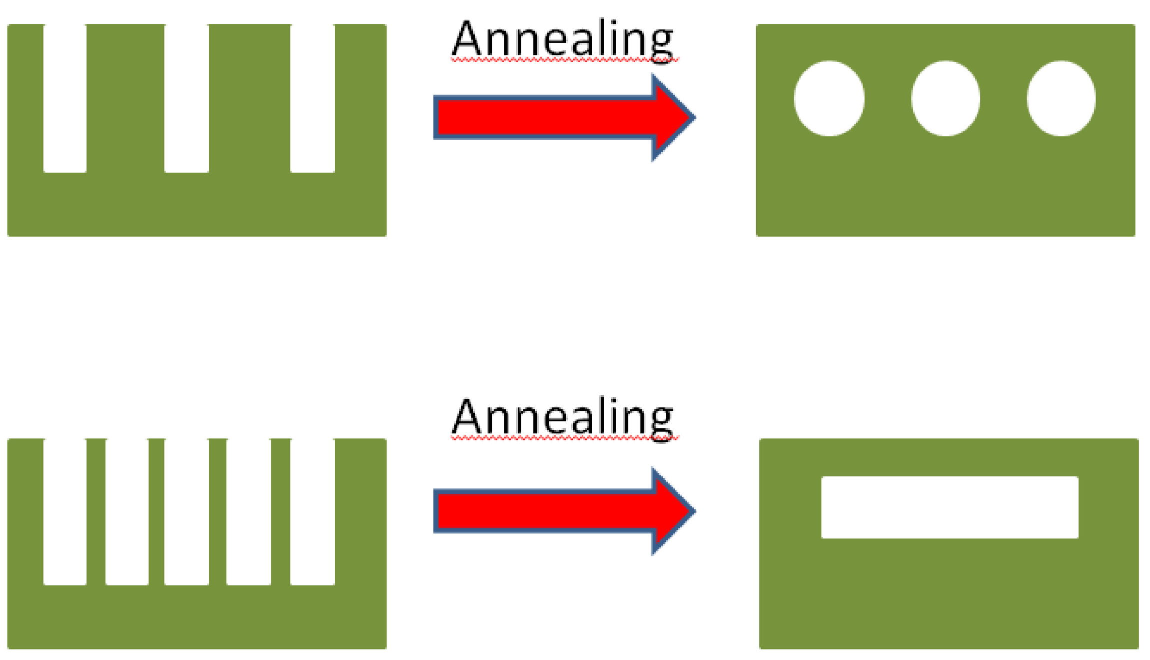

Figure 1. Void shape evolution scheme depending on the trench separation

Computational Methods: The method used for the simulations is the "Moving Mesh" (ALE) as it ensures volume preservation and direct surface variables calculation. This module needs, as an input, the velocity of the surface which is calculated by the surface diffusion equation [3, 4] where the normal velocity of the surface can be calculated as:

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

The previous equation have the following terms: D_S is the surface diffusion coefficient (Arrhenius form); Ω is the atomic volume; X_S is the atomic surface density; K is the curvature; Δ_S is the Laplacian on the surface domain; and k_B is the Boltzmann constant.

The curvature by its continuous equation (***K*= ∇*n***) cannot be directly used in this method as it yields numerical errors. In order to determine the curvature during the evolution, characteristic values from the process are employed where a time-dependent perturbation is added, giving as a result a function (being z_0 the bottom of the trench):

$$K = K_0 exp\left(-\frac{t}{\tau}\right) cos\left(\frac{2\pi}{\lambda}(z - z_0)\right)$$

The different terms are: λ is the wavelength based on Rayleigh instabilities [5]; z is the vertical coordinate; τ, which is the growth constant, and K_0 are functions of system parameters after a first order perturbation analysis.

Results: The geometry evolution changes with the length and radius of the trench and the temperature. In the examples given below (Figure 2), the longer the trench, the higher amount of void shapes are formed. Regarding the temperature (Figure 3), the process is faster at higher temperatures but they must be held below the fusion point (1414 ° C). These results agree with previous publications [1, 2, 6].

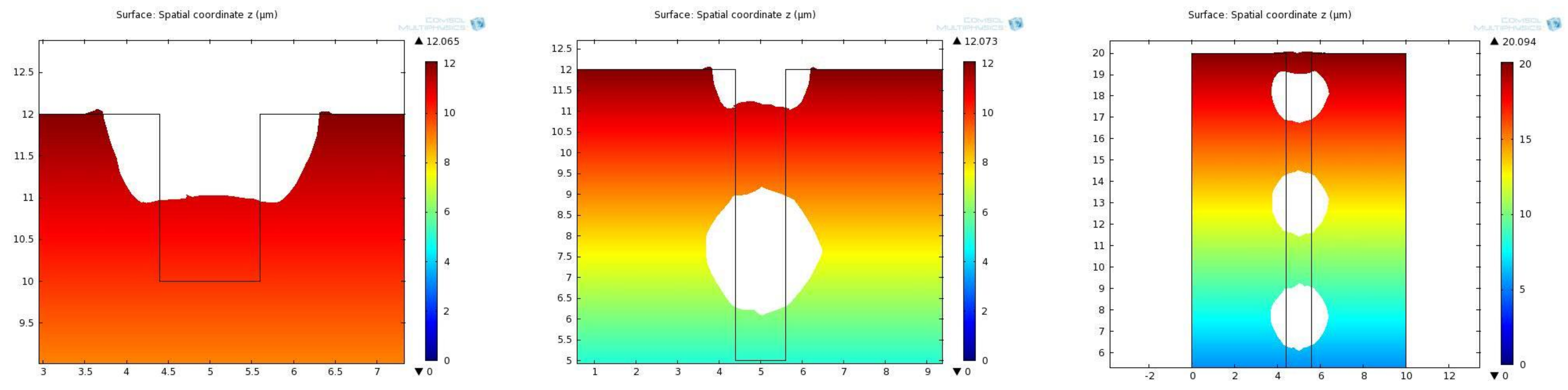

Figure 2. Number of final voids depending on the trench length/diameter ratio for values of (left to right) 1.67, 5.83 and 12.5

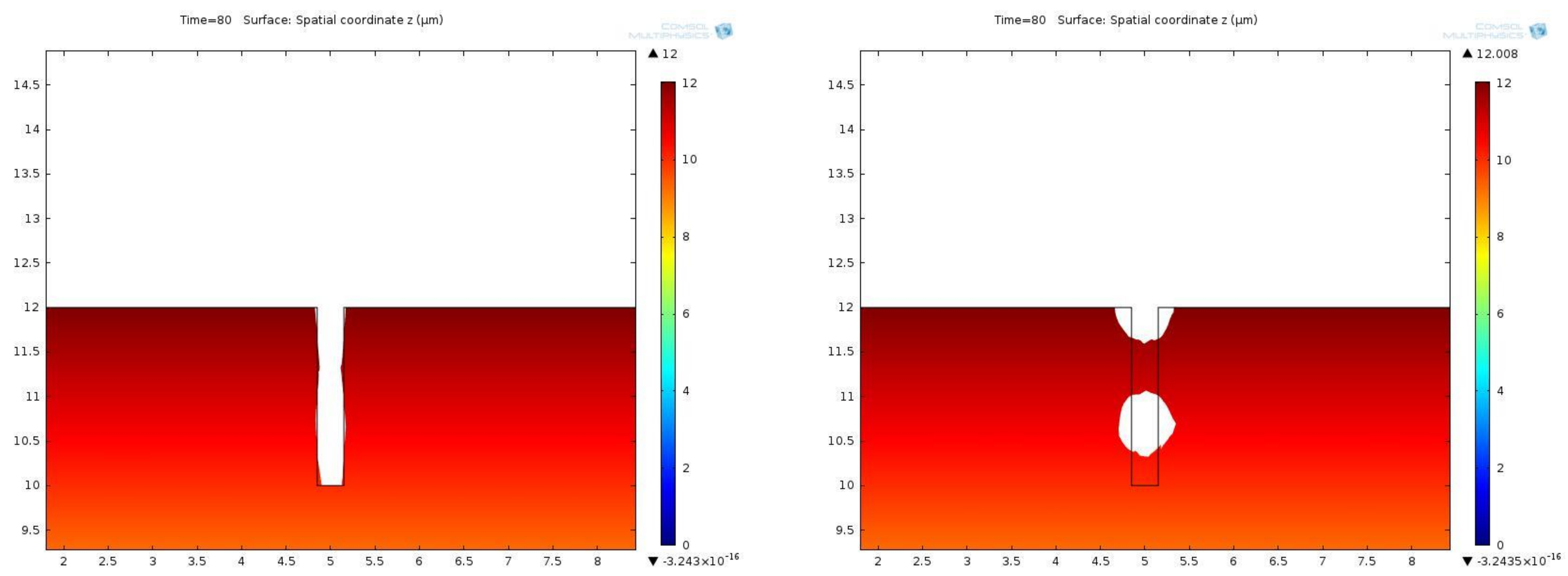

Figure 3. Evolution after 80 seconds annealing at a temperature of (left to right) 900 ° C and 1100 ° C

Variable	Value	Units
Atomic volume (Ω)	12.06	cm^3 / mol
Atomic surface density (X_S)	$1.13x10^{-9}$	mol / cm^2
Surface energy density (γ)	1.2	J / m^2
Pre-exponential term of D_S	0.1	m^2 / s
Activation energy of D_S	2.3	eV

Table 1. Common parameters

Conclusions: The geometry evolution could be simulated on single trenches while the coalescence between two or more trenches was not possible to address with the "Moving Mesh" method. The temperature and trench length dependence of the formation of void shapes were proved to be similar to those in literature [1, 2, 6]. A limitation of the moving mesh method was found as it could not simulate successfully the coalescence between two void shapes and the geometry mesh must be quite coarse to avoid instabilities on the geometry.

Further approaches for this specific problem are being currently investigated.

References:

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