Phase-Field Study of Interface Energy Effect on Quantum Dot Morphology

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Introduction

Phase-field method is powerful tool to simulate the complicated morphological evolution. In this study, we developed a multi-phase-field model which can take into consideration the surface energies of film and substrate and interface energy between film and substrate and can reproduce the faceted island, the island morphological transition and the deposition process during self-assembled quantum dots (QDs) growth. By performing 2D simulations, we investigated the effects of the interface energy on the surface morphological evolutions of film.

Multi-Phase-Field Model

Free energy functional

$$F=\int_V\left[\sum_{i=1}^{3}\sum_{j=i+1}^{3}\left(-\frac{a_{ij}^2}{2}\nabla\phi_i\cdot\nabla\phi_j+W_{ij}\phi_i^2\phi_j^2\right)+f_e\right]dV$$

Time evolution equation for ϕ_2

$$\frac{\partial\phi_2}{\partial t}=\nabla\cdot\left[M\nabla\frac{\delta F}{\delta\phi_2}\right]+V_d n_y\chi$$

$$\begin{aligned}\frac{\delta F}{\delta\phi_2}=&-\nabla\cdot\left(a_{12}^2\nabla\phi_2\right)+\frac{1}{2}\left[-\nabla\cdot\left(a_{12}^2\nabla\phi_3\right)+\nabla\cdot\left(a_{23}^2\nabla\phi_3\right)-\nabla\cdot\left(a_{31}^2\nabla\phi_3\right)\right]\\&+\frac{\partial}{\partial x}\left(a_{12}\frac{\partial a_{12}}{\partial\theta}\frac{\partial\phi_2}{\partial y}\right)-\frac{\partial}{\partial y}\left(a_{12}\frac{\partial a_{12}}{\partial\theta}\frac{\partial\phi_2}{\partial x}\right)\\&-\frac{\partial}{\partial x}\left(a_{12}\frac{\partial a_{12}}{\partial\theta}\frac{\partial\theta}{\partial\phi_{2,x}}\nabla\phi_3\cdot\nabla\phi_2\right)-\frac{\partial}{\partial y}\left(a_{12}\frac{\partial a_{12}}{\partial\theta}\frac{\partial\theta}{\partial\phi_{2,y}}\nabla\phi_3\cdot\nabla\phi_2\right)\\&+2W_{12}\phi_1\phi_2\left(\phi_1-\phi_2\right)+2W_{23}\phi_2\phi_3^2-2W_{31}\phi_3^2\phi_1+\frac{\partial f_e}{\partial\phi_2}\end{aligned}$$

Stress field

$$\sigma_{ij,j}=0$$

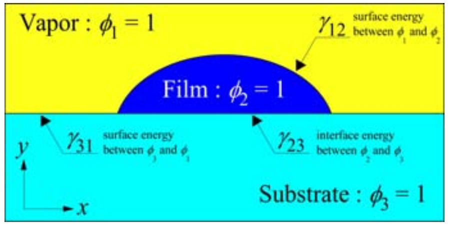
Elastic strain energy due to lattice misfit

$$f_e=\frac{1}{2}D_{ijkl}\left(\phi_2+\phi_3\right)\left(\varepsilon_{ij}-\varepsilon_{ij}^0\right)\left(\varepsilon_{kl}-\varepsilon_{kl}^0\right)$$

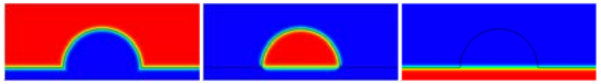
$$D_{ijkl}\left(\phi_2+\phi_3\right)=\frac{1}{2}\left[\tanh\frac{2\left(\phi_2+\phi_3\right)-1}{2\tau}+1\right]D_{ijkl}^0$$

Phase field and material parameters

$$a_{ij}=\sqrt{\frac{3\delta\gamma_{ij}}{b}}\quad\text{and}\quad W_{ij}=\frac{6\gamma_{ij}b}{\delta}$$



Phase field variables: ϕ_1, ϕ_2, ϕ_3



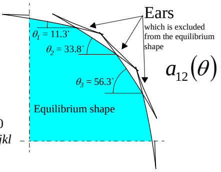
Vapor : $\phi_1=1,\ \phi_2=\phi_3=0$ Film : $\phi_2=1,\ \phi_3=\phi_1=0$ Substrate : $\phi_3=1,\ \phi_1=\phi_2=0$

$\phi_1+\phi_2+\phi_3=1$ must be satisfied.

$\phi_3=\frac{1}{2}\left[\tanh\left\{\frac{b}{\delta}\left(y_{subst}-y\right)\right\}+1\right]$ is constant.

Therefore, the independent variable is only ϕ_2.

Surface anisotropy to create faceted island

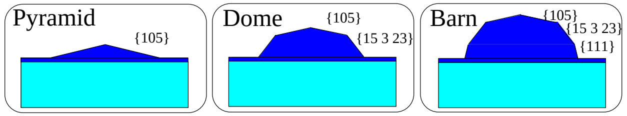


Ears which is excluded from the equilibrium shape

$$a_{12}(\theta)=\begin{cases}a_{12}^1(\theta)=\dfrac{\bar{a}_{12}}{1+\xi}\left\{1+\gamma\cos(k\theta)\right\}\\ \qquad\left(2\pi i/k+\theta_m\right)\le\theta\le\left(2\pi(i+1)/k-\theta_m\right)\\ a_{12}^2(\theta)=\dfrac{a_{12}^2\left(\theta_m\right)}{\cos\theta_m}\cos\theta\\ \qquad\left(2\pi i/k-\theta_m\right)<\theta<\left(2\pi i/k+\theta_m\right)\end{cases}$$

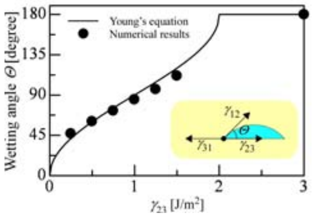
Multi-faceted island and island shape transition

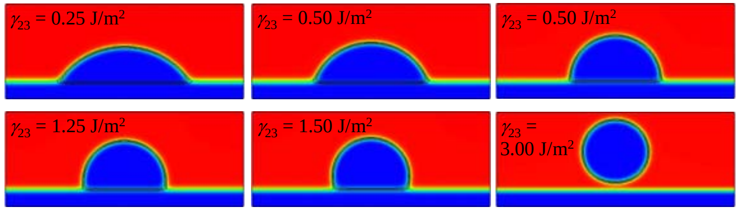
$$k=16$$



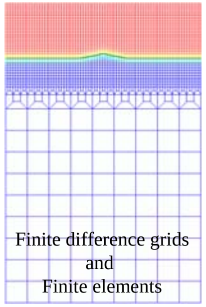
Numerical Results

<< Wetting angle >>

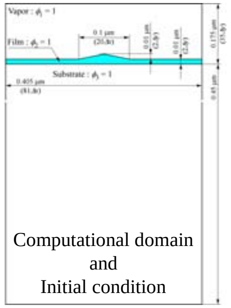




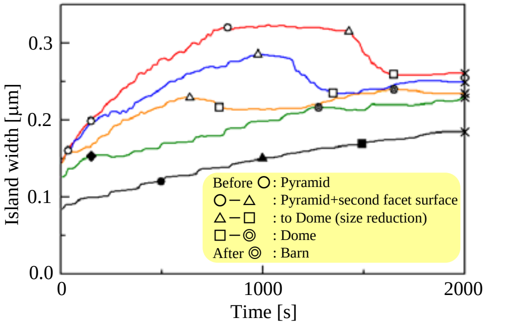
<< Single island growth simulation >>

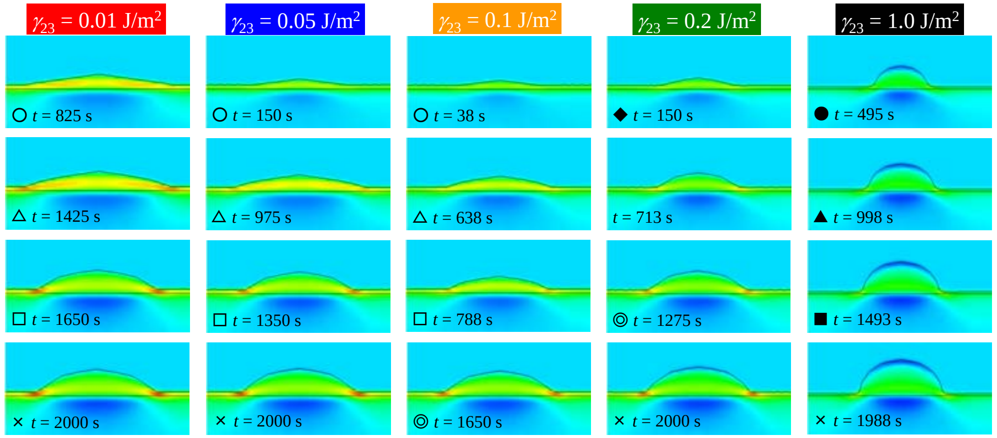


Finite difference grids and Finite elements

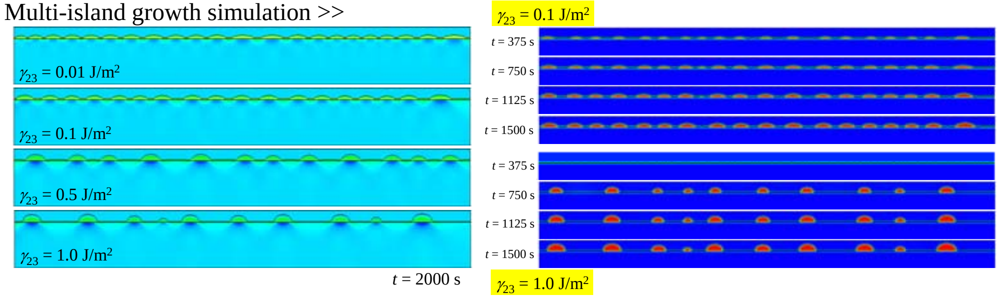


Computational domain and Initial condition





<< Multi-island growth simulation >>



<< Conclusions >>

In single island growth simulations, it is clarified that the morphological transition points occur at the earlier growth stage for the larger interface energy. Although the temporal reduction of the island width is observed at the transition point from pyramid to dome for the low interface energies, its magnitude reduces with increasing the interface energy. In the realistic interface energy, the island size evolution agrees well with the reported experimental result. In multi-island growth simulation, it is observed that the high interface energy result in the large island size fluctuation.