Two-Dimensional Phase-Field Simulation of Self-Assembled Quantum Dot Formation

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INTRODUCTION

Phase-field simulations are performed to investigate the effects of the growth parameters on island formation and island morphological evolution during deposition for SiGe/Si(001) system. In the phase-field model, facet morphologies are modeled using the generalized gradient correction coefficient for a crystal with a high anisotropy of surface energy. Furthermore, to enable computation of the island morphological change from faceted pyramids to multifaceted domes with increasing Ge coverage, we apply the sixteen-fold of the surface energy. The validity of the model developed is confirmed by comparing the numerical results demonstrated here with the reported experimental observations.

PHASE-FIELD MODEL

< Free-energy functional >

The morphologies of the thin film are assumed to be determined by the competition of the surface energy and the elastic strain energy. The Ginzburg-Landau-type free-energy functional of the system is assumed to have the form

$$F = \int_V \left\{ f_d(\phi) + f_e(\phi, \varepsilon_{ij}) + \frac{a^2}{2}|\nabla\phi|^2 \right\} dV$$

where

ϕ : phase field $\quad \phi = \begin{cases} 0 : \text{vapor phase} \\ 1 : \text{solid phase (= substrate + film)} \end{cases}$

f_d : double-well potential

$$f_d(\phi) = Wg(\phi) \qquad g(\phi) = \phi^2(1-\phi)^2$$

f_e : elastic strain energy

$$f_e(\phi, \varepsilon_{ij}) = \frac{1}{2} D_{ijkl}(\phi)(\varepsilon_{ij} - \varepsilon_{ij}^0)(\varepsilon_{kl} - \varepsilon_{kl}^0)$$

$$D_{ijkl}(\phi) = \rho(\phi) D_{ijkl}^0 \quad \text{: elastic coefficient}$$

$$\rho(\phi) = \frac{1}{2}\left[\tanh\frac{2\phi-1}{2\tau} + 1\right] \quad \text{: density of solid phase}$$

a : gradient correction coefficient

< Faceted island >

The surface anisotropy is considered by

$$a(\theta) = \bar{a}\{1 + \gamma\cos k\theta\}$$

where

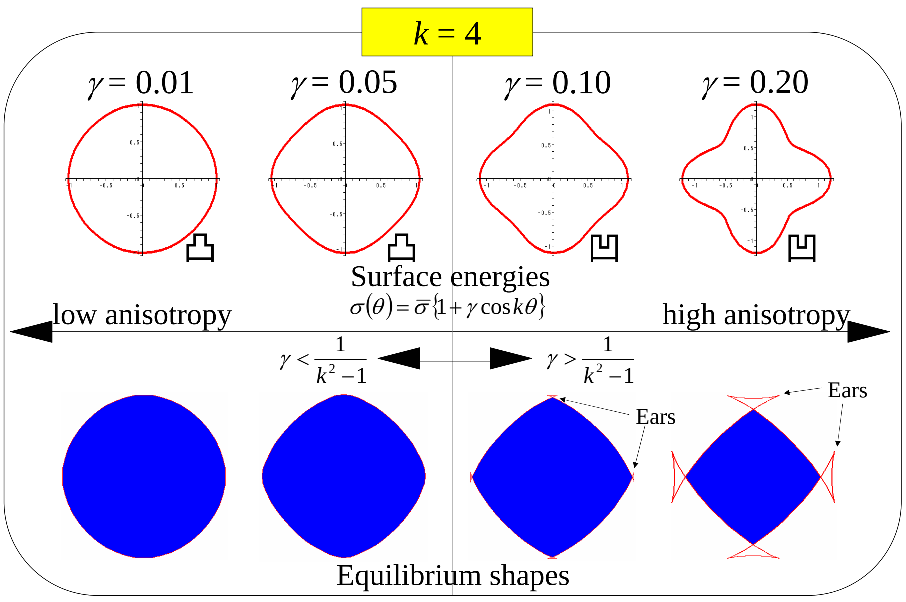
$\bar{a}$: constant related to the surface energy σ and the surface thickness δ

γ : strength of anisotropy

k : mode number

θ : angle between the surface normal and the x-axis

Faceted islands are created using a high anisotropy such as $\gamma > 1/(k^2-1)$



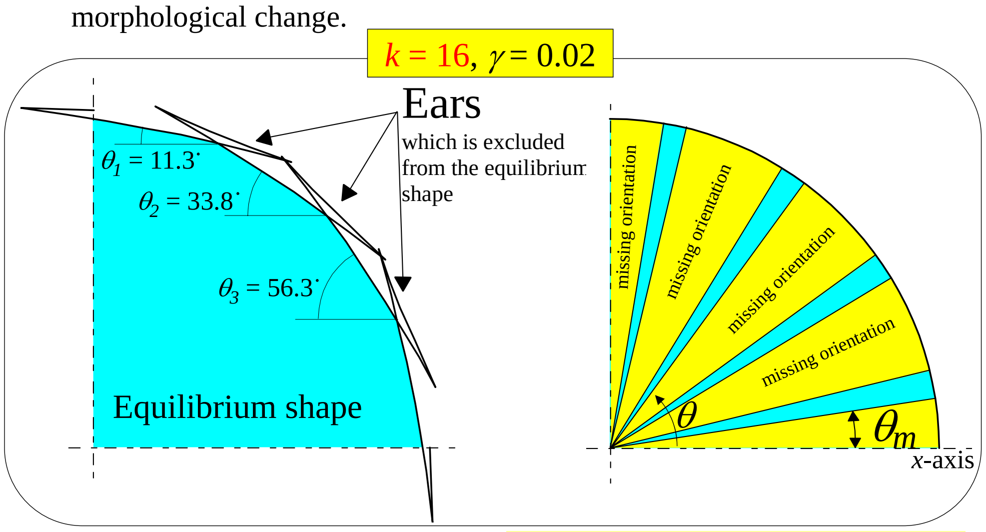
< Multifaceted island >

SiGe/Si(001) shows the following surface morphological change:

SiGe/Si(001) morphological change

2D wetting layer
↓
{105} faceted pyramid island
↓
Multifaceted dome island with {105}, {113} and {15 3 23} facets
↓
Barn island with additional {111} facet (for dilute alloy)

We introduce $k = 16$ to simulate the multifaceted islands and island morphological change.



The first missing orientation θ_m is calculated from

$$a(\theta_m)\sin\theta_m + a_\theta(\theta_m)\cos\theta_m = 0$$

$\theta_1 = 11.3°$ → {105} facet plane
$\theta_2 = 33.8°$ → {15 3 23} facet plane
$\theta_3 = 56.3°$ → {111} facet plane

< Generalized gradient coefficient >

To provide the island morphology without "ears" corresponding to the missing orientation, we use the regularized gradient coefficient for the missing orientation.

$$a(\theta) = \begin{cases} \bar{a}\{1 + \gamma\cos k\theta\} & \text{for } (2\pi i/k + \theta_m) \le \theta \le (2\pi(i+1)/k - \theta_m) \\ \dfrac{a(\theta_m)}{\cos\theta_m}\cos\theta & \text{for } (2\pi i/k - \theta_m) < \theta < (2\pi i/k + \theta_m) \text{ (missing orientation)} \end{cases}$$

where i denotes the integers from 0 to k–1.

< TDGL (Time-dependent Ginzburg-Landau) Equation >

$$\frac{\partial\phi}{\partial t} = \nabla\left(M\nabla\frac{\delta F}{\delta\phi}\right) + V_d n_y \chi$$

$$= M\nabla^2\left[2\phi(1-\phi)(1-2\phi)W + \frac{\partial f_e(\phi,\varepsilon_{ij})}{\partial\phi} + \frac{\partial}{\partial x}\left(a\frac{\partial a}{\partial\theta}\frac{\partial\phi}{\partial y}\right) - \frac{\partial}{\partial y}\left(a\frac{\partial a}{\partial\theta}\frac{\partial\phi}{\partial x}\right) - a^2\nabla^2\phi\right] + V_d n_y \chi$$

$$\sigma_{ij,j} = 0 \quad \text{: stress equilibrium condition}$$

where

M : mobility representing the surface diffusion

V_d : deposition rate

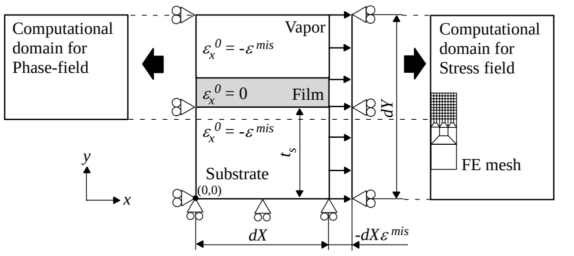
n_y : y-direction component of the surface normal

χ : random number

The phase field ϕ is assumed to be a conserved parameter. We assume the stress equilibrium conditions $\sigma_{ij} = 0$, since the elastic relaxation occurs much faster than the surface diffusion.

NUMERICAL SIMULATION

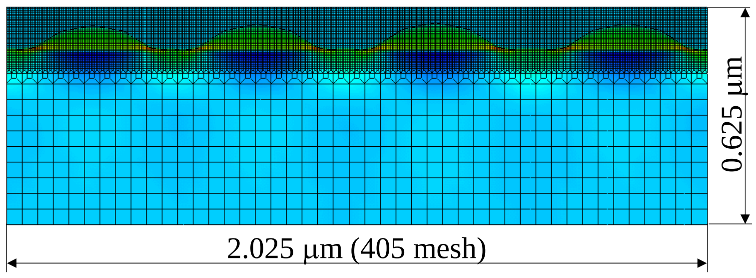
Phase field equation is descretized spatially using second-order finite difference method and explicit time differencing is employed for ϕ. Stress field is solved by finite element method as a plane strain problem.



< Parameters >

Surface energy σ = 1.23 J/m^2
Young's modulus E = 104 GPa
Poisson's ratio ν = 0.27
Strength of anisotropy γ = 0.1
Lattice mismatch strain ε^{mis} = 0.04x
(where x is Ge composition)
Mesh size dx = 5 nm
Time increment $dt = dx^4/(62.0a^2M)$

Computational domains and boundary conditions

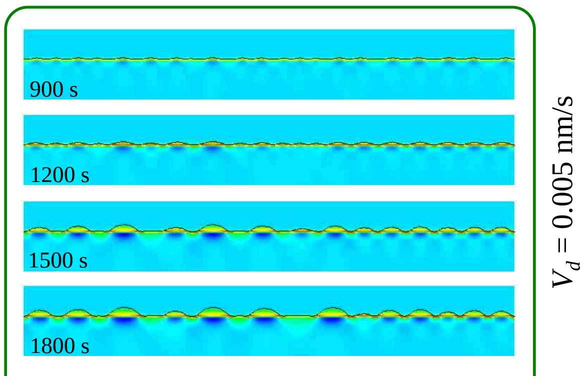


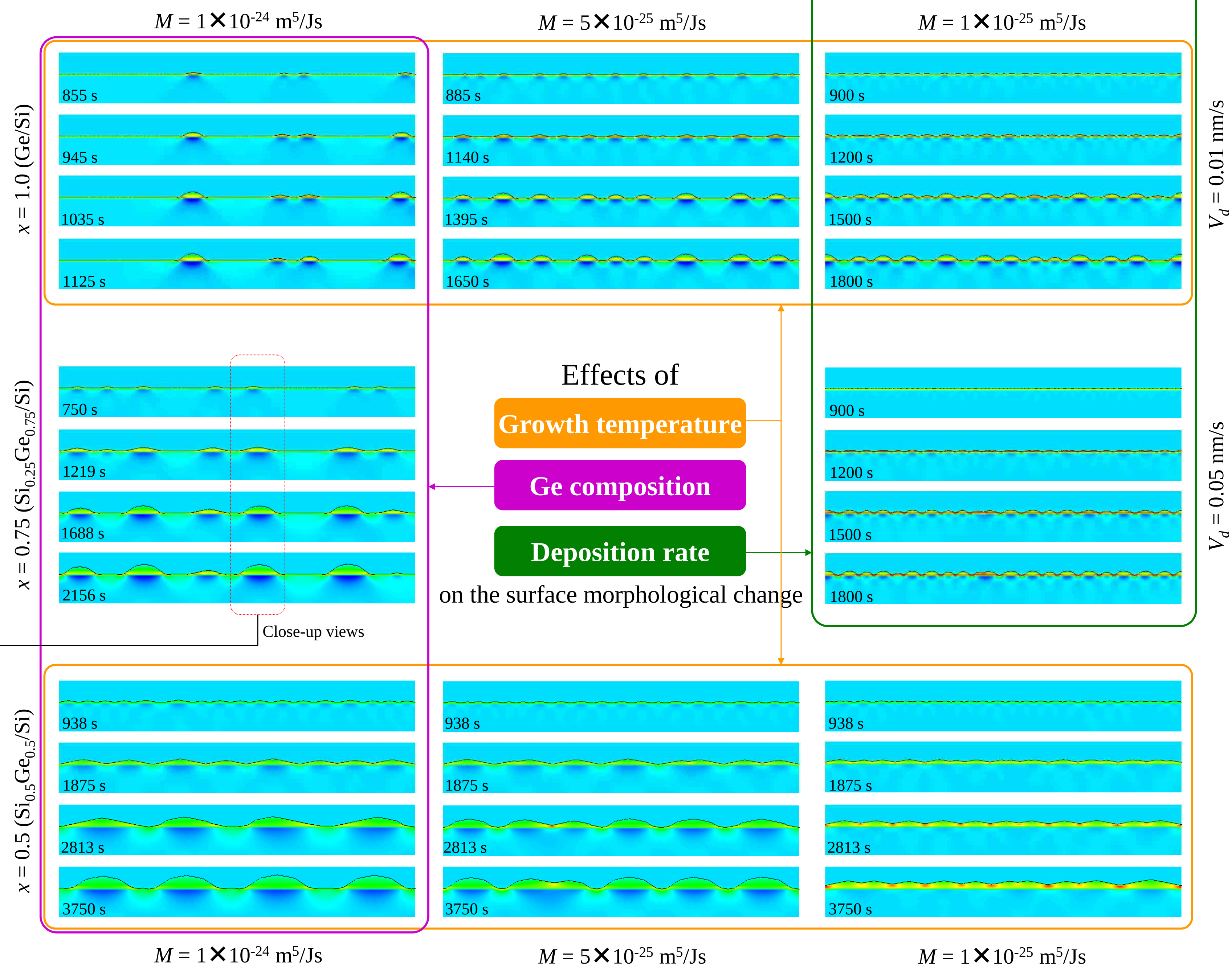
Finite element mesh and computational domain size

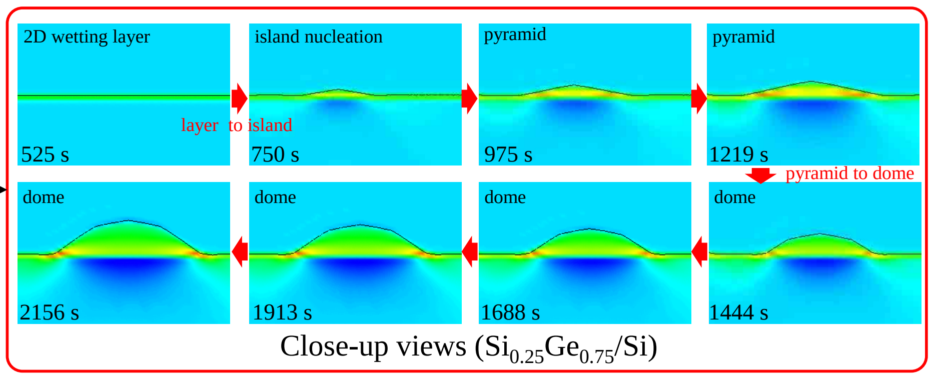
RESULTS

The effects of Ge composition, mobility and deposition rate on island formation and the evolution of surface morphology are investigated, and following results are obtained:

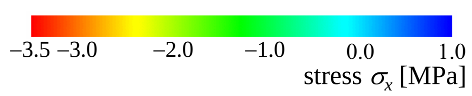
- For the 3D pyramid formation, it is observed that, at a low mismatch strain, 3D pyramid islands are formed from surface ripples as a result of strain-driven instability, while at high mismatch strain, islands are formed by nucleation.
- $Si_{0.5}Ge_{0.5}$ islands tend to show improved spatial ordering and a narrow size distribution compared to Ge islands.
- In the growth of a $Si_{0.5}Ge_{0.5}$ layer at low temperatures, a rippled surface morphology continues to grow without the formation of individual islands.







Close-up views ($Si_{0.25}Ge_{0.75}$/Si)



CONCLUSIONS

The heteroepitaxial growth of $Si_{1-x}Ge_x$/Si(001) alloys during deposition are simulated by the phase-field method as a two-dimensional problem, which is developed so as to simulate a typical sequential growth of a wetting layer, faceted pyramid islands and multifaceted dome islands. The effects of Ge composition, mobility and deposition rate on island formation and the evolution of surface morphology are investigated. It is confirmed that the phase-field model developed can simulate some typical and important phenomena for the formation and evolution of SiGe islands grown on Si, as observed in previous experiments. We believe that this model can be applied to the analysis of other heteroepitaxial systems for the formation of faceted 3D islands and can be expanded to solve more realistic three-dimensional problems.