Surface Diffusion Driven Evolution of Periodic Arrays of High Aspect Ratio Holes: Experiment and Simulation

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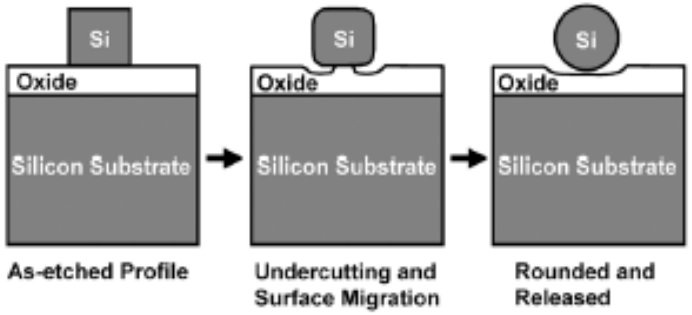
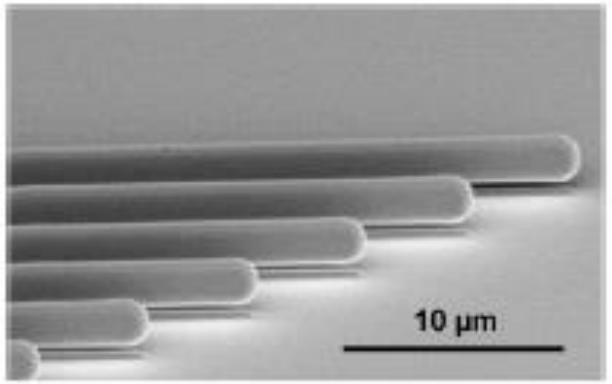
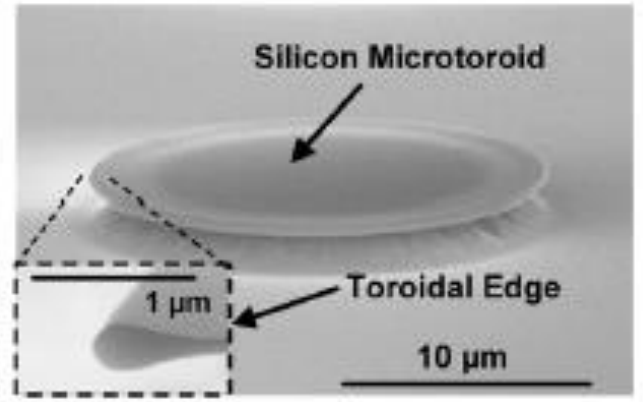
Shape Control of Si Microstructures by High-Temperature Annealing

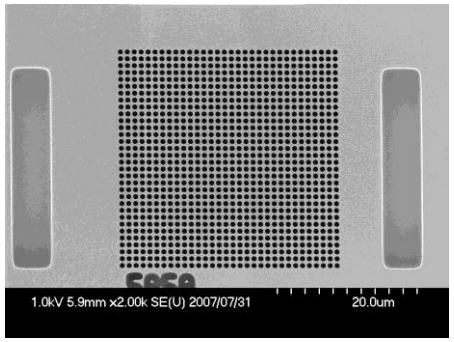




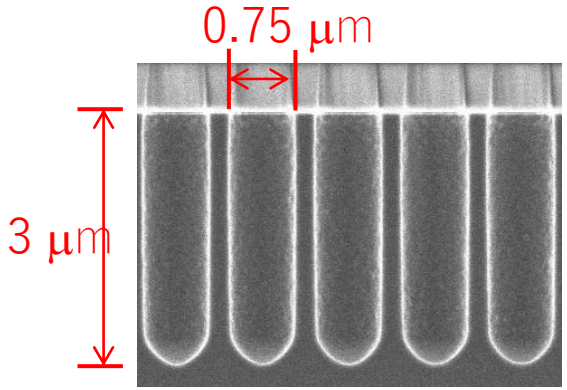


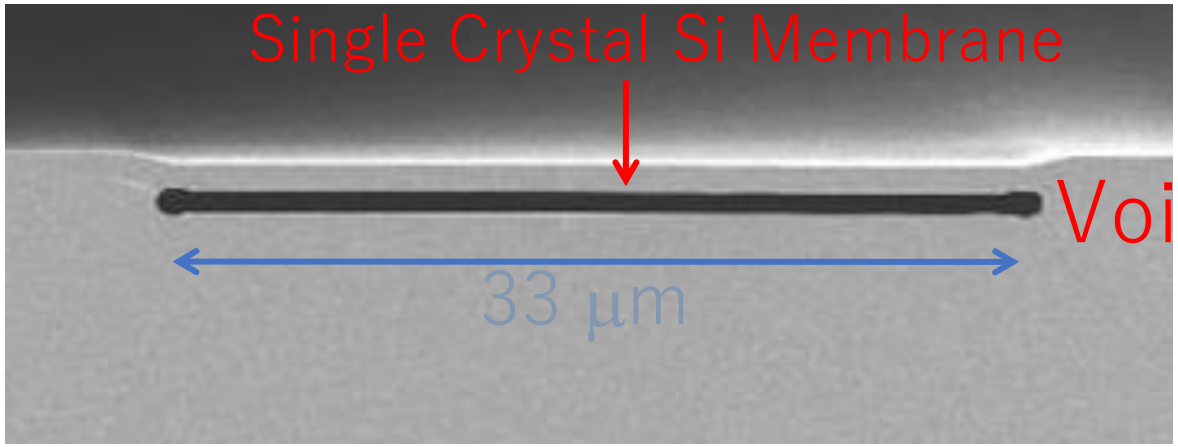
M. M. Lee and M. C. Wu:
J. Microelectromech. Sys. 15, 338 (2006).

Silicon-on-nothing (SON) Structure



Periodic Hole Array on Si



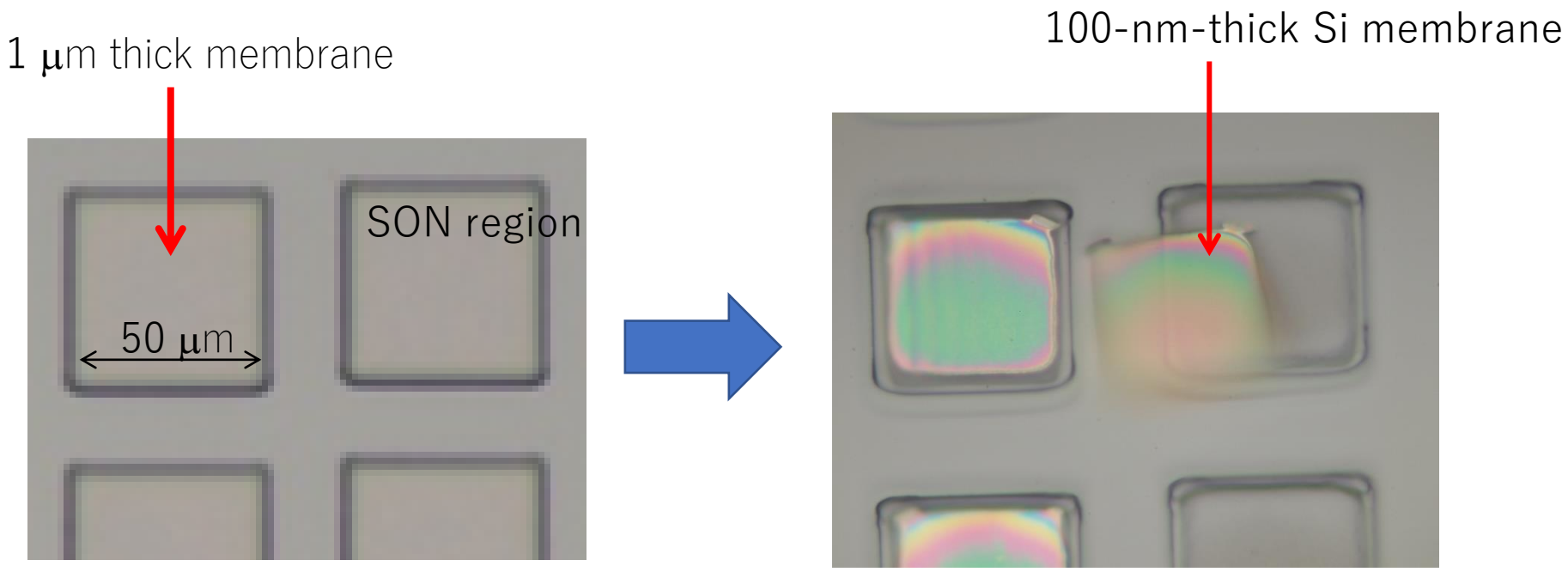


Silicon-on-nothing (SON) Structure

after annealing at 1100 C

I. Mizushima et al., Appl. Phys. Lett, 77 (2000) 3290.
T. Sato et al., Jpn. J. Appl. Phys. 43 (2004) 12.
K. Sudoh et al., J. Appl. Phys. 105 (2009) 083536.

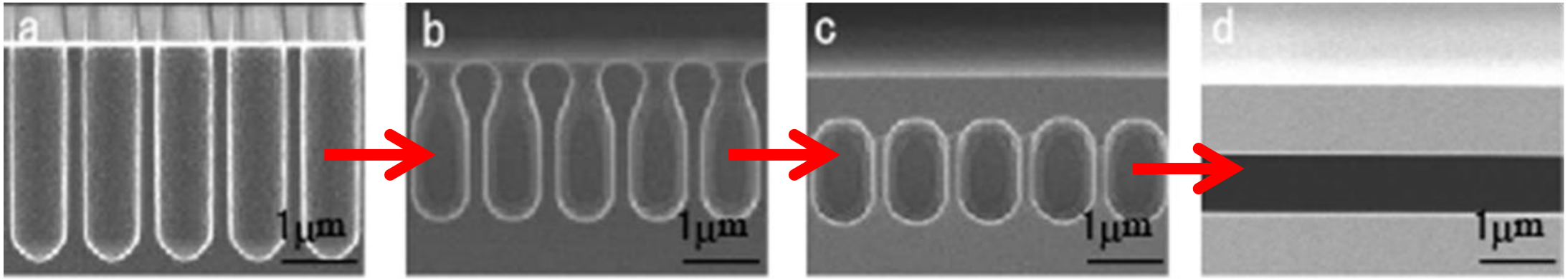
Fabrication of Si Nano-membrane



Reactive Ion Etching

Process of SON Formation

K. Sudoh et al., J. Appl. Phys. 105 (2009) 083536.



Aspect ratio = 3.5

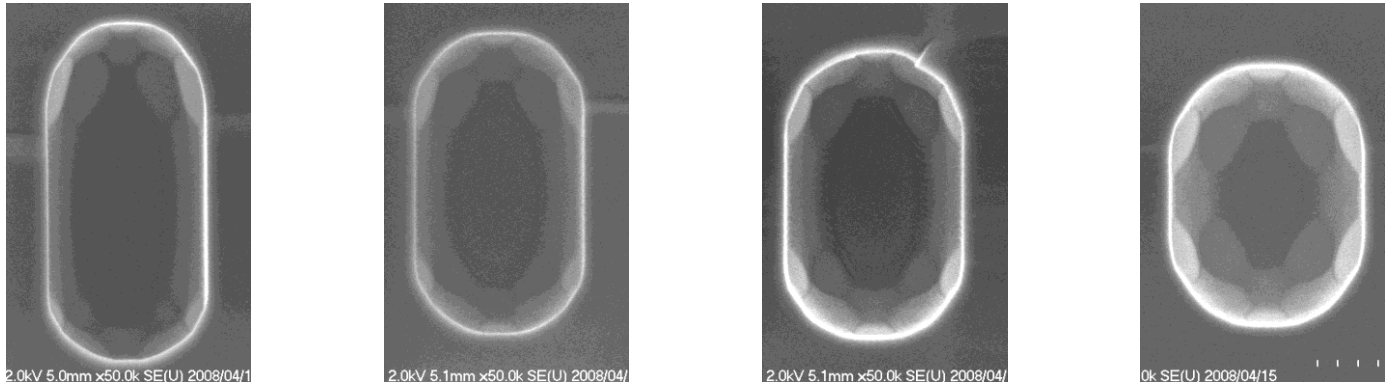
Closure of the hole inlets

Coalescence of voids

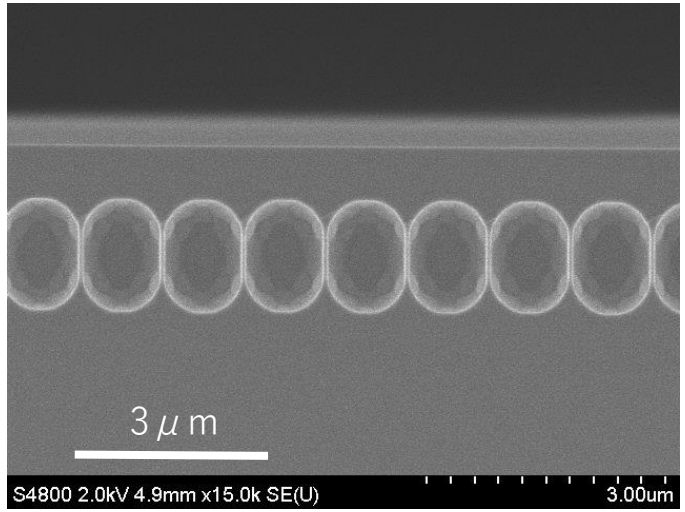
- The SON structures are formed through two steps:

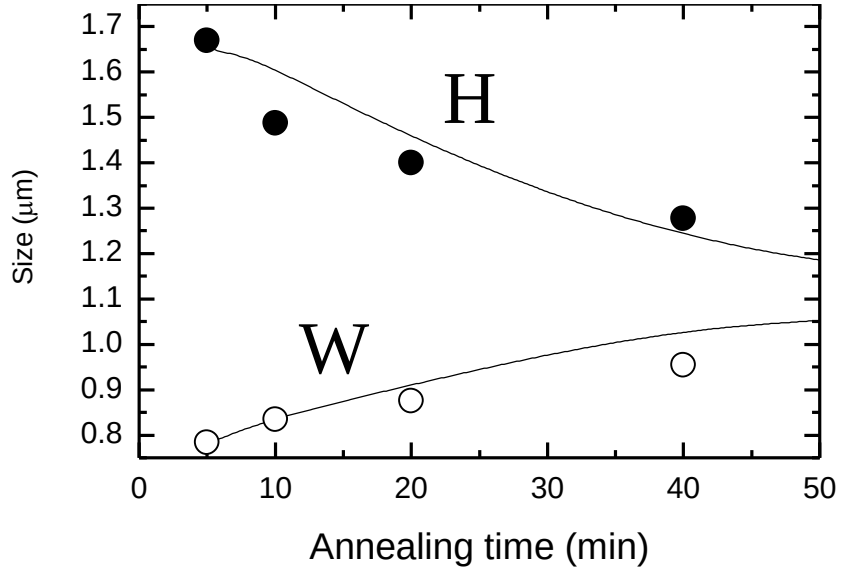
(1) Closure of the hole inlets, forming an array of closed voids.
(2) Coalescence of the closed voids.

Coalescence of Voids through Shape Relaxation



Volume preserving shape relaxation of individual voids.

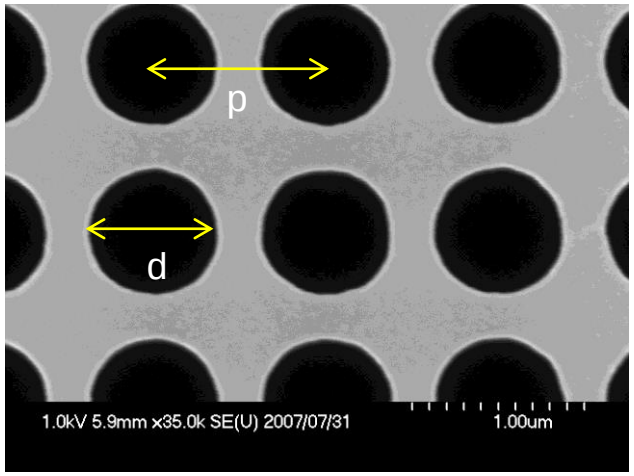


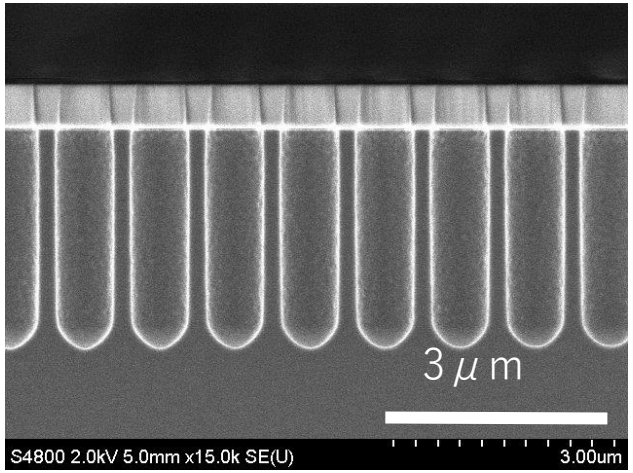


K. Sudoh et al., J. Appl. Phys. 105 (2009) 083536.

Characteristic Sizes of SON

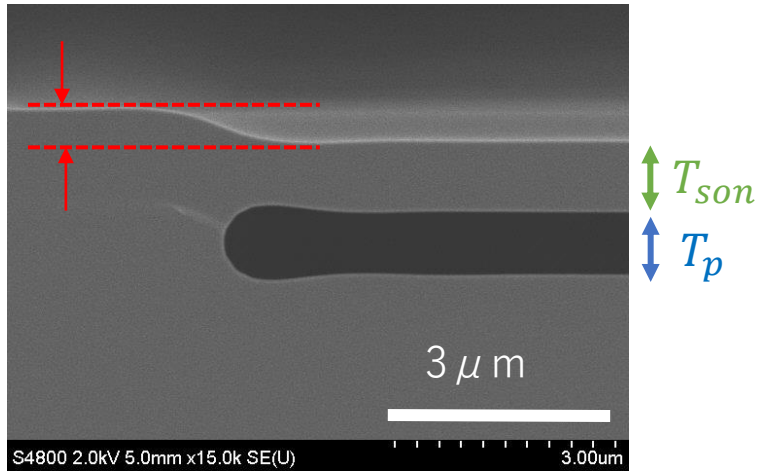
(d, p, l)





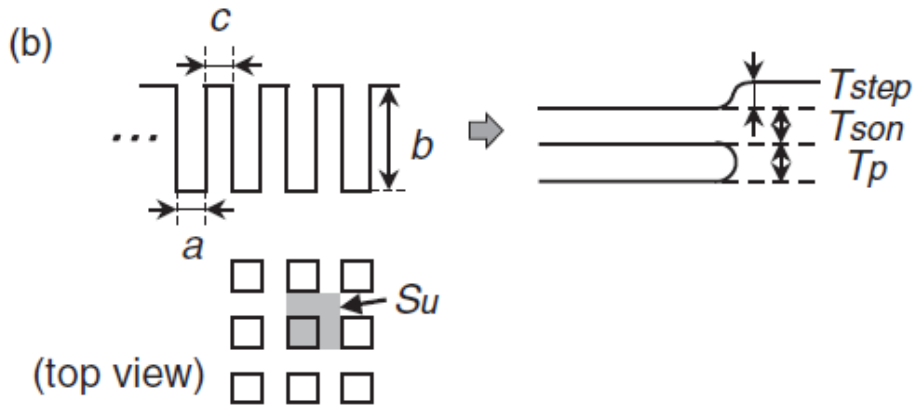
d=0.8 um, s = 0.3 um, l = 3 um

(T_{step}, T_{son}, T_p)



Dependence of the obtained SON structures on initial hole arrays

T. Sato et al., Jpn. J. Appl. Phys. 43, 12 (2004)



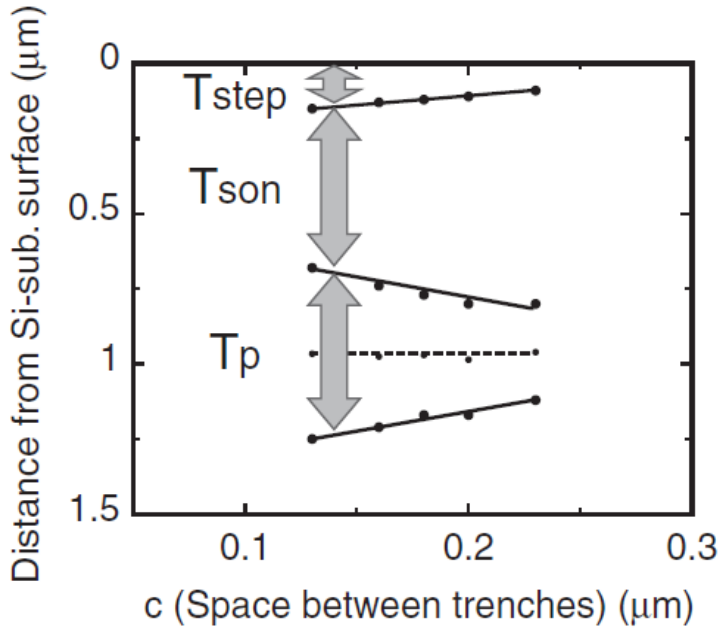
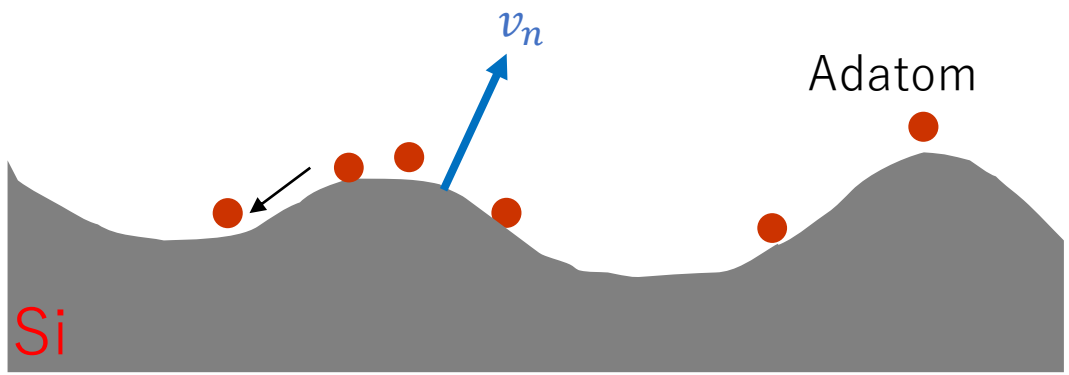


Fig. 6. Initial trench layout dependency of the plate-shaped ESS. The results of the trenches, the diameter of which was 0.22 μm and the aspect ratio was 7.9, are plotted. The thickness of the SON layer decreases as the distance between neighboring trenches decreases. The thickness of the ESS region and the step on the ESS region increase as the distance between neighboring trenches decreases. It was found that the position of the center of the plate-shaped ESS was constant independent of the distance between the trenches and was the same as that of the spherical ESS.

Surface diffusion driven morphological evolution



Gibbs-Thomson Chemical Potential

$$\mu = \gamma \Omega K$$

Mullins Equation

$$v_n = B \Delta_s K$$

v_n: normal velocity of the surface

K: mean curvature of the surface

Δ_s: surface Laplacian

W. W. Mullins, J. Appl. Phys. 28, 333 (1957).

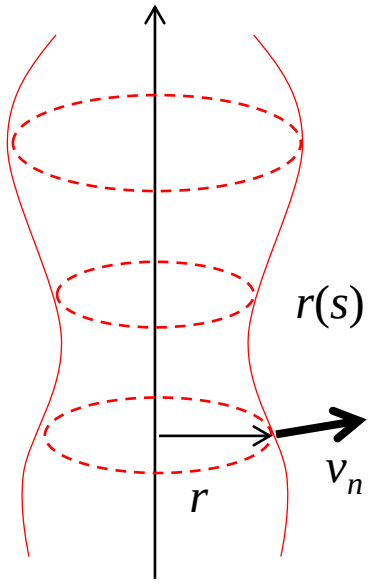
Evolution Equation for Surfaces of Revolution

$$v_n = B\Delta_s K$$

$$v_n = \frac{D_s C_{eq}\Omega}{kTr}\frac{\partial}{\partial s}\left(r\frac{\partial \mu}{\partial s}\right)$$

$$\mu = \gamma\Omega K$$

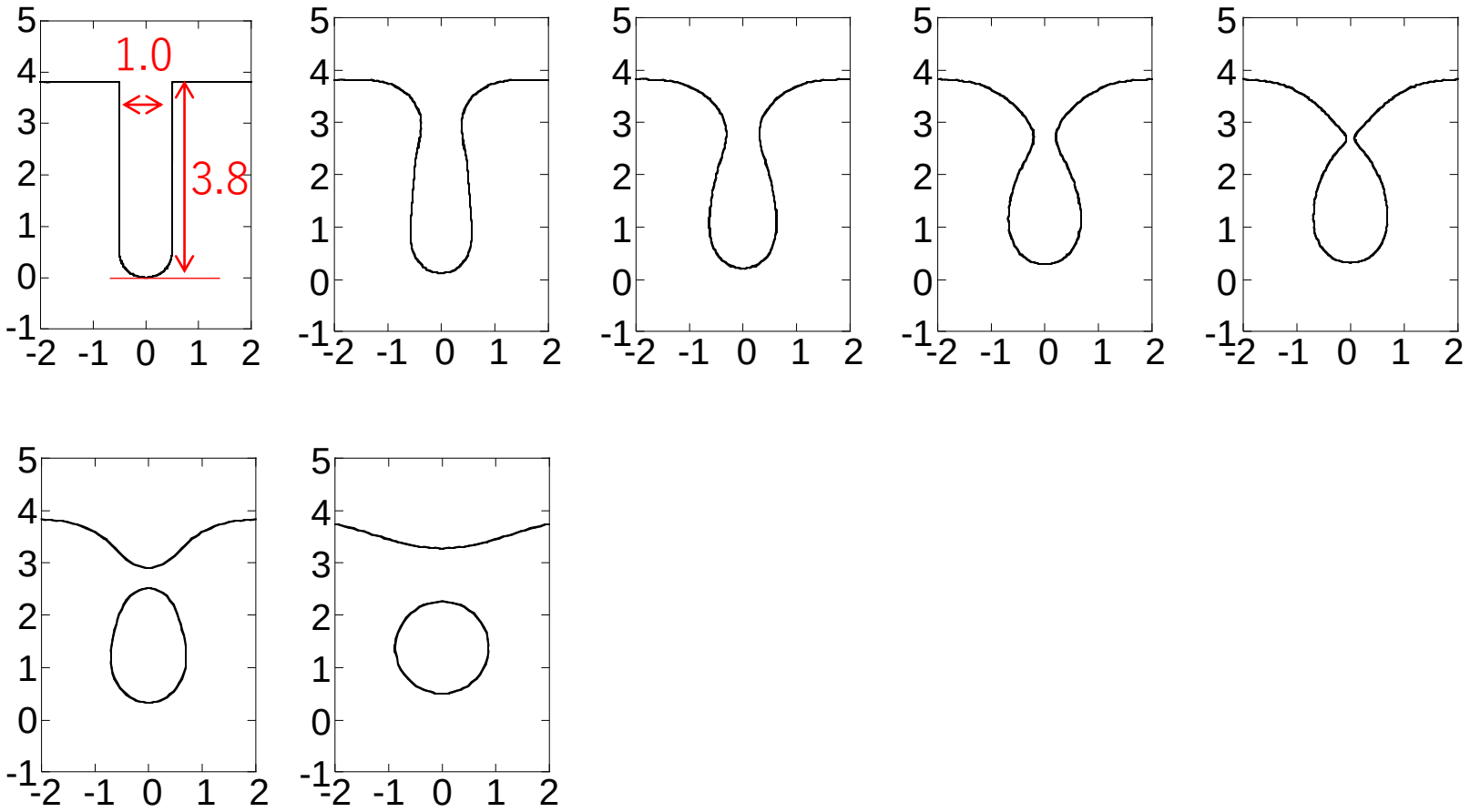
$$K = K_1 + K_2 = \frac{\partial \theta}{\partial s} + \frac{\cos\theta}{r}$$



Cylindrical Coordinates

F. A. Nichols and W. W. Mullins, J. Appl. Phys. 36, 1826 (1965).

Simulation Result: Void Formation



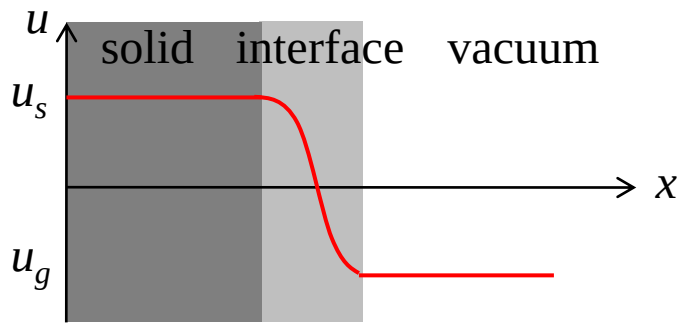
K. Sudoh et al., J. Appl. Phys., 114 (2013) 183512

Phase Field Model

Ref: J.W. Cahn, C.M. Elliott, A. Novick-Cohen, Euro. J. Appl. Math. 7, pp. 287-301 (1996).

Order Paramter: u

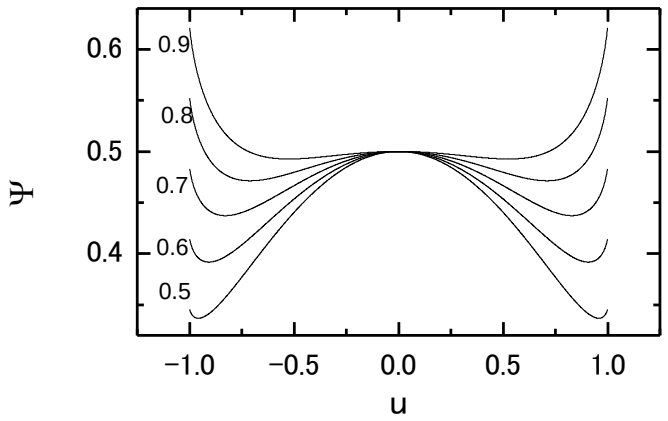
$u = u_s$: solid phase(silicon)
$u = u_g$: vacuum (environment)



Free energy function: $\Psi(u)$

$$\Psi(u) = \frac{1}{2}\theta\{(1+u)\ln(1+u) + (1-u)\ln(1-u)\} + \frac{1}{2}(1-u^2)$$

θ: absolute temperature



Double well form potential

Ginzburg-Landau free energy

$$E\{u(\vec{r})\} = \int \left(\frac{\gamma}{2}|\nabla u|^2 + \Psi(u)\right) d\vec{r}$$

Cahn-Hilliard Equation with Degenerate Mobility

Ref: J.W. Cahn, C.M. Elliott, A. Novick-Cohen, Euro. J. Appl. Math. 7, pp. 287-301 (1996).

$$\frac{\partial u}{\partial t} = -\nabla \cdot \mathbf{J}$$

$$\mathbf{J} = -M(u)\nabla w$$

Chemical Potential

$$w = -\gamma \Delta u + \Psi'(u)$$

Concentration dependent mobility

$$M(u) = 1 - u^2$$

Requirement for θ, γ

Setting $\gamma = \epsilon^2$

Assuming $\theta(\epsilon) = O(\epsilon^\alpha), \alpha > 0$

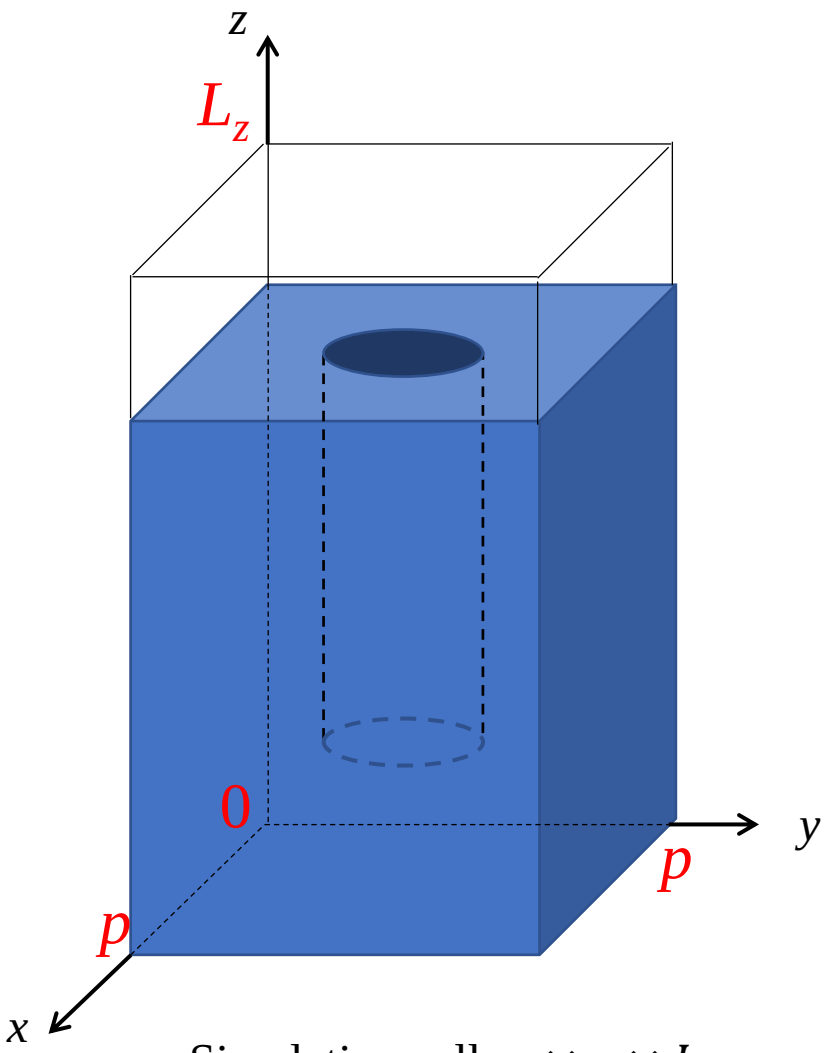
Rescaling time $t \to \epsilon^2 t$

As $\epsilon \to 0$, interface motion is approximately given by

Mullins Equation: $V = -\frac{\pi^2}{16}\Delta_s K$

We need to determine the values of γ and θ that approximately achieve the deep quench limit for numerical calculation.

Setting of the Numerical Calculation



Simulation cell: $p \times p \times L_z$

Initial structure

Square array of cylindrical holes

Boundary condition

x and y: periodic

z:

$$u(x, y, 0) = u_s$$

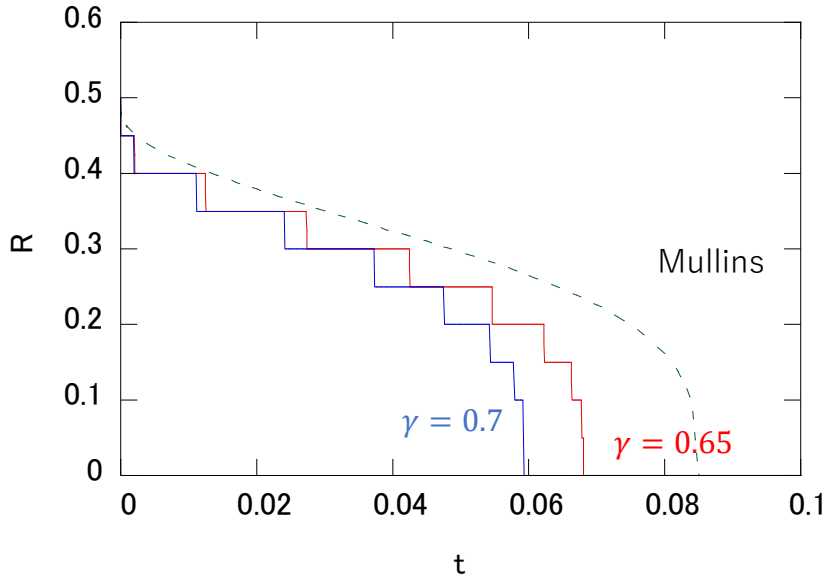
$$u(x, y, L_z) = u_g$$

$$j_z(x, y, 0) = 0$$

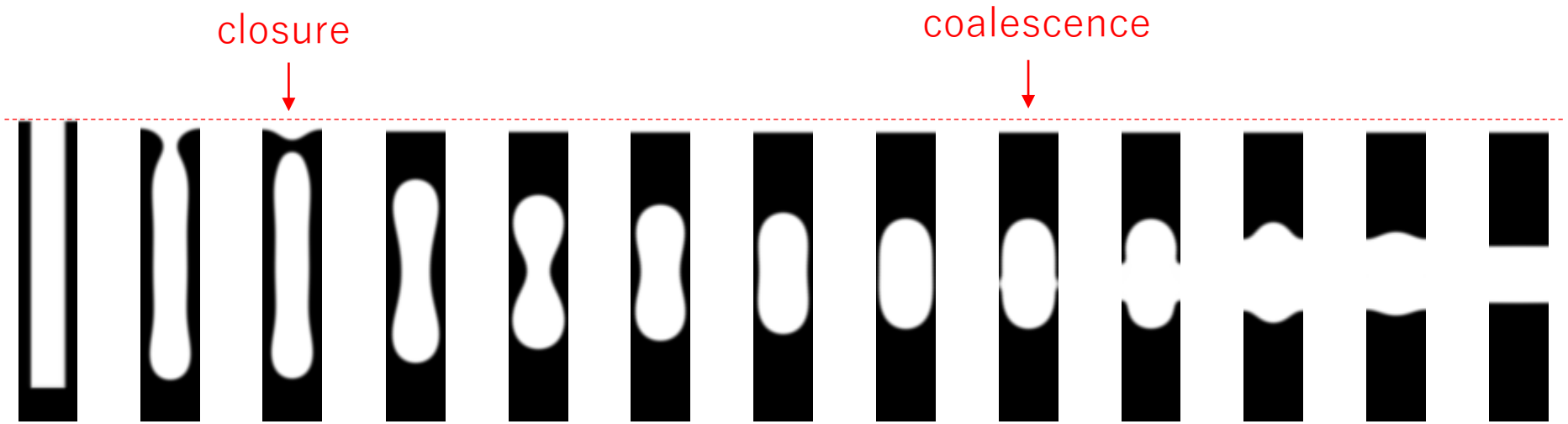
$$j_z(x, y, L_z) = 0$$

Comparison of the phase-field simulations with the sharp interface simulation

$\theta = 0.3$
$\gamma = 0.7$



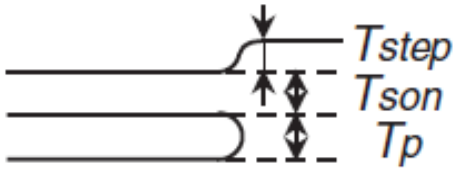
Simulation result of SON formation

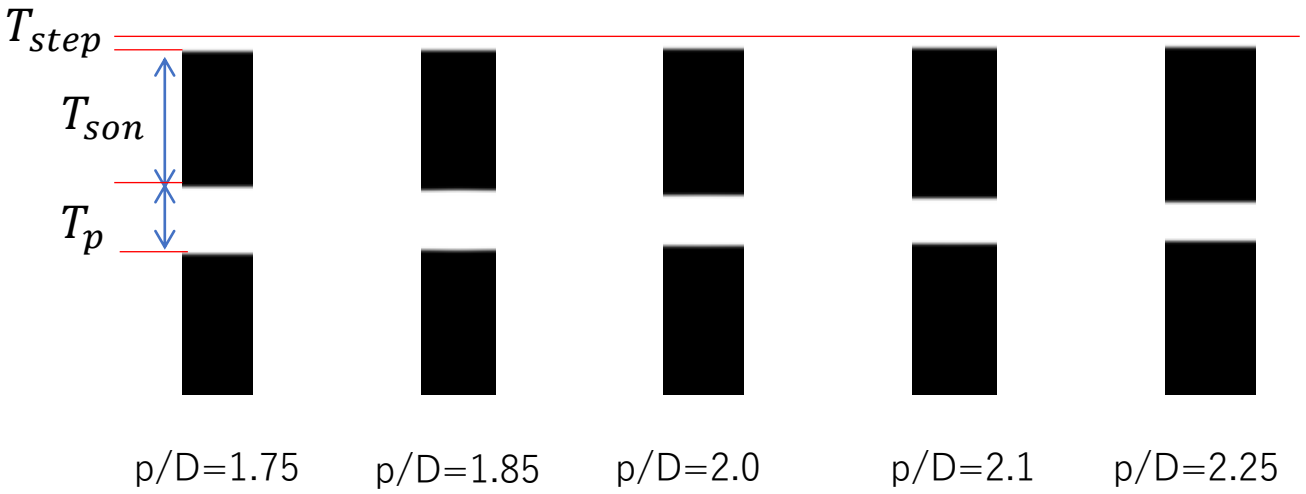


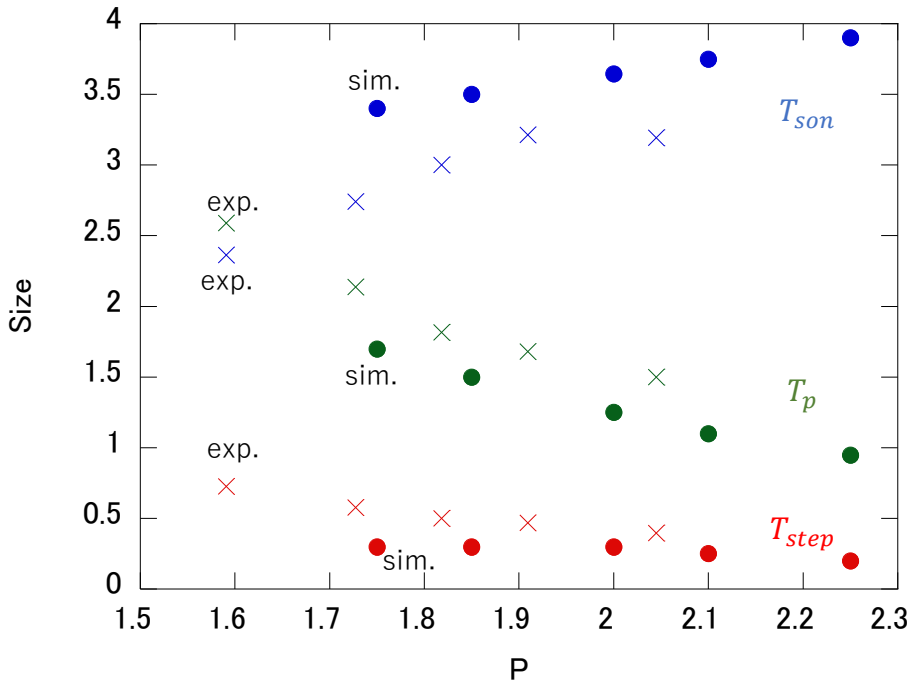
$\theta = 0.3$
$\gamma = 0.7$

AR=7.9, p/D=1.75

Dependence of the sizes of SON structures on the period of the initial hole array

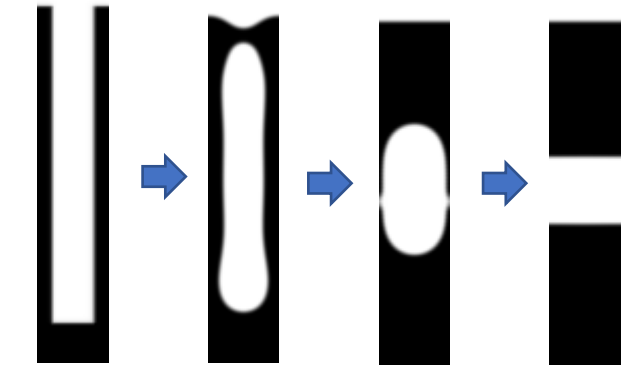


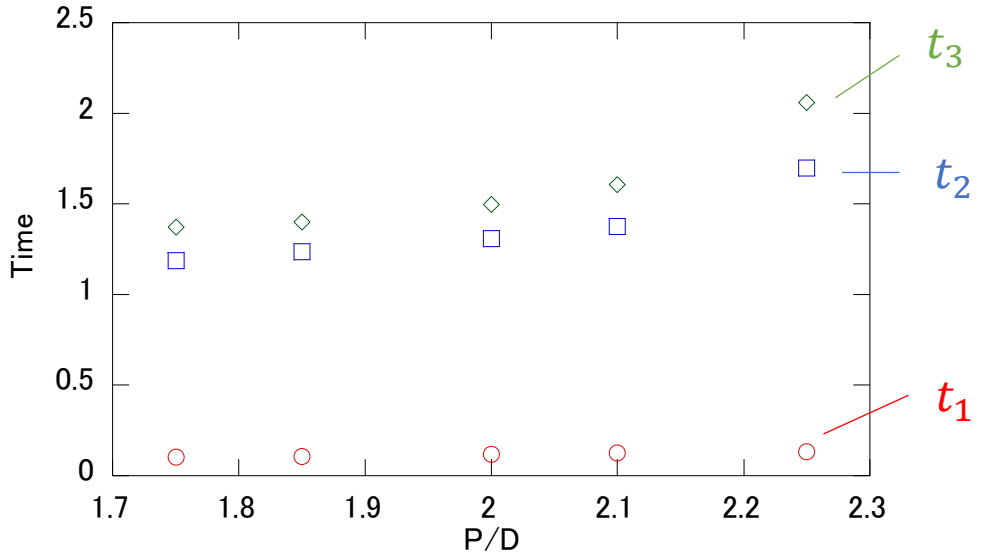




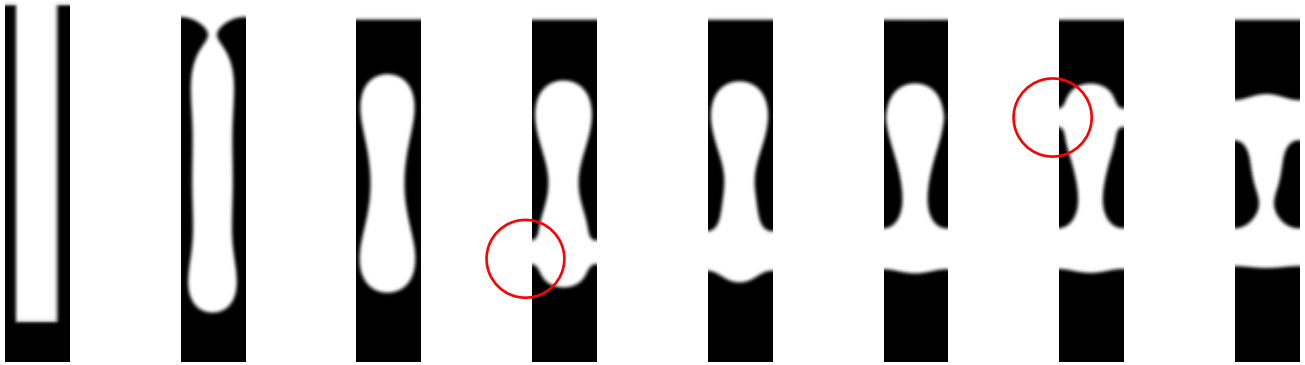
T. Sato et al., Jpn. J. Appl. Phys. 43 (2004) 12.

Prediction of the required annealing time for SON formation





Evolution of a hole array with a smaller period



AR=7.9, p/D=1.6

Summary

When periodic arrays of high-aspect-ratio holes on silicon substrates are annealed at high temperatures, SON structures are formed through surface-diffusion-driven structural evolution.

We have investigated the complicated structural evolution involving topological changes in the SON formation by phase-field simulations.

We have demonstrated that the experimentally observed SON formation processes are well reproduced by the phase-field simulation.

The phase-field simulation can be used to predict the surface-diffusion-driven evolution of the periodic structures.