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Modelling of Surface Diffusion in Structured Silicon

U. Bethers, J. Seņņikovs, A. Timuhins, J. Virbulis, D. Zablockis

Abstract

We present a three – dimensional model of surface diffusion which describes the time evolution and topography changes of deep trenches under low pressure hydrogen anneal and compare the results with experimental observations. An anneal process for regular arranged cylindrical trenches was investigated using a genetic optimization algorithm. Seven different structural phases of the final bubble / layer arrangement out of the trench array anneal could be predicted.

Introduction

In the pioneering work of Sato & Mizushima et al. [1-4] a new simple approach to establish large –Scale empty spaces in silicon (ESS) basing on microstructure transformation of silicon (MSTS) is demonstrated. Trench patterned silicon surfaces were annealed in hydrogen ambient at low pressures and result in formation of empty bubbles, pipes or plates underneath a refilled and closed silicon top layer. It is stated that the self-organizing surface migration of silicon acts in that way that the surface energy is minimized. Depending on the spacing (or pitch), width and depth of the initial trenches they coalesce and form in two dimensions an empty plate under the surface.

It is important to develop simulation models to study the transformation of the trench into single bubbles or empty plates in detail. Thus, predictions could be made about the limitations of this “silicon – on-nothing” technique e.g. the minimum allowable silicon top layer for the given trench geometry. Developing a “phase” diagram spanned by the two fundamental geometrical parameters (depth and radius) for a simple cylindrical trench array would give information about stable conditions to derive a single silicon top layer.

1. Numerical Models

1.1 Surface diffusion model

Surface diffusion as the fundamental process for this silicon on nothing (SON) technology can be macroscopically described by a Mullin’s equation [5]:

$$\frac{\partial n}{\partial t} = B \Delta_S k \, , \tag{1}$$

whereas k is the sum of the two principal surface curvatures (mean curvature), n is the surface position in normal direction and Δ_S is the surface Laplace operator. Coefficient B is defined as:

$$B = \frac{D_S \, \gamma \, \nu \, \Omega^2}{k_B T} \tag{2}$$

whereas D_S is the surface diffusion coefficient, γ is the surface tension (surface energy density), k_B is the Boltzmann's constant, Ω and ν are atomic volume and atomic surface density, respectively. The surface diffusion coefficient is given by Keefe [6] as

$$D_S = 0.1\exp(-\frac{2.3eV}{k_B T}), \qquad (3)$$

with pre-exponential constant of 0.1 and activation energy of 2.3 eV.

The following algorithms are used for the surface development modelling in 3D, i.e. for the triangular meshes on surfaces. The algorithm for mean surface curvature (k) is adapted from Zinchenko et. al [7]. It allows determination of curvature and normal vector (**n**) at mesh nodes.

The algorithm for calculating the surface Laplace operator is adapted from Mayer [8]. It finds the value of the surface Laplace operator at node (i) as

$$(\Delta\kappa)_i \approx \frac{1}{\Delta S}\int_S \Delta\kappa dS = \frac{1}{\Delta S}\oint_C \frac{\partial\kappa}{\partial n} d\Gamma \approx \frac{1}{\sum_j S_j}\sum_j \frac{1}{2}\left(\frac{\kappa_{1j}-\kappa_i}{|\vec{r}_{1j}-\vec{r}_i|} + \frac{\kappa_{2j}-\kappa_i}{|\vec{r}_{2j}-\vec{r}_i|}\right)|\vec{r}_{2j}-\vec{r}_{1j}|, \qquad (4)$$

and integration is done along the boundary of the triangular patch (C). Summation is performed over all triangles (j) of the patch. Indexes 1 and 2 correspond to two other nodes of the triangle, **r** are the co-ordinates of the nodes.

Moving of the mesh is performed by the first order approximation of the equation of motion:

$$\frac{d\vec{r}}{dt} = v_n \vec{n} \qquad (5)$$

Mesh restructuring uses the algorithms of mesh refinement [9], edge merging (length smaller than prescribed minimum) and edge swapping [10].

Topological changes of surface are described as splicing and joinning. Mesh (surface) splicing occurs during the narrowing of the surface neck. Mesh (surface) joining occurs if two parts of a mesh are moving towards each other.

The symmetry boundary conditions are implemented i.e. the triangles touching the symmetry planes are mirrored against these planes and mirrored vertices are used in calculations. This condition allows simulating infinite symmetric areas of trenches.

A specialized simulation software Surver was developed using these described algorithms.

1.2. Genetic optimization algorithm

The numerical model of surface diffusion is used for parameter studies of layer thickness and uniformity. The aim is to find out the optimum configuration of the trench array which gives the minimum thickness and maximum stability of the upper Si layer after the anneal process. Due to the required large number of simulations the genetic optimization method was used and it's adaptation to this problem is described here. The genetic optimization algorithms, initiated in 1960-ies (for instance by Bremermann et al [11]) and theoretically developed in 1970-ies (for instance by Rechenberg [12], Schwefel [13]), nowadays are considered among the most efficient methods in finding the global minimums of the target functions (Goldberg [14]).

The task is to minimize the function f(P_1, P_2 , …. , P_n). whereas f is the upper Si layer thickness and P_1 to P_n are the n process parameters. The algorithm used in our work is described in detail in [15].

The genetic algorithm was realized numerically, and implemented as a server process in the cluster of workstations. The server program distributes the parallel calculation tasks to the workstations. The Si surface development is calculated by Surver software [16] on the workstations returning the target function – the final upper layer Si thickness – to the server.

2. Results

2.1. SON layer formation

The principle of layer formation during the trench annealing is illustrated by presenting the simulated shapes developing after subsequent time increments. Fig. 1 shows one trench in an array of trenches in cross-section perspective (trench pitch = 1 μm, trench diameter = 0.6 μm and trench depth = 4 μm). In the first stage of annealing the main effect of the surface diffusion is the formation of a neck near the wafer surface (a). The radius of the neck decreases, the trench has been closed and the underlying bubble structure is formed (b) (furtheron calling this process "splicing"). Afterwards, the surface diffusion changes the bubble shape, its height decreases and the diameter increases (c). If the distance between the neighbouring trenches is smaller than the diameter of the sphere the bubbles will join each other (d) and form a continuous empty layer (e).

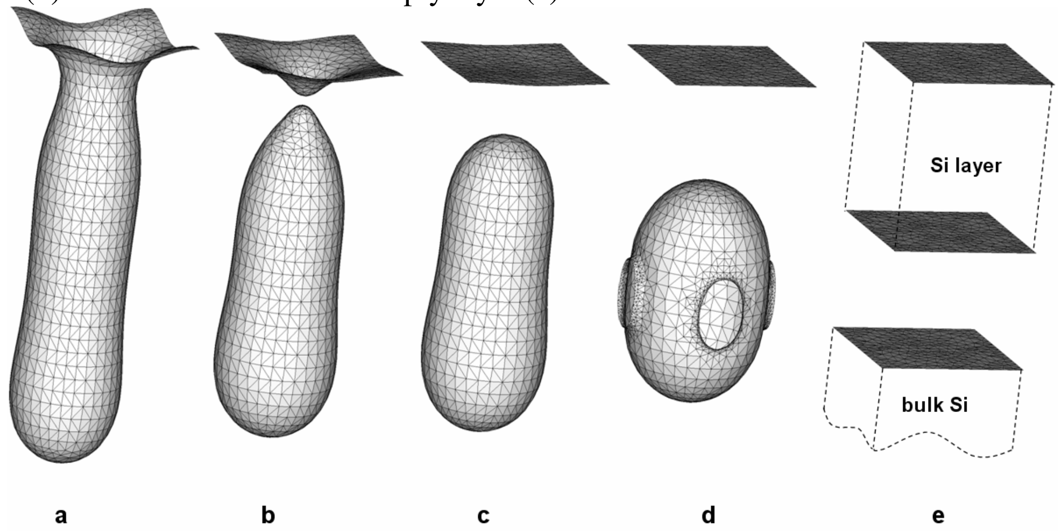

Figure 1. Time development of an SON layer represented by one trench out of an infinite calculated trench layer: neck formation (a), splicing of neck and bubble formation (b), bubble surface minimization (c), bubble joining with neighbouring bubbles (d), continuous layer formation (e).

2.2. Comparison of bubble formation with experimental data from literature

The experiments [2] presenting bubble formation from trench annealing were used as a starting point for our verification of the developed SON surface diffusion model. An experimentally obtained trench geometry (rounded trench with an aspect ratio of 30 see Fig.2) and it's annealing conditions were taken from [2] as initial simulation parameter. The silicon nitride / silicon dioxide film on the upper surface can be considered as a specific feature in this study. This film prevents the diffusion on the plane silicon surface and the closing of the trench starts from the bottom. As a consequence bubbles are formed in regular distances starting from the bottom, too. The simulation was able to verify this effect and the same final shapes of the bubbles could be derived by our simulation approach (lines in Fig. 2).

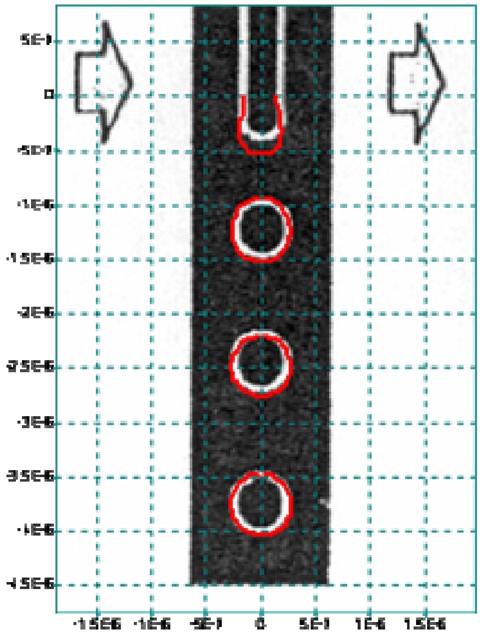

Figure 2. Comparison of simulation results (lines) with experimental bubble shapes taken from [2].

__2.3 Study of layer uniformity__

The optimization studies were performed by the developed genetic optimization method for cylindrical trenches only. The target of the optimization was defined as minimisation of the upper Si layer thickness Δz. Cylindrical trenches have only two (optimization) parameters – the trench radius R and the trench depth H. The used pitch of the trench array was set to 1 µm; however due to the linear process of the surface annealing a linear scaling of the geometric parameters is allowed.

The different structure types occurring after the anneal process are presented as a “phase diagram” *radius* vs. *depth* in fig. 3. Each point represents one simulation and seven individual structural types (Fig. 4)/ phase diagram zones (Fig. 3) can be isolated:

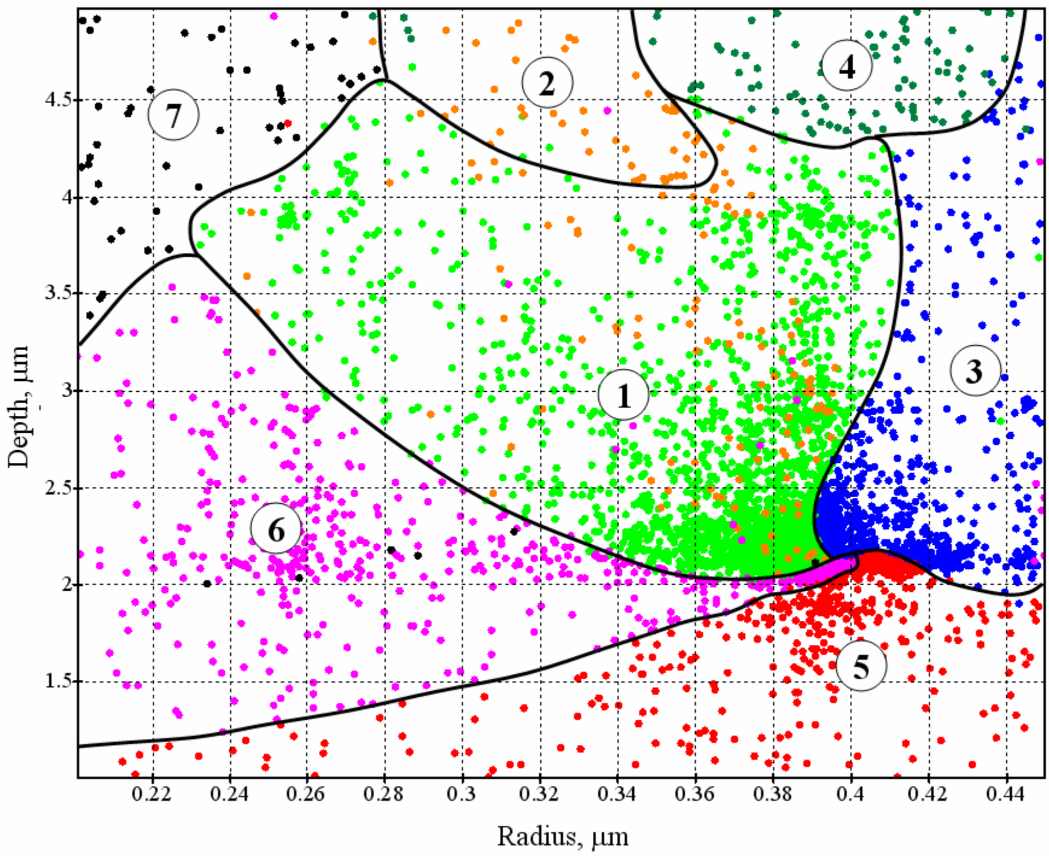

Figure 3. Phase diagram of surface near structures after trench anneal: SON layer (1), SON layer and spheres (2), SON layer with trench joining first (3), two SON layers (4), plane Si surface (5), bubbles (6), two bubbles (7).

- (1) SON layer: the closure of the upper trench openings (splicing) occurs first, the cavities beneath the upper Si layer join each other later;

- (2) SON layer and spherical objects: this development is characteristic for the rather deep medium-radius trenches;
- (3) SON layer with trench joining first: the joining of the deeper parts of the neighbouring trenches occurs before the closure of the upper trench openings and the upper Si layer develops through the rather complicated stages of the surface diffusion process; we consider this process rather unstable;
- (4) Two SON layers: two upper Si layers (and, respectively, 2 layers of an empty space) develop for rather deep and wide trenches;
- (5) plane Si surface: the trenches disappear, and the final Si wafer surface is plane for the shallow trenches;
- (6) Bubbles: the trenches evolve into spherical enclosures which do not join each other for the thin trenches;
- (7) Two bubbles: increasing of the depth of the thin trenches leads to the evolution of two spherical enclosures which do not join the neighboring spheres.

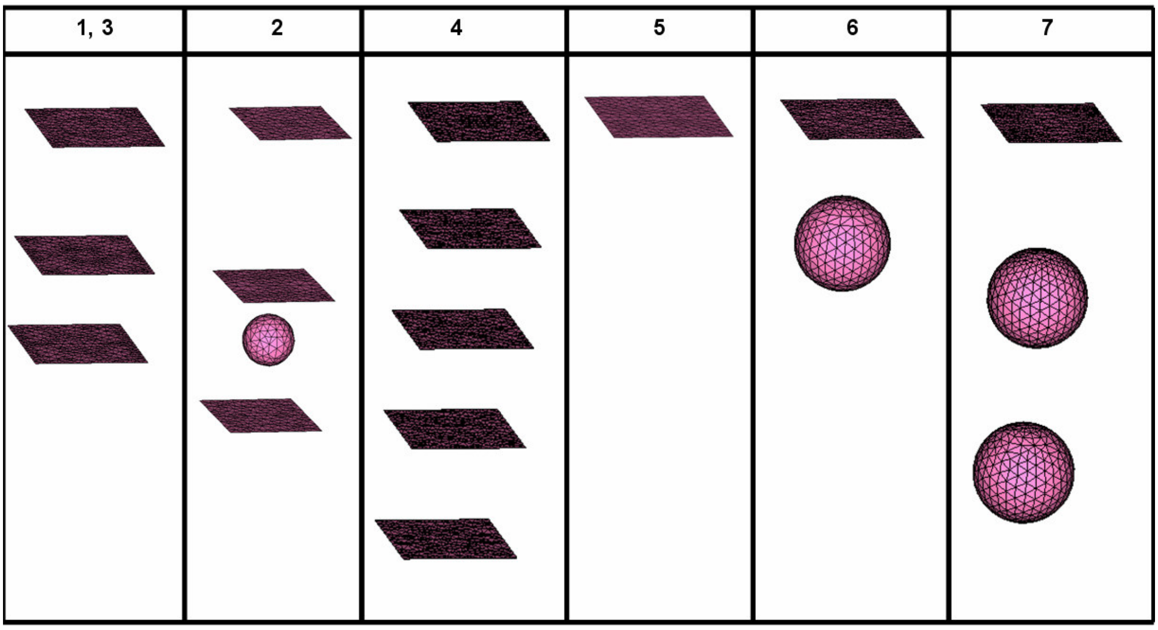

Figure 4. Shapes of surface near structures after trench anneal. Numbers correspond to the depiction of the zones given in Fig. 3-a.

An important result is the dependence of the thickness of the SON layer on the trench shape. The summary of seven optimization campaigns for the cylindrical trenches is given in Table 1. **The 1st to 3rd optimization campaigns** were performed for the standard genetic situation using the standard optimization algorithm. These campaigns illustrate the high stability of the genetic algorithm. The minimum of the upper layer thickness (412 nm) was found at the maximum allowed trench radius and at a trench depth of 1.65 µm. The **4th optimization campaign** considered only the straightforward upper Si layer development when the splicing of the trench entrance occurred first followed by the forming of the joint empty space beneath it. One may consider that the straight genetic algorithm is efficient for the search of the global minimum value but in the same time may be less efficient in minimizing the target function in the vicinity of the local minimum. Therefore **the 5th optimization campaign** was initiated to test the hybrid optimization method combining the standard genetic optimization algorithm and the SIMPLEX algorithm by Nelder&Mead (1965) [17]. One may conclude that the convergence of the hybrid method is faster in comparison with pure genetic algorithm. At the same time there was rather insignificant improvement of the achieved minimum of the upper layer thickness (1.3 %, see Table 1). The configuration leading to a minimum layer thickness (0.63 μm) for zone 1 (splicing first) is located close to the borders of zones 3 and 5, see Fig. 3.

TABLE I. Summary of the optimization campaigns for cylindrical trenches

No	Geometry range	Splicing first	Simplex	Number of runs	Min Δz	R_{opt}	H_{opt}
1	R:0.25-0.45 H: 1- 4	-	-	713	0.466	0.450	1.656
2	R:0.25-0.45 H: 1- 4	-	-	2059	0.415	0.449	1.675
3	R:0.1-0.45 H: 1- 7	-	-	4563	0.412	0.449	1.648
4	R:0.2-0.45 H: 1- 5	X	-	1960	0.639	0.395	2.008
5	R:0.2-0.45 H: 1- 5	X	X	2192	0.631	0.396	2.023

Conclusions

An efficient numerical model of the surface diffusion allows calculating complicated surface restructuring of cylindrical trench arrays during the SON anneal. Very good agreement between experimental and simulated shapes was achieved. The allowed parameter space for layer formation is found and the necessary parameter set to obtain a minimum layer thickness could be predicted. The studies of layer uniformity show that the formation of a continuous layer is possible for rather large range of geometric parameters (radius and depth).

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Authors

Dr.-Phys. Bethers, Uldis
Sennikovs, Juris
Timuhins, Andrejs
Dr.-Phys. Virbulis, Janis
Zablockis, Dmitrijs
Center for Processes analysis and research
Zellu str. 8
LV-1002 Riga, Latvia
E-mail: janis@paic.lv