Evolution of micro-structures on silicon substrates by surface diffusion

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Microstructure Fabrication applying Spontaneous Shape Transformation by Annealing

Collaboration with:

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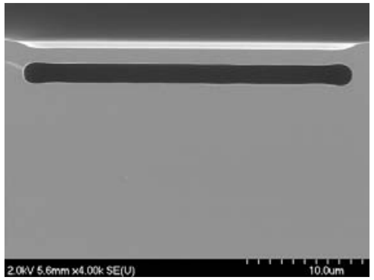
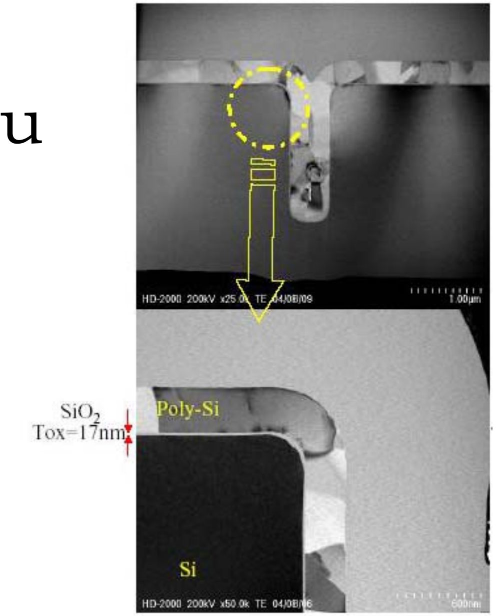
Fuji Electric Group
H. Iwasaki Osaka University



Silicon-on-nothing

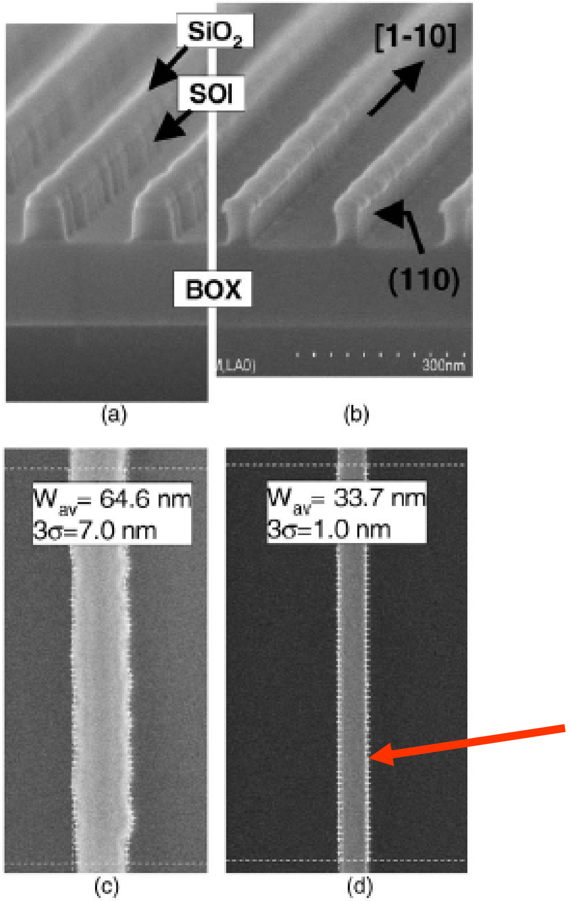


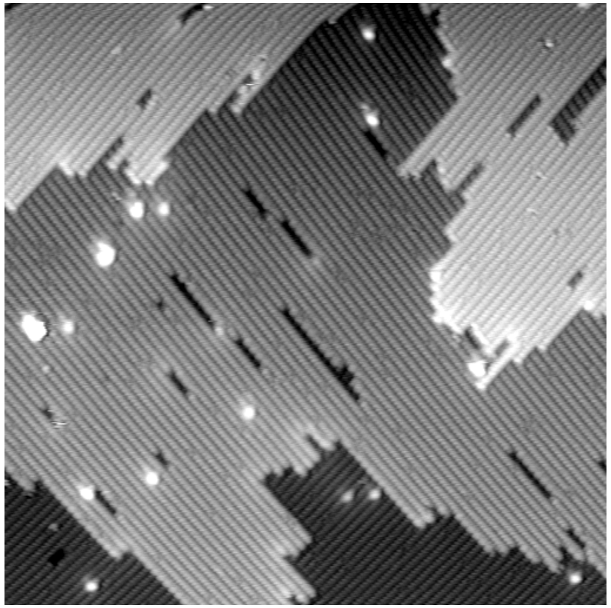
Trench MOSFET

Useful in fabrication of 3D structures on Si surfaces

- Trench corner rounding
- Formation of empty space in Si

Flattening of Surfaces

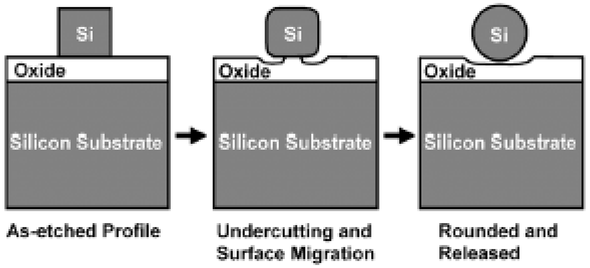


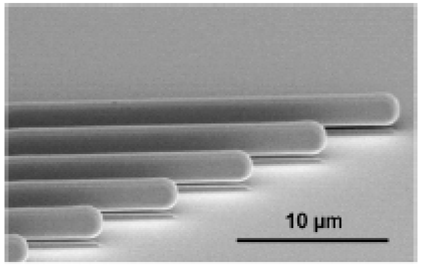


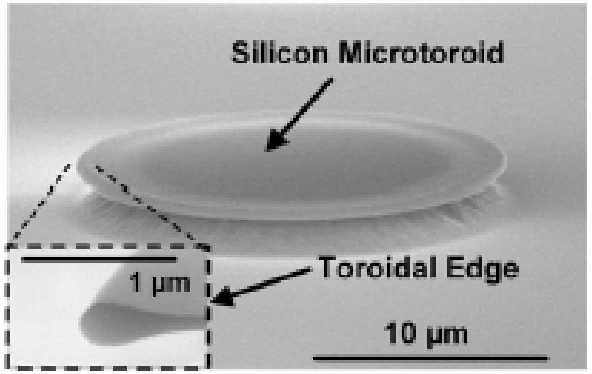
(110) facet formation on sidewall of fin structures

T. Tezuka et al., Appl. Phys. Lett. 92, 191903 (2008).

Shape Modification







toroidal structure

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

Outline

I. Shape transformation of 1D gratings

Trench corner rounding during annealing

Mass transport mechanism for shape transformation

Analysis based on Mullins' equation

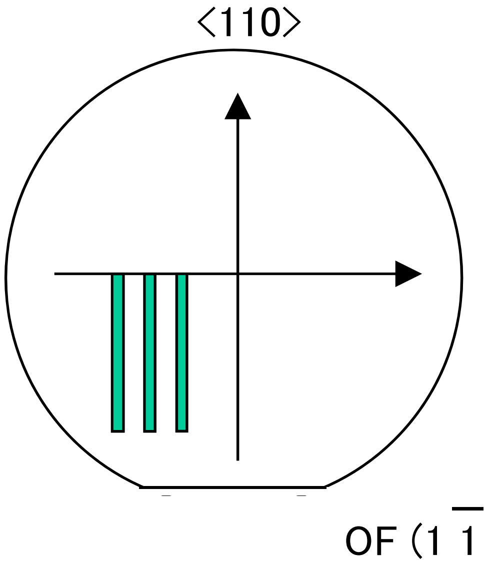
II. Shpe transformation of high –spect-ratio hole patterns

Void formation via shape transformation

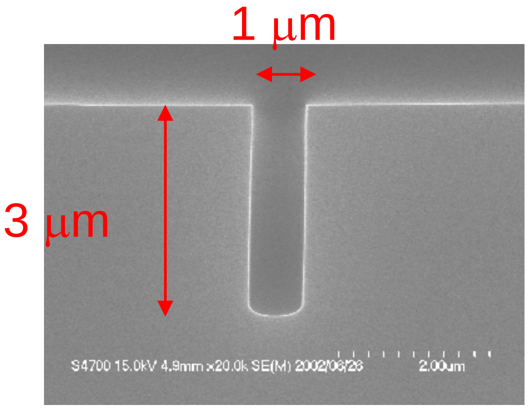
Shape change of faceted voids

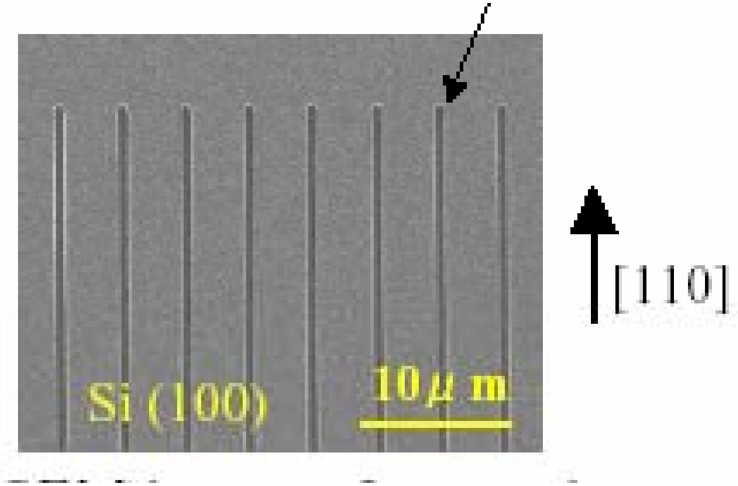
Modeling of the evolution of faceted structures

Fabrication of 1D gratings on Si(001)



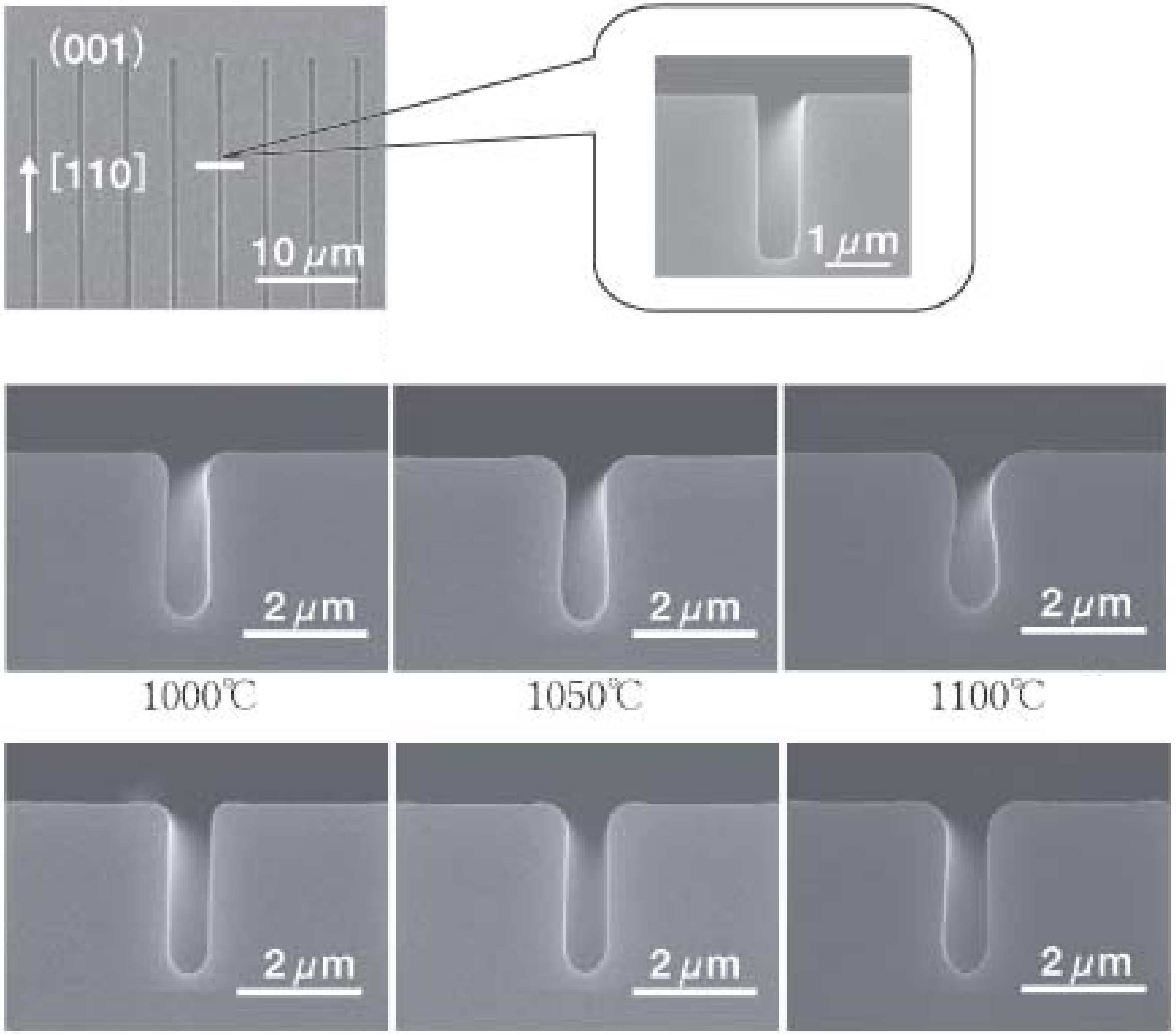
6inch ϕ
N−Si(100)
2～3Ω cm





Fabrication of a 1D trench array
by reactive ion etching on Si(001)

Trench corner rounding by annealing

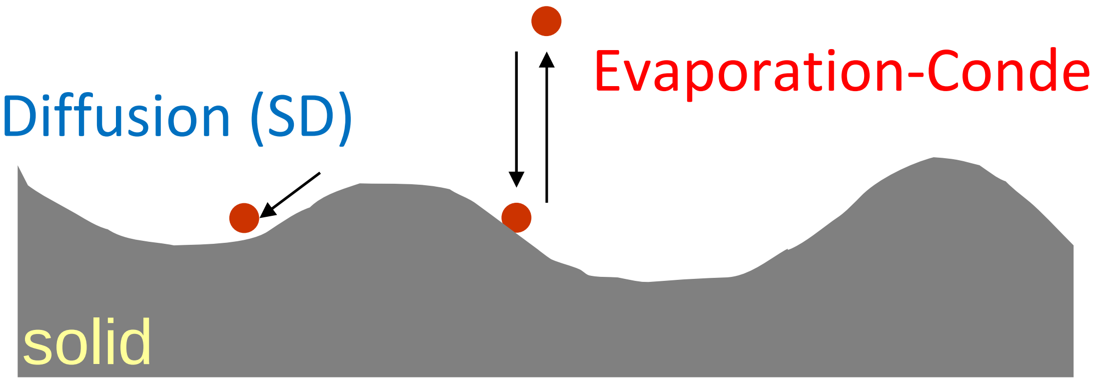


for 3 min

1 min
3 min
10 min

at 1000 C

Mechanism of Morphological Evolution



Surface Diffusion (SD)

Evaporation-Condensation(EC)

solid

Gibbs-Thomson Effect

Curvature Dependence of Chemical Potential

$$\mu(K) = K\gamma\Omega$$

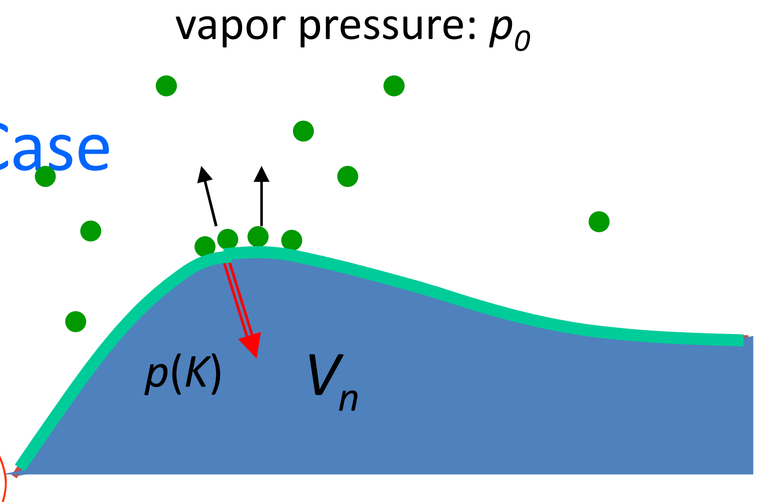
Curvature Dependence of Vapor Pressure: $P_{eq}(K)$

$$\ln\frac{P_{eq}(K)}{P_0} = \frac{\gamma\Omega}{kT}K$$

Mullins Equation for Evolution of Isotropic Surfaces

W. W. Mullins: J. Appl. Phys.

1) Evaporation-Condensation Case

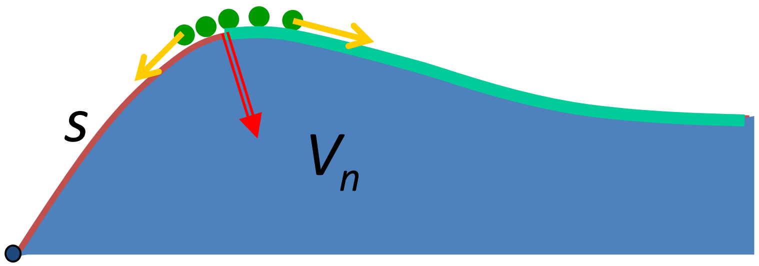


$$v_n = \vartheta_0 \Omega \left[1 - \exp\left(\frac{\gamma\Omega}{kT} K\right)\right]$$

$$v_n = A_1\left[1 - \exp\left(A_2 K\right)\right] \approx -A_1 A_2 K$$

Curvature

2) Surface Diffusion Case



$$v_n = \frac{D_s \gamma \Omega^2 X_s}{kT} \frac{\partial^2 K}{\partial s^2} = B \frac{\partial^2 K}{\partial s^2}$$

Predictions from Scaling Argument

Time scaling of the trench corner radius: $R \propto t^{\alpha}$

1) Evaporation-Condensation Case

$$v_n \propto \quad K = \frac{1}{R}$$

$$\frac{dR}{dt} \propto R^{-1}$$

$$R \propto t^{1/2}$$

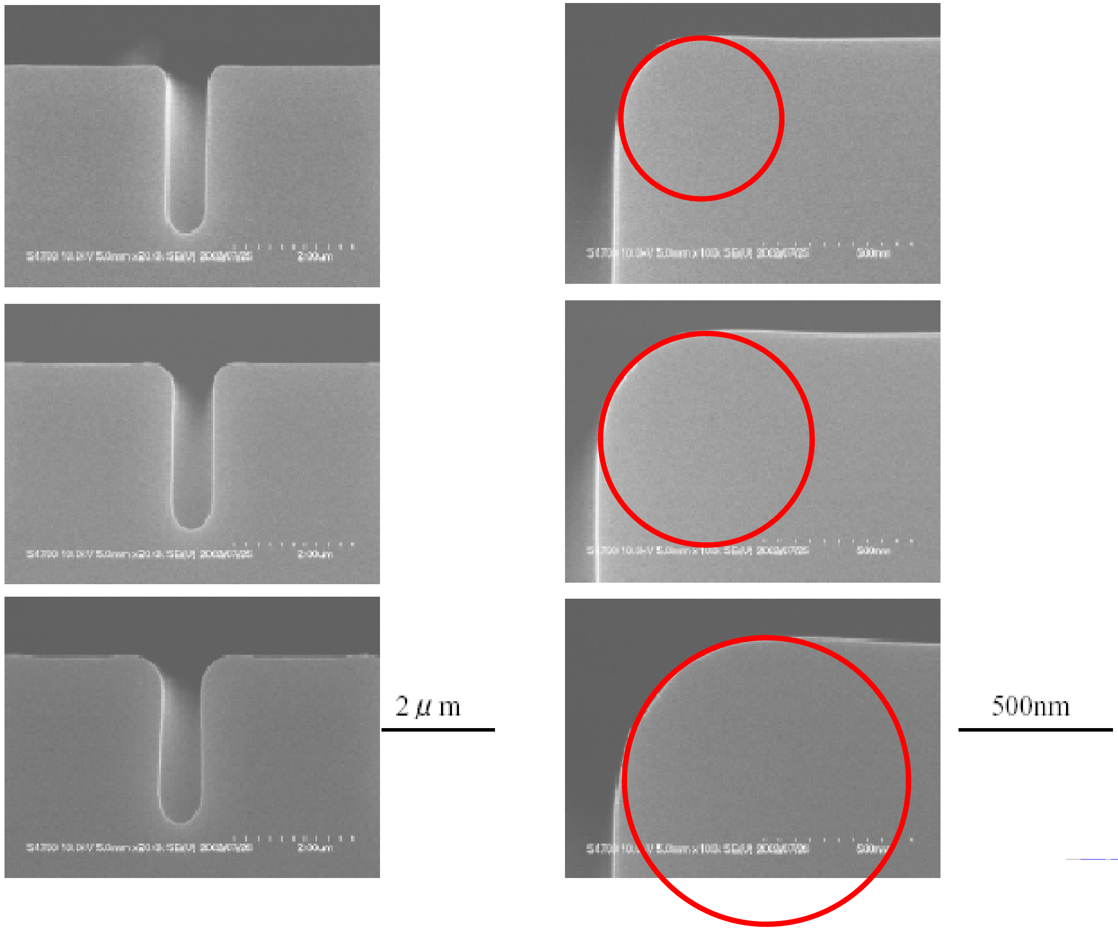
2) Surface Diffusion Case

$$v_n \propto \frac{\partial^2 K}{\partial s^2}$$

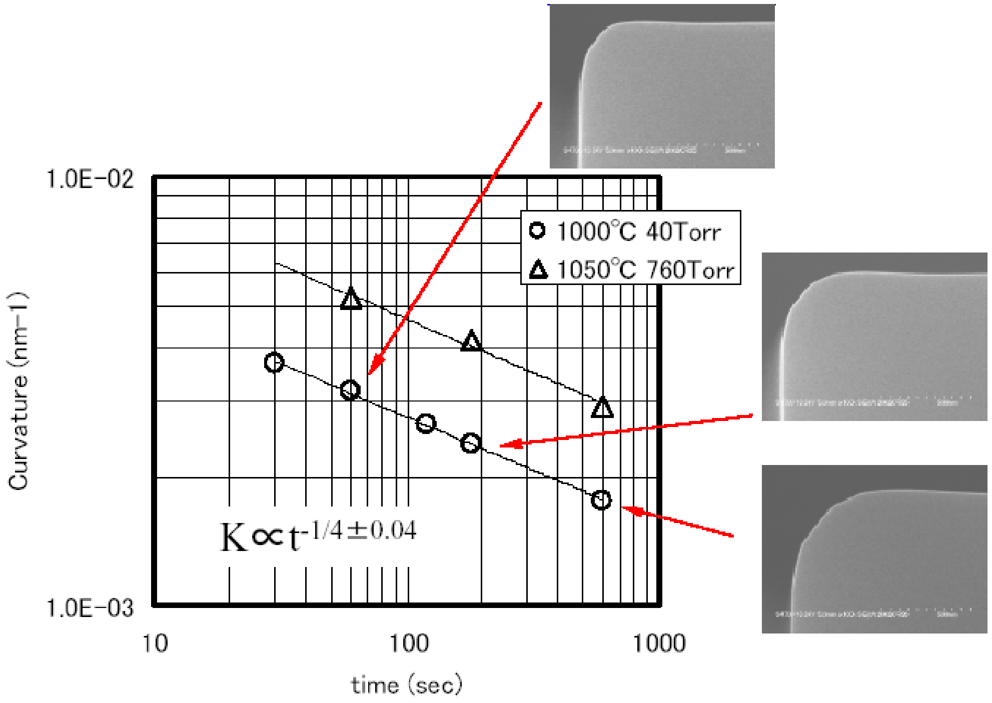
$$\frac{dR}{dt} \propto R^{-3}$$

$$R \propto t^{1/4}$$

Corner Rounding of 1D Trenches

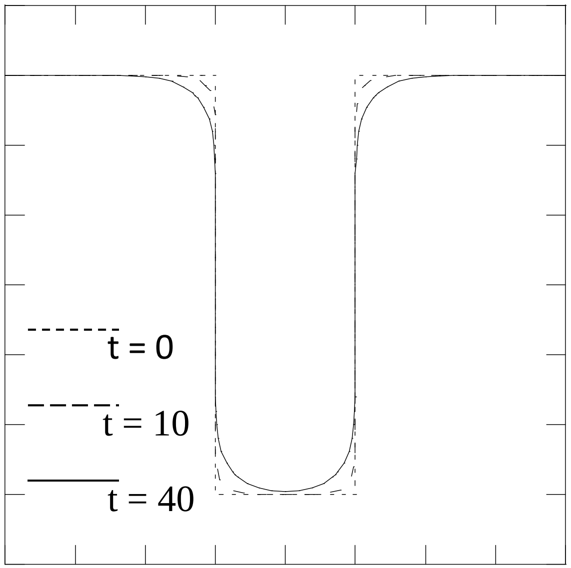


Annealing time dependence of curvatures of trench corners

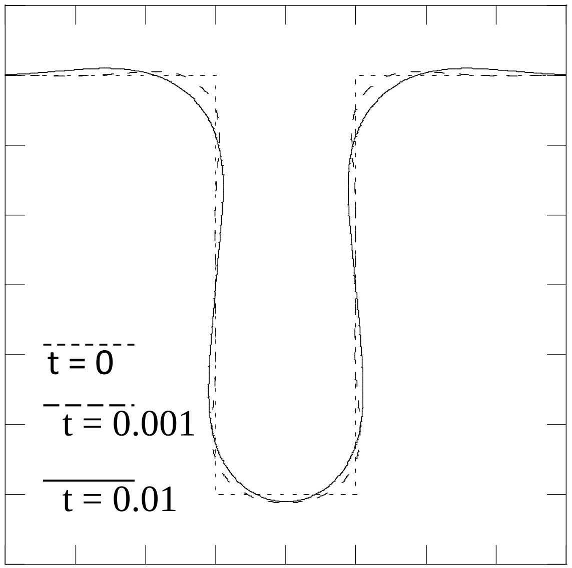


$R = t^{1/4}$ → Surface Diffusion

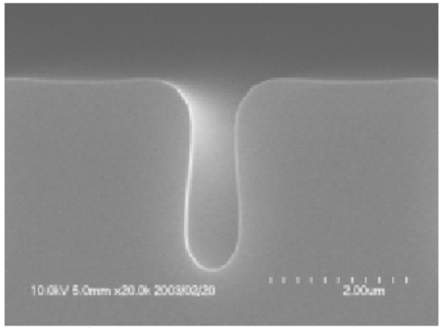
Shape Transformation by Mullins Equation for EC and SD



Evaporation-Condensation

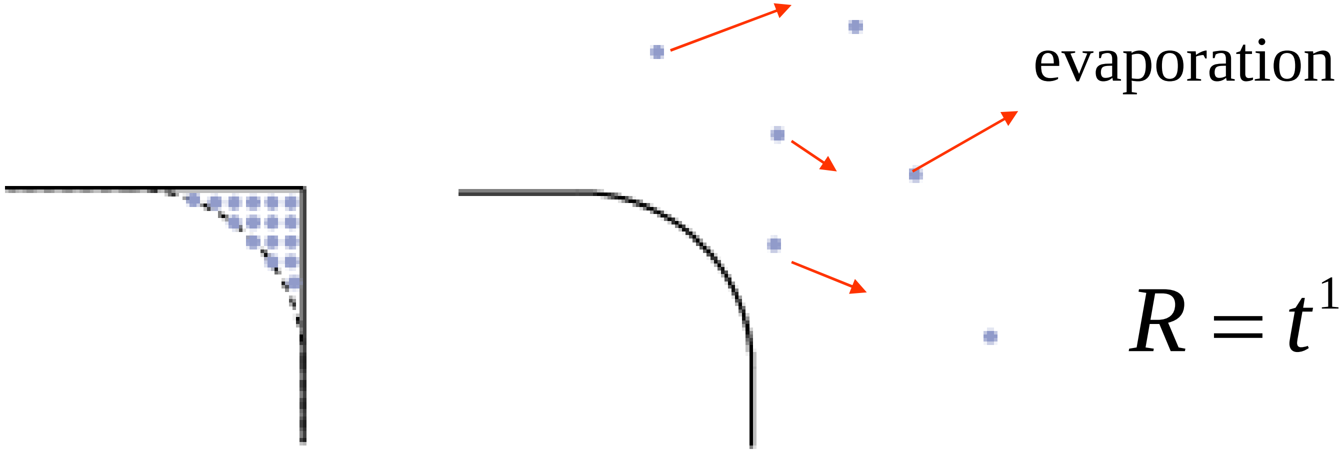


Surface Diffusion



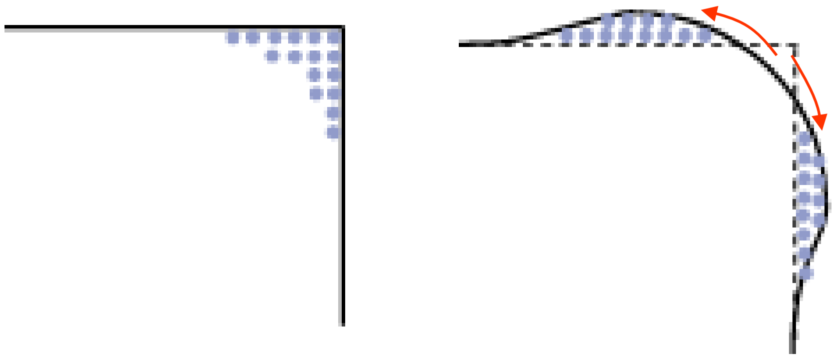
ArH 1000°C760Torr600s

Difference between EC and SD



$$R = t^{1/2}$$

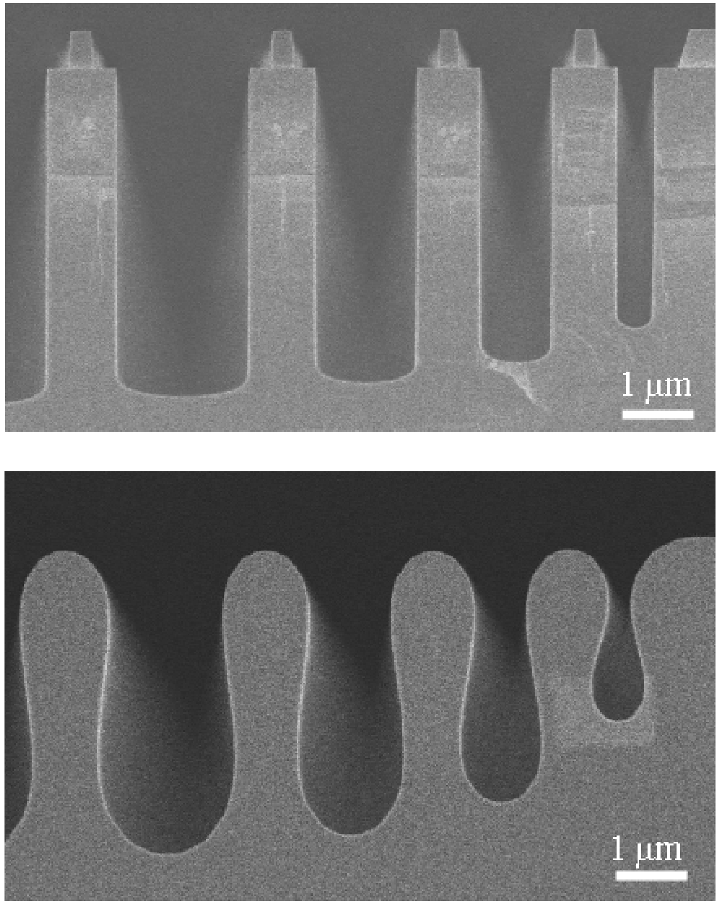
Evaporation and Condensation



$$R = t^{1/4}$$

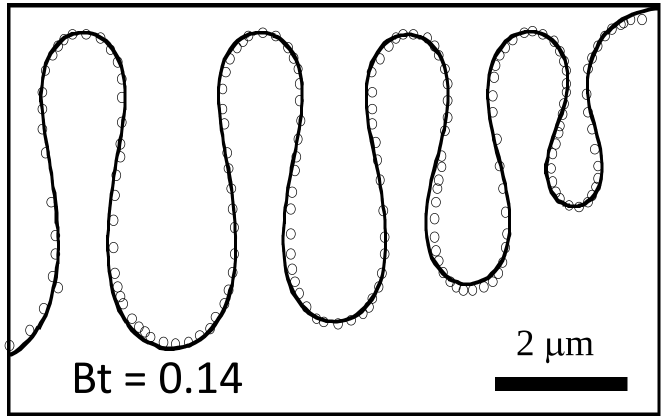
Surface diffusion

Simulation using Mullins Equation



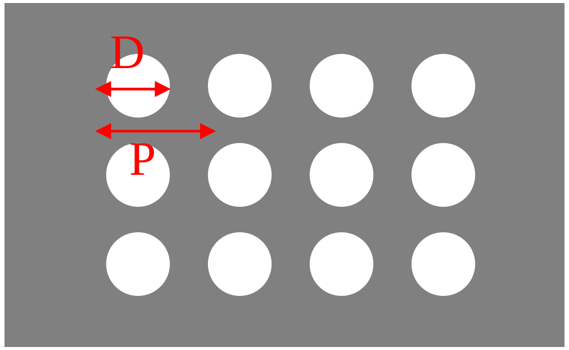
SEM Images

4%H_2/Ar 760Torr
1150 ºC
5min

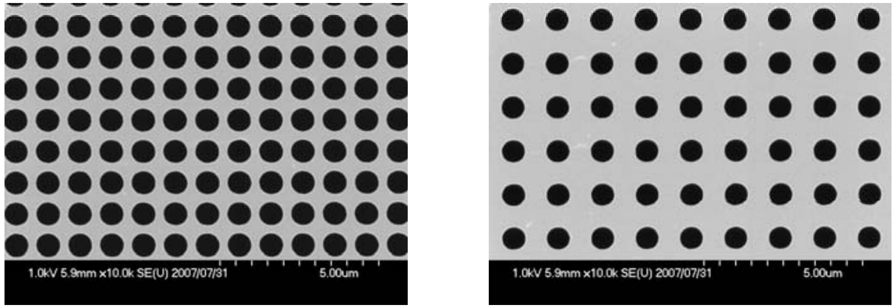


Simulation

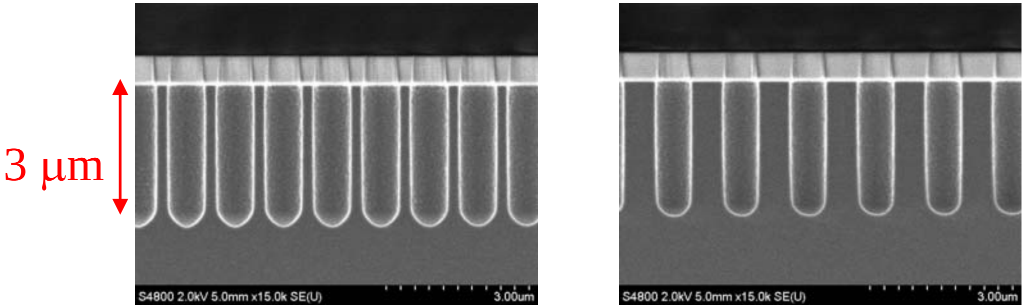
Square Array of Cylindrical Holes



Top View



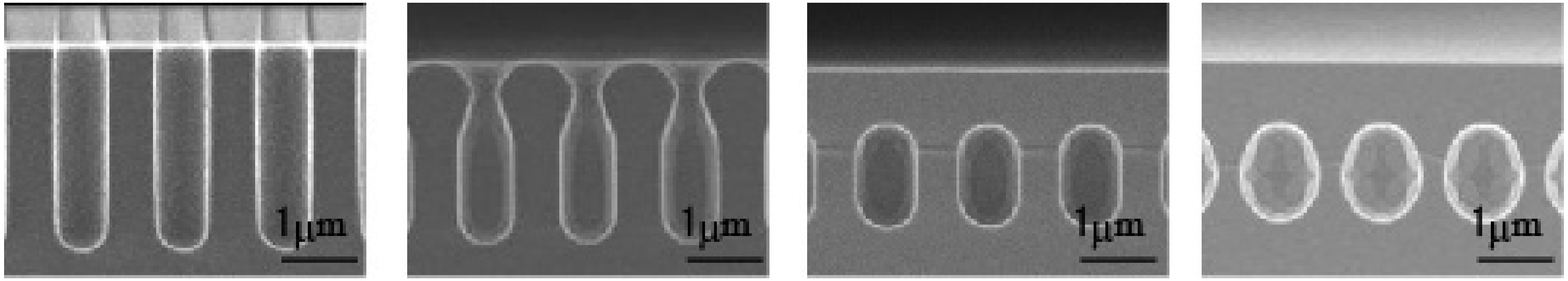
top view



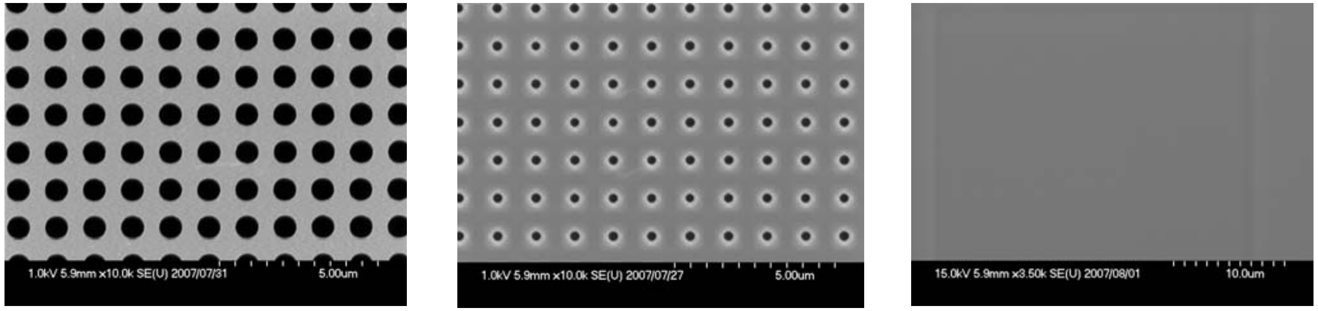
cross section

D = 0.75 μm, P = 1.0 μm   D = 0.75 μm, P = 1.8 μm

Void Formation by Shape Transformation of Hole Array

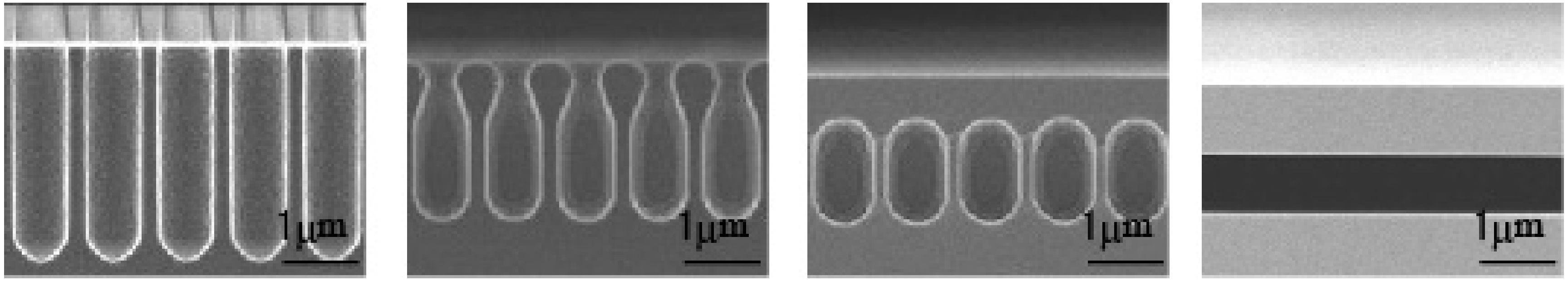


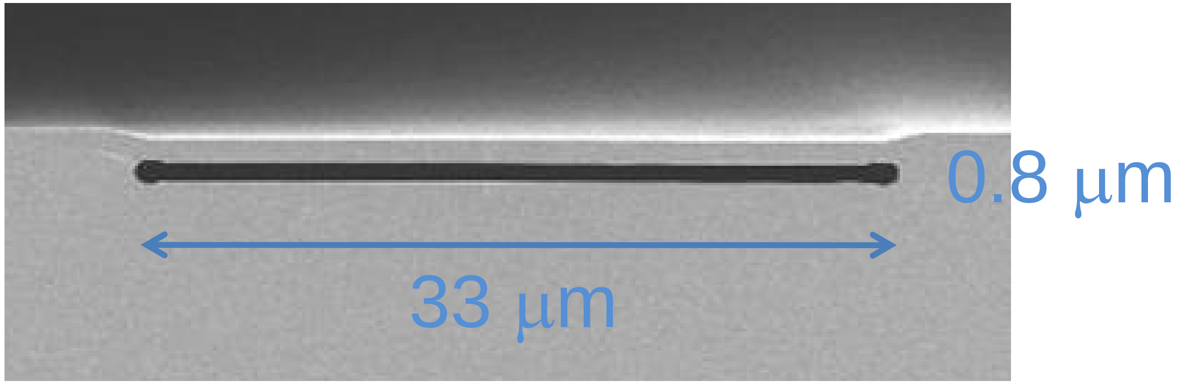
Cross section



Top view

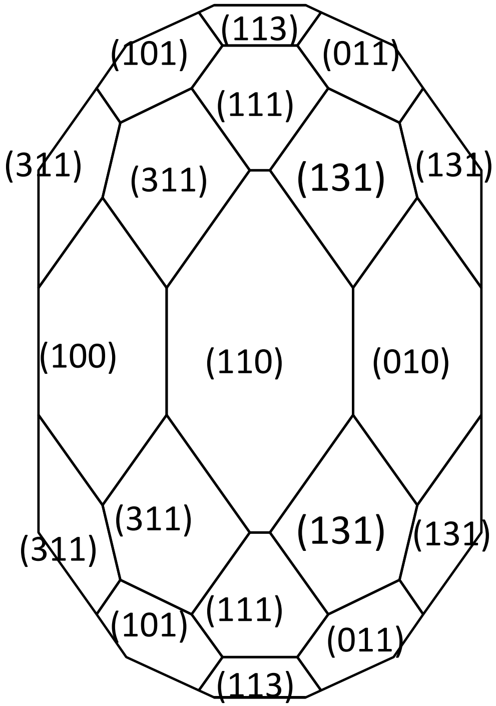
Silicon-on-Nothing (SON) Structure

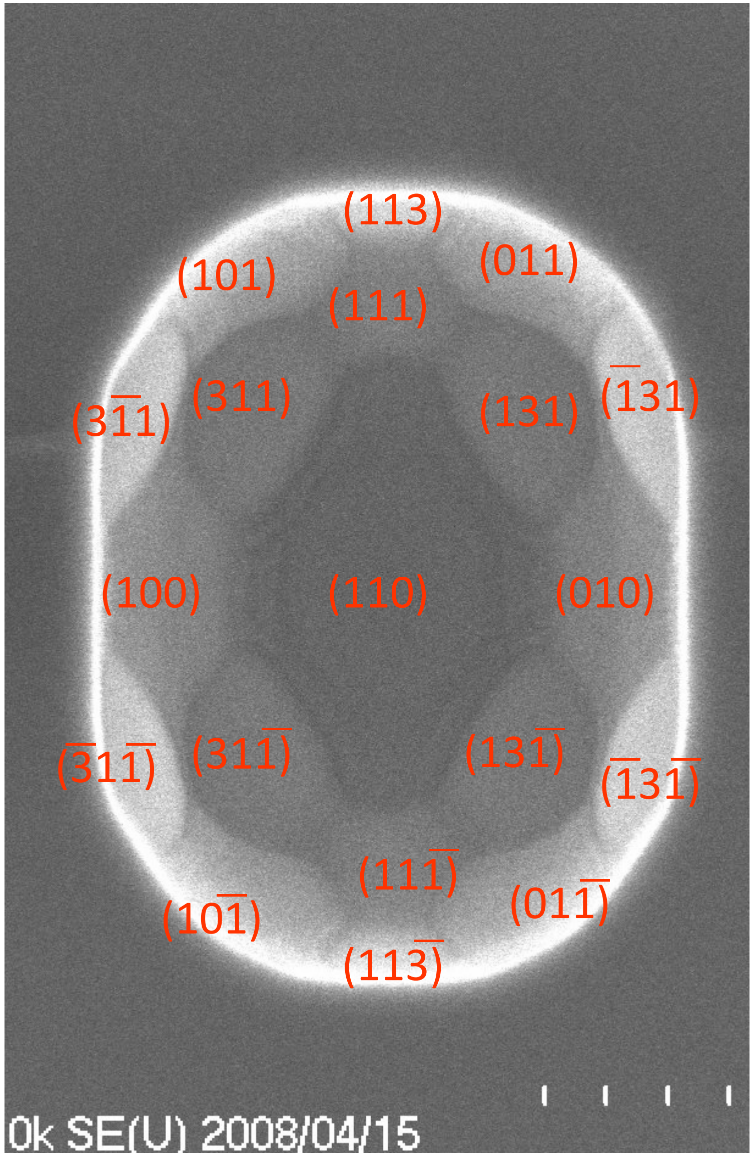




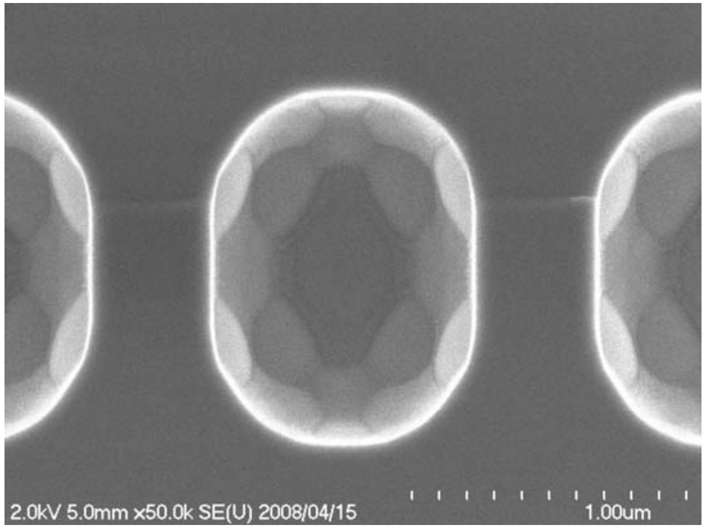
SON structure

Facets on the Void Surface

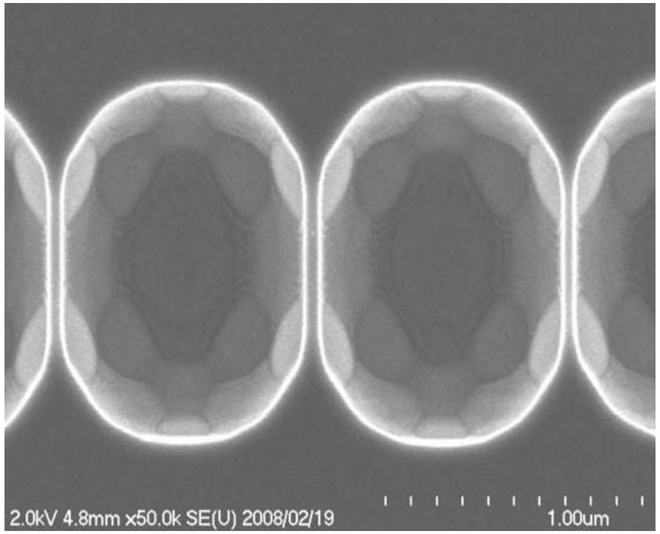




Effects of the adjacent voids



P = 1.8 μm

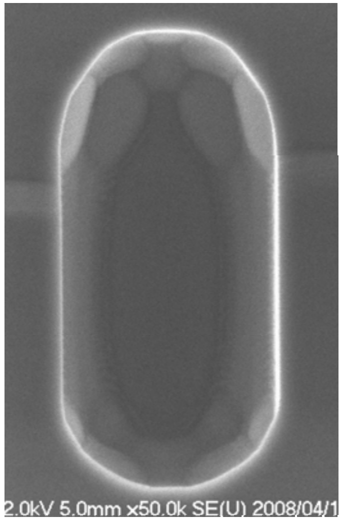


P = 1.0 μm

Shape change of individual voids occur independently without affected by the neighboring voids.

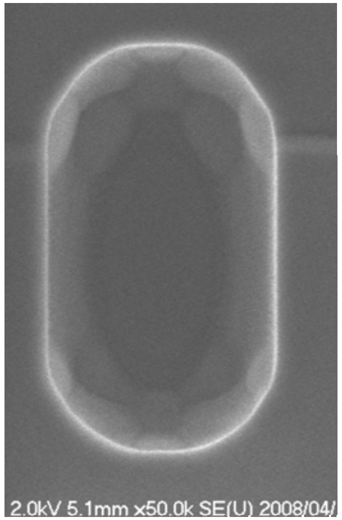
Evolution of void shape during annealing

at 1100 ºC in 60 Torr H_2 gas



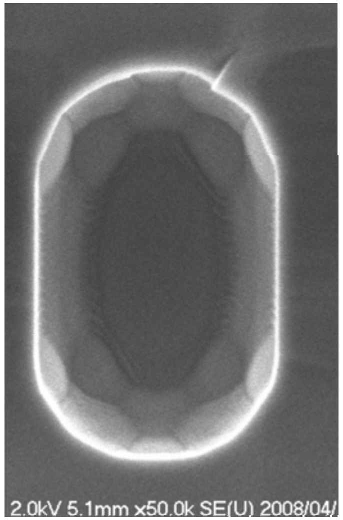
5 min

0.70 μm³



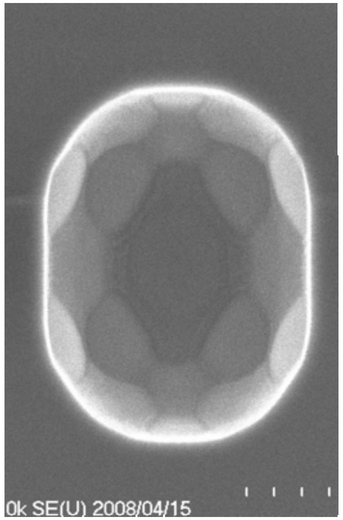
10 min

0.70 μm³



20 min

0.71 μm³

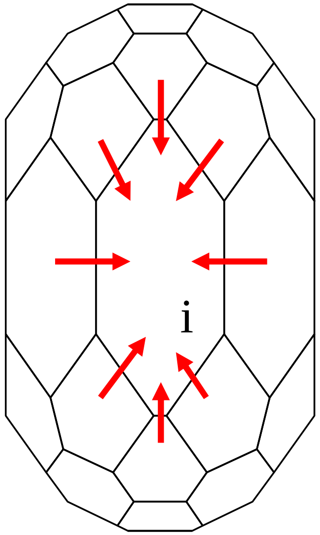


40 min

0.72 μm³

The volume of a void is preserved during shape change

Mean chemical potential of a facet



Chemical potential of a faceted crystal
(J. E. Taylor, Acta Metall. Mater. 40 (1992) 1475.)

$$\mu_i = \mu_0 + \Omega K_i$$

Weighted mean curvature

$$K_i = \frac{1}{S_i} \sum_{j \neq i} f_{ij} l_{ij}$$

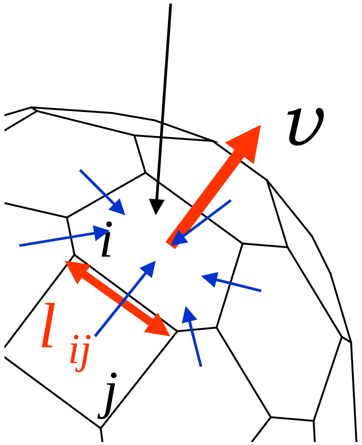
$$f_{ij} = \left[\gamma_j - c_{ij}\gamma_i\right] / \sqrt{1 - c_{ij}^{\,2}}$$

$$c_{ij} = \mathbf{n}_i \cdot \mathbf{n}_j$$

$$v_i = \frac{\Omega}{S_i} \sum_{j \neq i} J_{j \to i}$$

Numerical Simulation of Void Shape Change

Area of i-th facet: S_i



Normal velocity of the i-th facet

$$v_i = \frac{\Omega}{S_i} \sum_{j \neq i} l_{ij} J_{ij}$$

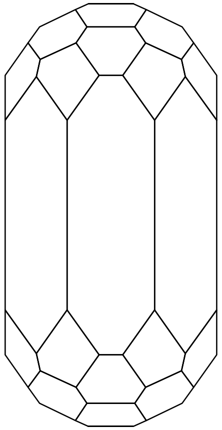
Atomic current from j-th to i-th facet

$$J_{j \to i} = \frac{Dc_0}{kT} \frac{\mu_j - \mu_i}{\Delta x_{ij}}$$

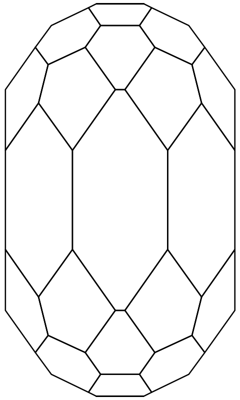
$$\Delta x_{ij} = \sqrt{S_i} + \sqrt{S_j}$$

M. Kitayama, J. Am. Ceram. Soc. 83 (2000) 2561.

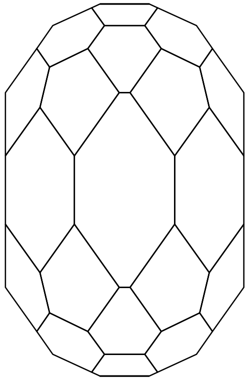
Simulation Results



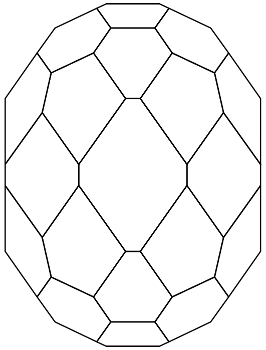
0



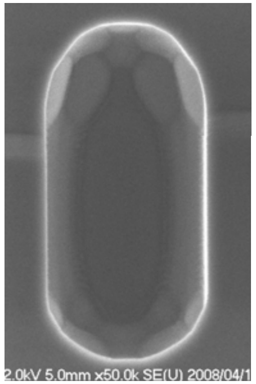
1500

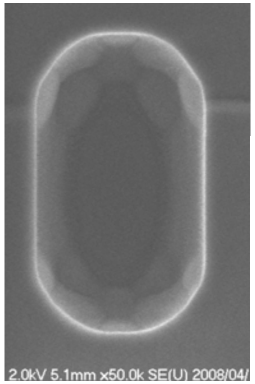


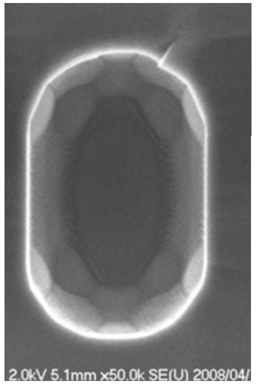
3000

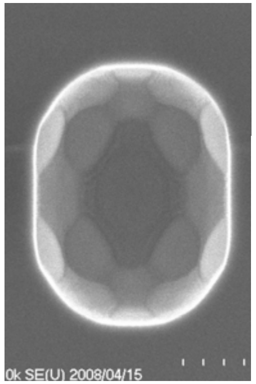


5000

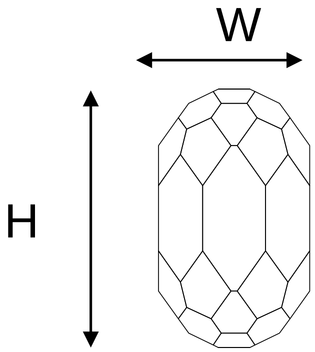


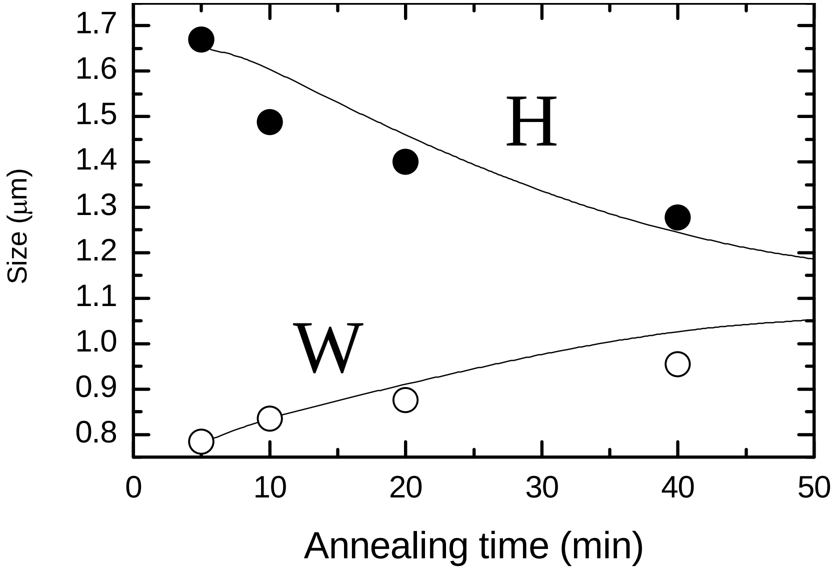






Annealing time dependence of the height and width of voids





Summary

Shape transformation of 1D gratings

Dominant mass transport mechanism for the shape transformation is surface diffusion.

The evolution of trench profiles can be predicted by numerical simulation based on the Mullins equation.

Shape transformation of hole arrays

Empty spaces can be created in the bulk Si by annealing of hole arrays.

Modeling for the evolution of polyhedral crystals reproduces the evolution of a faceted void in Si substrate.