Evolution of micro-structures on silicon substrates by surface diffusion

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Microstructure Fabrication applying Spontaneous Shape Transformation by Annealing

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Useful in fabrication of 3D structures on Si surfaces
- Trench corner rounding
- Formation of empty space in Si

Silicon-on-nothing

Trench MOSFET
Flattening of Surfaces

(110) facet formation on sidewall of fin structures

Shape Modification

M. M. Lee and M. C. Wu:
Outline

I. Shape transformation of 1D gratings
   - Trench corner rounding during annealing
   - Mass transport mechanism for shape transformation
   - Analysis based on Mullins’ equation

II. Shape transformation of high-спект-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)

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

for 3 min at 1000°C
Mechanism of Morphological Evolution

Surface Diffusion (SD) \quad \text{Evaporation-Condensation (EC)}

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


1) Evaporation-Condensation Case

\[ v_n = \sigma_0 \Omega \left[ 1 - \exp \left( \frac{\gamma \Omega}{kT} \right) \right] \]

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

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

\[
v_n \propto K = \frac{1}{R}
\]

\[
\frac{dR}{dt} \propto R^{-1}
\]

2) Surface Diffusion Case

\[
v_n \propto \frac{\partial^2 K}{\partial s^2}
\]

\[
\frac{dR}{dt} \propto R^{-3}
\]
Corner Rounding of 1D Trenches

H₂ 1000°C, 40 Torr

1 min

3 min

10 min

2 μm

500 nm
Annealing time dependence of curvatures of trench corners

\[ R = t^{1/4} \quad \longrightarrow \quad \text{Surface Diffusion} \]
Shape Transformation by Mullins Equation for EC and SD

Evaporation-Condensation

Surface Diffusion
Difference between EC and SD

Evaporation and Condensation

Surface diffusion

\[ R = t^{1/2} \]

\[ R = t^{1/4} \]
Simulation using Mullins Equation

SEM Images 4%H$_2$/Ar 760Torr 1150 °C 5min

Simulation

Bt = 0.14
Square Array of Cylindrical Holes

Top View

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
Facets on the Void Surface
Effects of the adjacent voids

Shape change of individual voids occur independently without affected by the neighboring voids.
Evolution of void shape during annealing at 1100 °C in 60 Torr H₂ gas

The volume of a void is preserved during shape change
Mean chemical potential of a facet

Chemical potential of a faceted crystal

\[ \mu_i = \mu_0 + \Omega K_i \]

Weighted mean curvature

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

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

\[ c_{ij} = \mathbf{n}_i \cdot \mathbf{n}_j \]
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

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

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

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.