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Design of silicon-on-nothing structure based on multi-physics analysis

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Abstract. The formation of silicon-on-nothing (SON) structure during an annealing process from the silicon substrate including the trench structures has been considered as an effective technique to construct the structure that has an empty space under the closed flat surface. Previous studies have demonstrated the mechanism of the formation of SON structure, which is based on the surface diffusion driven by the minimization of their surface energy. Also, it has been fragmentarily shown that the morphology of SON structure can be affected by the initial design of trench (e.g., size, number) and the annealing conditions (e.g., temperature, pressure). Based on the previous studies, here, we report a comprehensive study for the design of the cavity-embedded structure (i.e., SON structure). To do this, a dynamic model has been developed with the phase field approach. The simulation results represent that the morphology of SON structures could be detailedly designed, for example the position and thickness of cavity, the thickness of top and bottom layer, according to the design parameters. This study will give us an advantage in the effective design of SON structures.

Keywords: SON structure; morphological design; phase field model; multi-physics analysis

1. Introduction

The fabrication of silicon on nothing (SON) structure from the silicon substrate including the trench structures has been considered as an effective technique to make the empty space under the closed flat silicon surface (Sudoh *et al*. (2009), Ogura (2003), Kuribayashi *et al*. (2003), Kuribayashi *et al*. (2004), Sudoh *et al*. (2004), Lee and Wu (2006)). In order to understand the formation mechanism of SON structure, the theoretical studies have been done and it has been revealed that the mechanism of SON structure formation is based on the surface diffusion driven by the minimization of their surface energy under the annealing process (Sudoh et al. (2004), Mullins (1957), Martin (2009)). The previous studies report that the design of the initial trenches has an important role to determine the final morphology of SON structures (Tanaka *et al*. (1996)). For example, the formation of the empty space in silicon have three typical structures (i.e., sphere,

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pipe and plate) which are based on the design of trench structures (i.e., size of trench and number of trenches) (Mizushima *et al*. (2000)). On the other hand, the morphological evolution of silicon substrate can be well controlled under such appropriate environmental conditions (Tanaka *et al*. (1996), Sato *et al*. (2000), Homma *et al*. (1996)). For instance, the surface migration of silicon atoms is enhanced as the annealing temperature increases (Sato *et al*. (2000)). Also, the annealing needs to be kept in an appropriate pressure condition to remove native oxide and promote smooth surface migration (Sato *et al*. (2004)). The low pressure ambient is efficient since they provide the necessary dangling bonds and promote removal of surface oxide.

Here, we report a comprehensive study for the design of the void-embedded structure (i.e., SON structure). To do this, a dynamic model for the morphological evolution of silicon structure has been developed with the phase field approach. The simulation results shows the various formation of SON structures according to the variation of design parameters. Details of numerical modeling are as follows.

2. Modelling

2.1 Numerical model

In order to describe the formation of SON structure, a three-dimensional (3D) dynamic model based on the phase field approach (Song and Kim (2010), Zhang *et al*. (2011), Song and Kim (2013), Han *et al*. (2014), Yang *et al*. (2015)) was developed. In general, phase field approach is based on the free energy variation to describe the evolution of system. To express the free energy of system, the concentration field, $c(x,y,z,t)$, is introduced and it is defined by the volume fraction of the silicon in the system. The total free energy of the system can be express as (Cahn (1958))

$$G = \int_V [\, f(c) + \frac{1}{2} h(\nabla c)^2 \,] dV \tag{1}$$

where the first term is the bulk free energy and the second term represents the surface energy of the silicon with the phase boundary energy, h. The driving force could be represented by the free energy as $\mathbf{F} = -\nabla(\delta F / \delta c)$ and the total flux generated by the driving force is given by $\mathbf{J} = -M\nabla(\delta F / \delta c)$. M is the mobility of the silicon at 1150 °C. The total flux combined with the conservation of mass requirement obeys a Cahn-Hilliard equation and it gives the governing equation. The governing equation normalized with a characteristic length L_c and time $t_c = L_c^{\,2} / M_c f_0$ and can be written as

$$\frac{\partial c}{\partial t_n} = \nabla \cdot \left\{ M_n \nabla (4c^3 - 6c^2 + 2c - \mathrm{Ch}^2 \nabla^2 c) \right\} \tag{2}$$

where the mobility, M_n, is dimensionless numbers normalized by M_c. The significance of the surface energy of silicon is described by the Cahn number, $\mathrm{Ch} = \sqrt{h / f_0} / L_c$.

To resolve the high-order derivatives in the Eq. (2), a semi-implicit Fourier spectral method is implemented to have a high spatial resolution as well as the large gradients at the interface region.

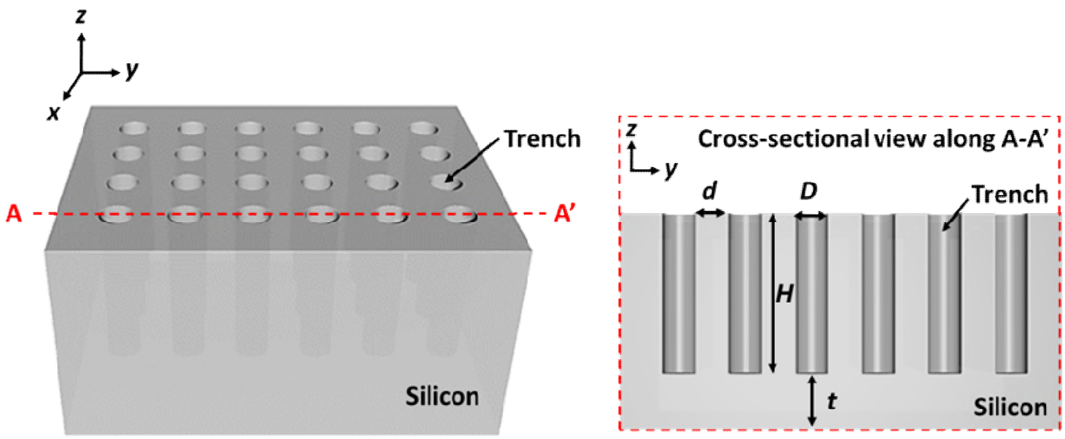

Fig. 1 Schematic illustration of silicon substrate including trenches. Design of silicon structure with the diameter of trench (D), the height of trench (H), the distance between trenches (d), and the thickness of initial bottom layer (t).

The approach satisfies the requirements for the numerical effectiveness and allows the larger time steps without losing numerical stability. Meanwhile focusing on solving the mathematical problems without a harsh time-step constraint, we employed Semi-implicit Backwards Differentiation Formula (SBDF) scheme that has the strongest high-modal decay among the second-order multistep methods (Ascher *et al*. (1995)).

2.2 Scale

The schematic draw of initial silicon structure for the formation of SON structure is illustrated in Fig. 1. An initial silicon structure is represented with the design parameters, such as the diameter (D) of trench, the height (H) of trench, the distance (d) between trenches, and the thickness of initial bottom layer (t). The characteristic length (L_c) is taken to be 100 nm. The simulation domain is set to be 40 × 240 × 100 and, thus, it corresponds the volume of 4 μm × 24 μm × 10 μm. The characteristic diffusivity, D_c, is selected to be 1.0 $\mu m^2/s$ according to the diffusivity of silicone at 1150 °C under the hydrogen pressure of 10 torr (Lee and Wu (2006), Wijaranakula (1990)). The characteristic time, $t_c = L_c^2 / M_c f_0 = 2L_c^2 / D_c$, becomes 2 × 10^{-2} s.

3. Result and discussion

The formation of void-embedded microstructure (i.e., SON structure) from the silicon substrate is numerically investigated with the developed dynamic model. The computational simulations were performed to describe the morphological evolution. Fig. 2 shows the time-dependent simulation results for the formation of SON microstructure. The diameter of the initial trench is 1.0 μm and the height is 4.7 μm. The distance between the trenches is set to be 0.6 μm. During annealing process, array of trenches are transformed to the small voids, and then they are merged to a large plate shaped void. This result agree well with experimental results that the plate shaped

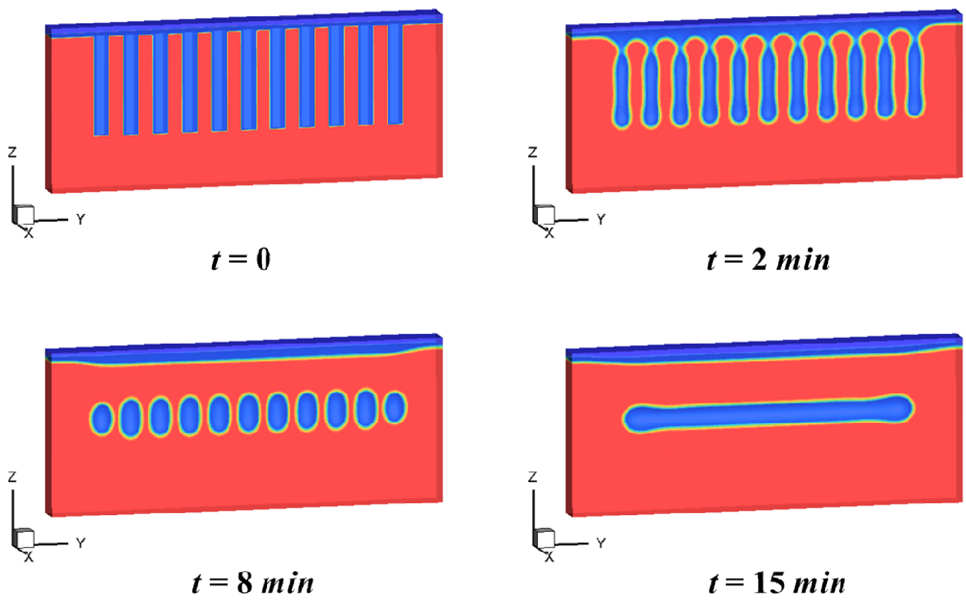

Fig. 2 Time-dependent simulation results for the formation of void-embedded microstructure (i.e., SON structure) during an annealing process. The red and blue regions represent the silicone and air, respectively. Aspect ratio (*H*/*D*) of the initial trenches is 4.7.

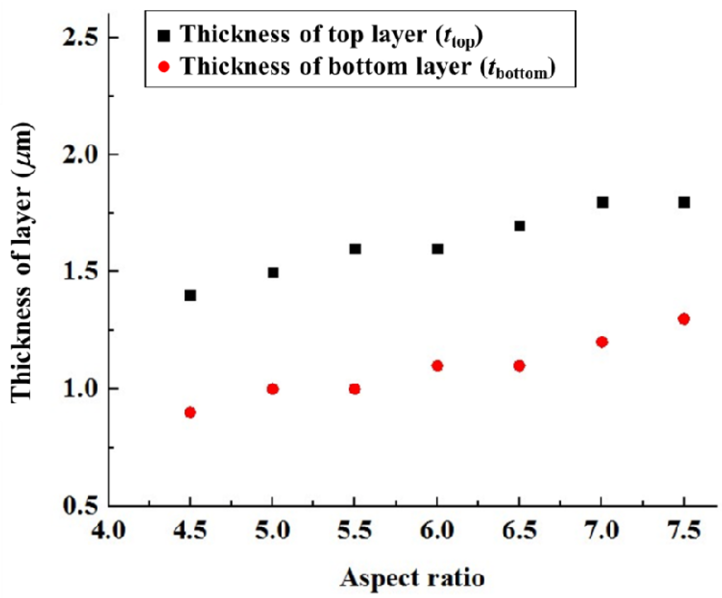

Fig. 3 Thickness of top layer (t_{top}) and of bottom layer (t_{bottom}) of SON structure with respect to various aspect ratios of the initial trenches.

cavity formed in silicon under the aspect ratio (*H*/*D*) ranges approximately from 3.0 to 9.5 (i.e., our aspect ratio is 4.7) (Sato *et al*. (2004)). In addition, we observed that SON structure can be

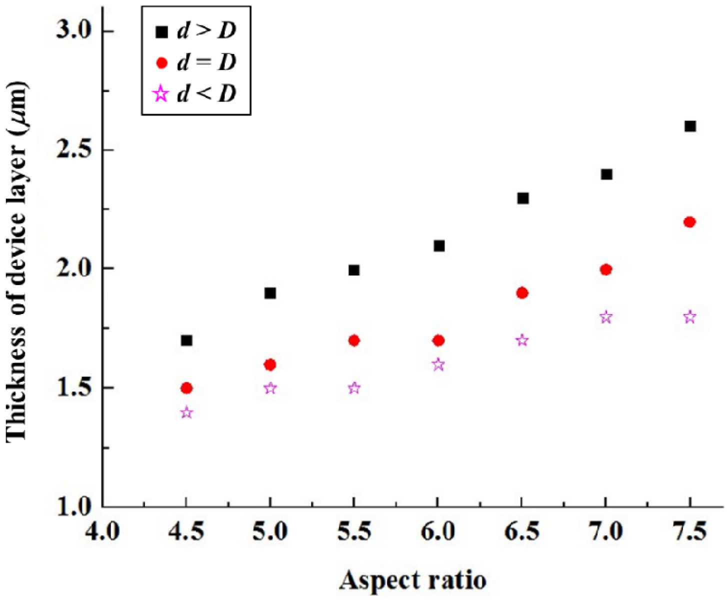

Fig. 4 t_{top} of SON structure according to the relation between the trench distance (*d*) and the diameter of trench (*D*). *D* is fixed as 1.0 μm in all of simulations.

differently formed, such as plate shaped cavity, multiple plate shaped cavity, array of circular shaped voids, and multiple array of circular shaped voids, according to the various combination of design parameters (data not shown).

To analyze quantitatively the final morphology of SON microstructure, the simulations are systematically performed with respect to the initial design of trenches. The transformed microstructure consists of the top layer, the cavity, and the bottom layer. It is necessary to analyze the relationship between the top layer and the bottom layer in the formed microstructure in order to control the position of the cavity. Fig. 3 represents the thickness of top layer (t_{top}) and the bottom layer (t_{bottom}) with the different aspect ratio of the initial trenches. As the aspect ratio increases, the thickness of top and bottom layers increases.

The effect of *D* of the initial trench and *d* between the trenches to the thickness of top layer of microstructure is represented in Fig. 4. *D* is fixed as 1.0 μm in all of the cases and only *d* is varied in a size of 0.6, 1.0, and 1.3 μm, respectively. The result indicates that the thickness of top layer of microstructure is to be thicker as *d* between trenches is increased. The increase of between trenches means the increase of silicon material to form SON structure. Because the total mass of silicon is conserved, the thickness of top layer increases as *d* between trenches increases. Also in the same manner, the thickness of top layer increases with the increase of aspect ratio.

To suggest the strategy for the design of SON microstructure, a series of simulations were performed with various design parameters as shown in Fig. 5(a). In the current work, *D* and *d* are assumed to be same value as 1.0 μm in order to ignore the effect of these two parameters on the device layers. Also, from the various simulations, the relation between the thicknesses of layer of final structure (i.e., t_{top} and t_{bottom}) and thickness of bottom layer of initial structure (*t*) is emerged as $\left(t_{bottom} - 3t_{top}/4\right) < t < \left(t_{bottom} - t_{top}/2\right)$ (data not shown). With this relation, the same thickness of

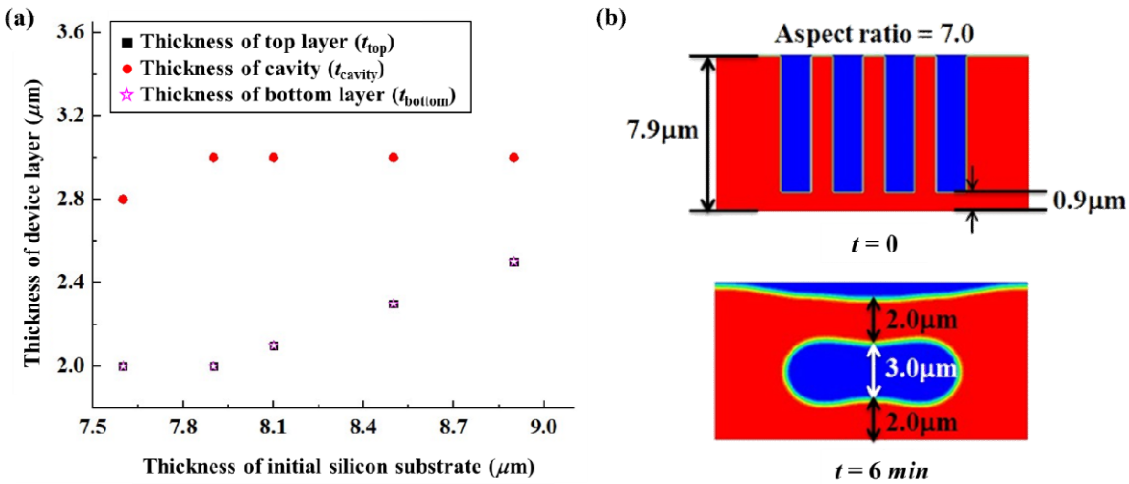

Fig. 5 Different morphological formation of SON structure according to the various design parameters. (a) The position of cavity can be controlled to be located at the center of SON structure (i.e., t_{top} = t_{bottom}). (b) The aspect ratio of the initial trench corresponds to the summation of thickness of transformed three layers (t_{top}, t_{cavity}, and t_{bottom}).

t_{top} and t_{bottom} are achieved. It means that the cavity is placed at the center of the fabricated microstructure. Furthermore, it was revealed that the aspect ratio of the initial trench corresponds to the summation of thickness of transformed three layers (i.e., t_{top}, t_{cavity}, and t_{bottom}). For example, the microstructure that has about 2.0 μm of t_{top} and t_{bottom} is achieved by the selection of t to be 0.9 μm as following above relation. Also, with 2.0 μm of t_{top} and t_{bottom}, 3.0 μm of t_{cavity} is achieved from the initial trench structure that has 7.0 of aspect ratio as shown in Fig. 5(b).

4. Conclusions

The fabrication of void-embedded microstructure from the silicon substrate induced by the annealing process have been investigated with the developed dynamic model. The numerical simulations have demonstrated that the transformation of silicon substrate bases on the surface diffusion which is driven by the minimization of surface energy. The simulation results have shown a reliable design to control the position of the cavity and the size of device layers (t_{top}, t_{cavity}, and t_{bottom}) in the formation of SON microstructure. We believe that our results will give the advantages in an effective design for the fabrication of SON structures.

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