Modeling and Simulation for Solid-State Dewetting Problems

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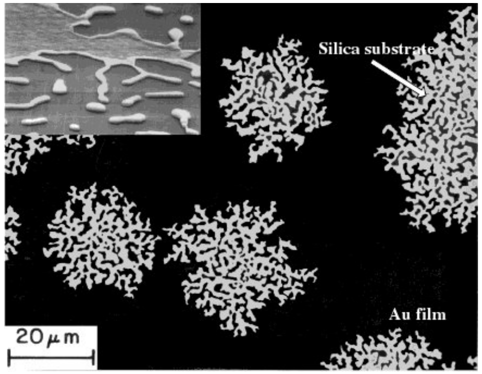
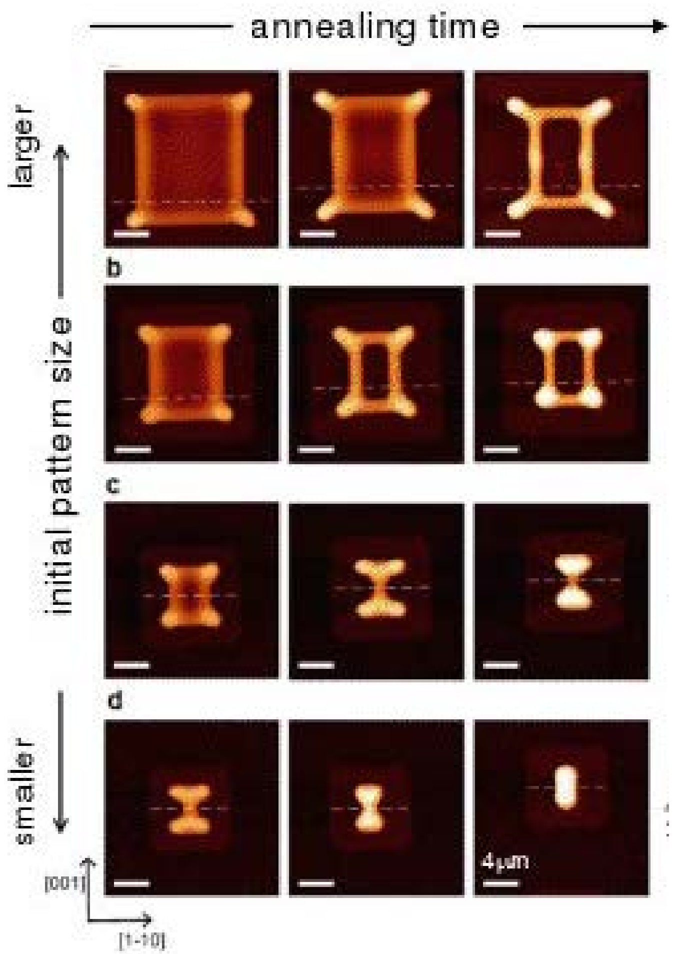


Collaborators: Wei Jiang (Wuhan), David J. Srolovitz (U. Penn); Carl V. Thompson (MIT); Yan Wang (NUS); Quan Zhao (NUS)

Outline

- Motivation
- Sharp Interface models (SIMs)
  - Isotropic surface energy
  - Anisotropic (weak/strong) surface energy
  - Numerical methods & results in 2D
- Phase field/Diffuse interface model
  - Mathematical model
  - Numerical methods
  - Results in 3D
- Conclusion & future works

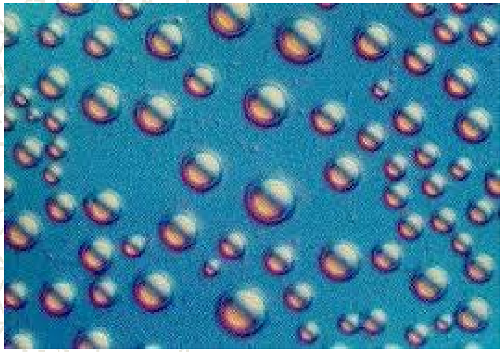
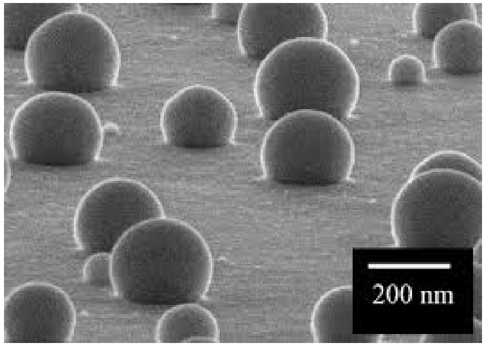
Patterned Ni(110) square patche

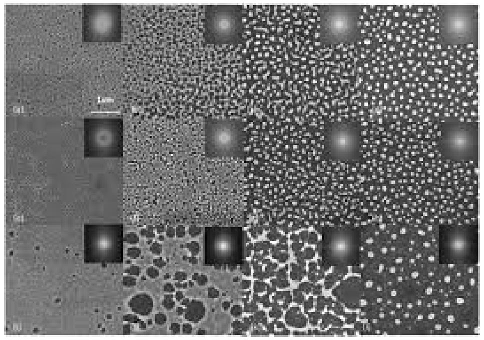


Wetting / Dewetting in Fluid Mechanics

- Wetting– spread of a liquid on a substrate

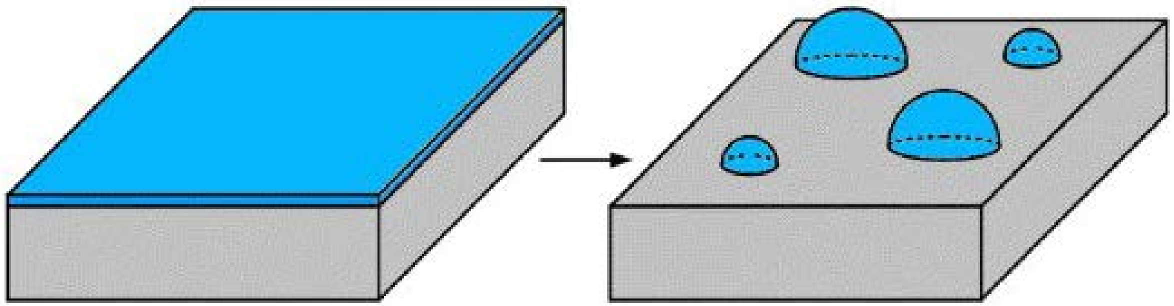

- Dewetting – the rupture of a thin liquid film on a substrate

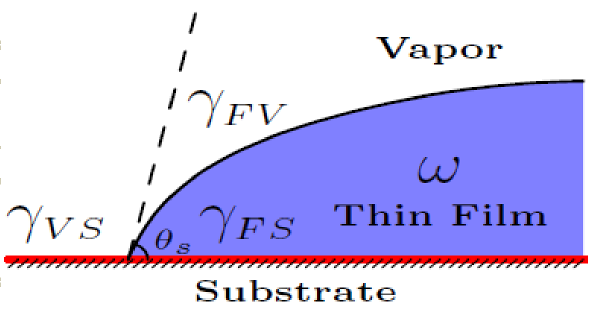


Solid-State Dewetting of Thin Films

- Most thin films are metastable in as-deposited state & dewet to form particles



- This occurs when the temperature is high enough for surface self diffusion, which can be well below the film's melting temperature

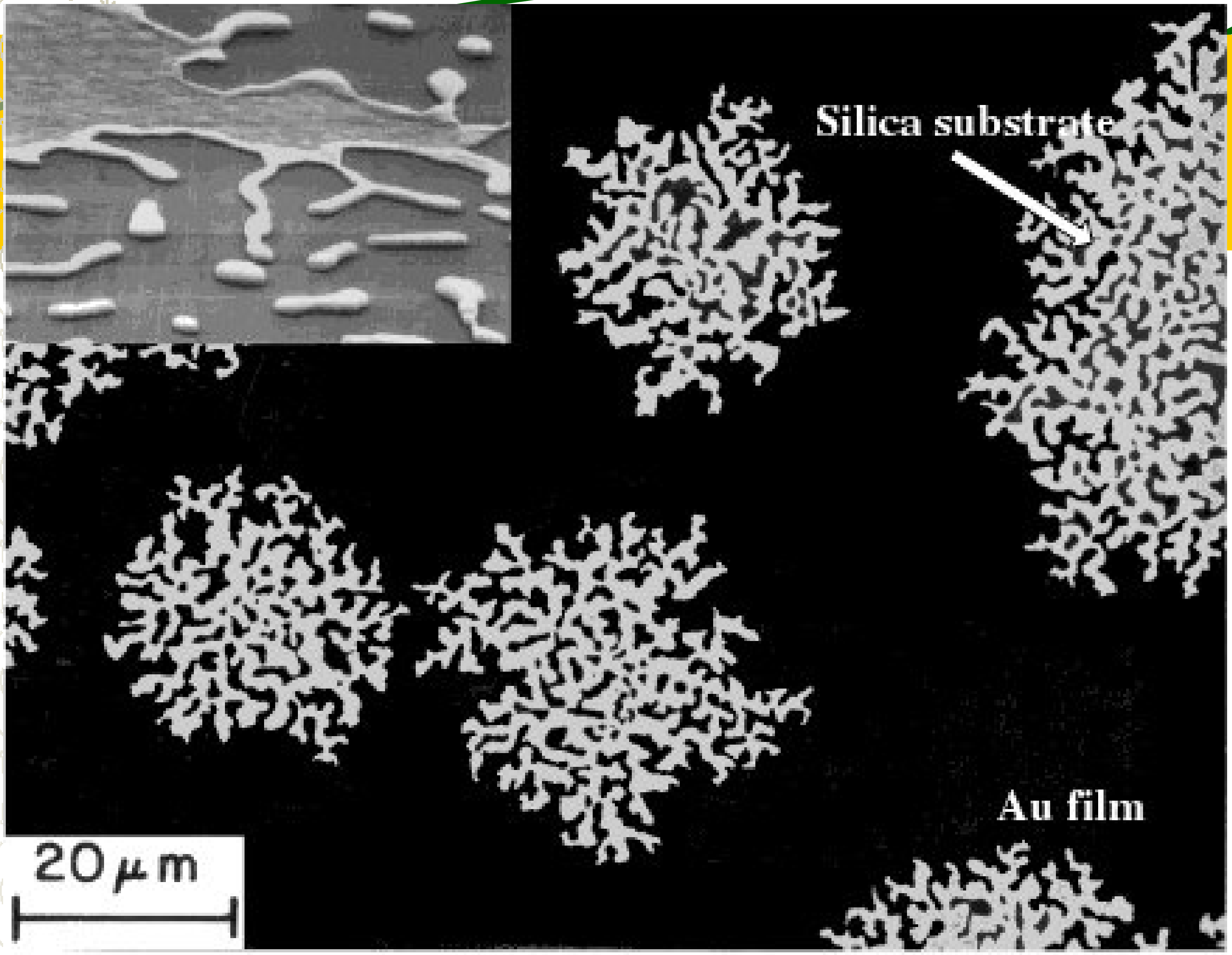


$$\gamma_{VS} = \gamma_{FS} + \gamma_{FV}\cos(\theta) \text{ -- Young}$$

γ_{VS} : substrate free surface energy

γ_{FV} : film free surface energy

γ_{FS} : film-substracte interface energy



Dewetting on a flat substrate

[1] E. Jiran & C. V. Thompson, Journal of Electronic Materials, 19 (1990), pp. 1153-1160.

[2] E. Jiran & C. V. Thompson, Thin Solid Films, 208 (1991), pp. 23-28.

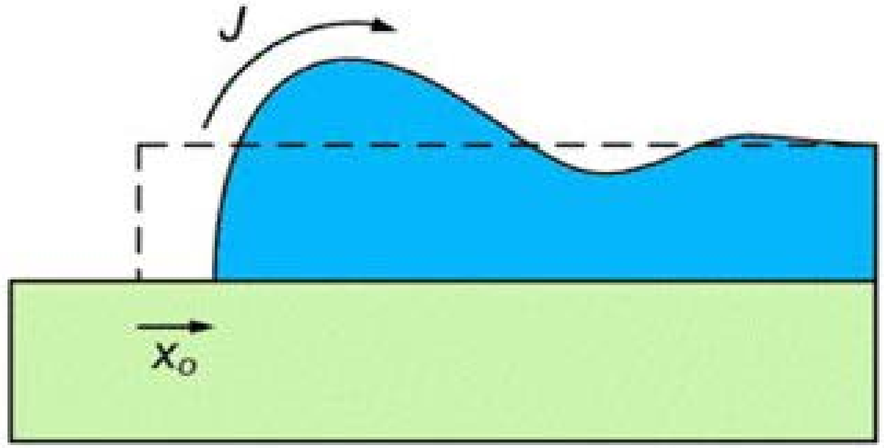
Solid-State Dewetting Problems

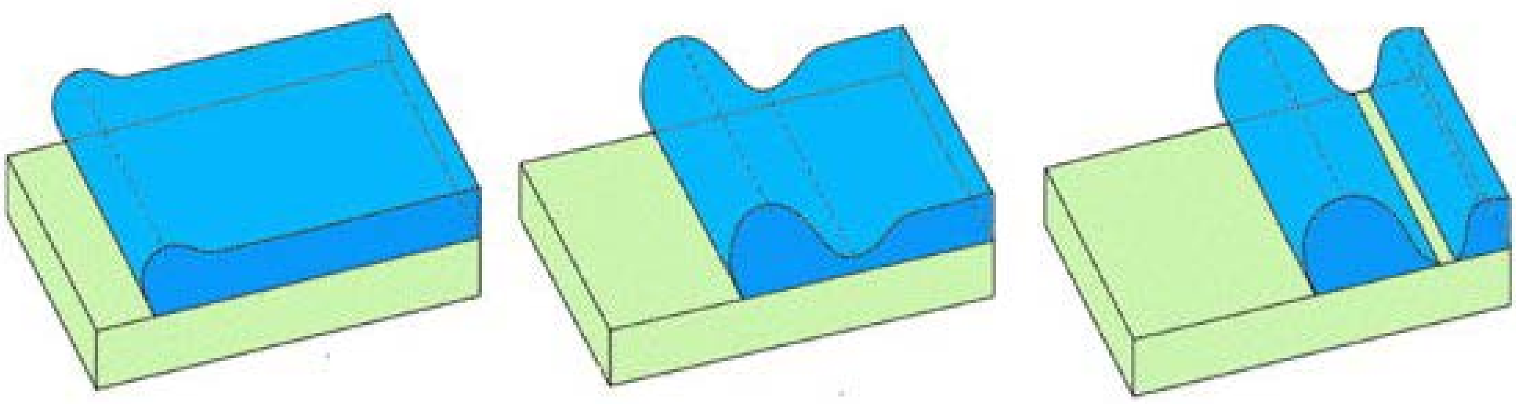
- Solid-state dewetting
  - Is driven by capillarity effects
  - Occurs through surface diffusion controlled mass transport
  - Belongs to capillarity-controlled interface/surface evolution problems
  - Surface diffusion + contact line migration
- Applications of dewetting of thin films
  - Play an improtant role in micorelectronics processing
  - A common method to produce nanoparticles
  - Catalyst for the growth of carbon nanotubes & semiconductor nanowires
- Recent experiments -– [1]
  - Geometric complexity, capillarity-driven instabilities, faceting
  - Crystalline anisotropy, corner-induced instabilities, pinch-off, ….
- Wetting/dewetting in fluids: TZ Qian, XP Wang&P Sheng; W. Ren&W E, ...

[1] J. Ye & C.V. Thompson, Acta Mater. 23 (2011), 1567; 59 (2011), 582; Appl. Phys. Lett. 97 (2010), 071904

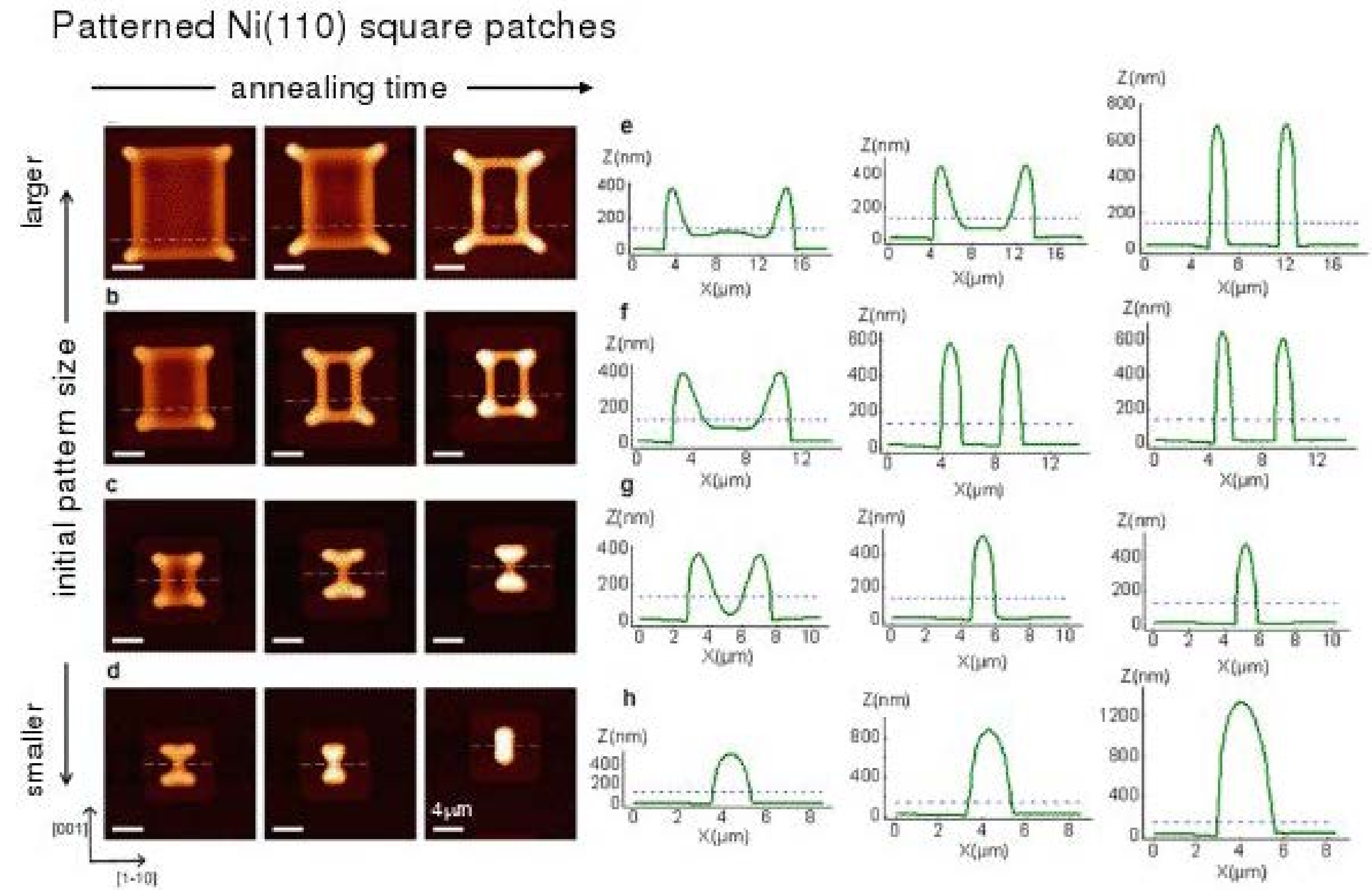
Pinch-off

$$\vec{J}_S = -\frac{D^S \gamma^S}{kT} \frac{\partial \kappa}{\partial s}$$



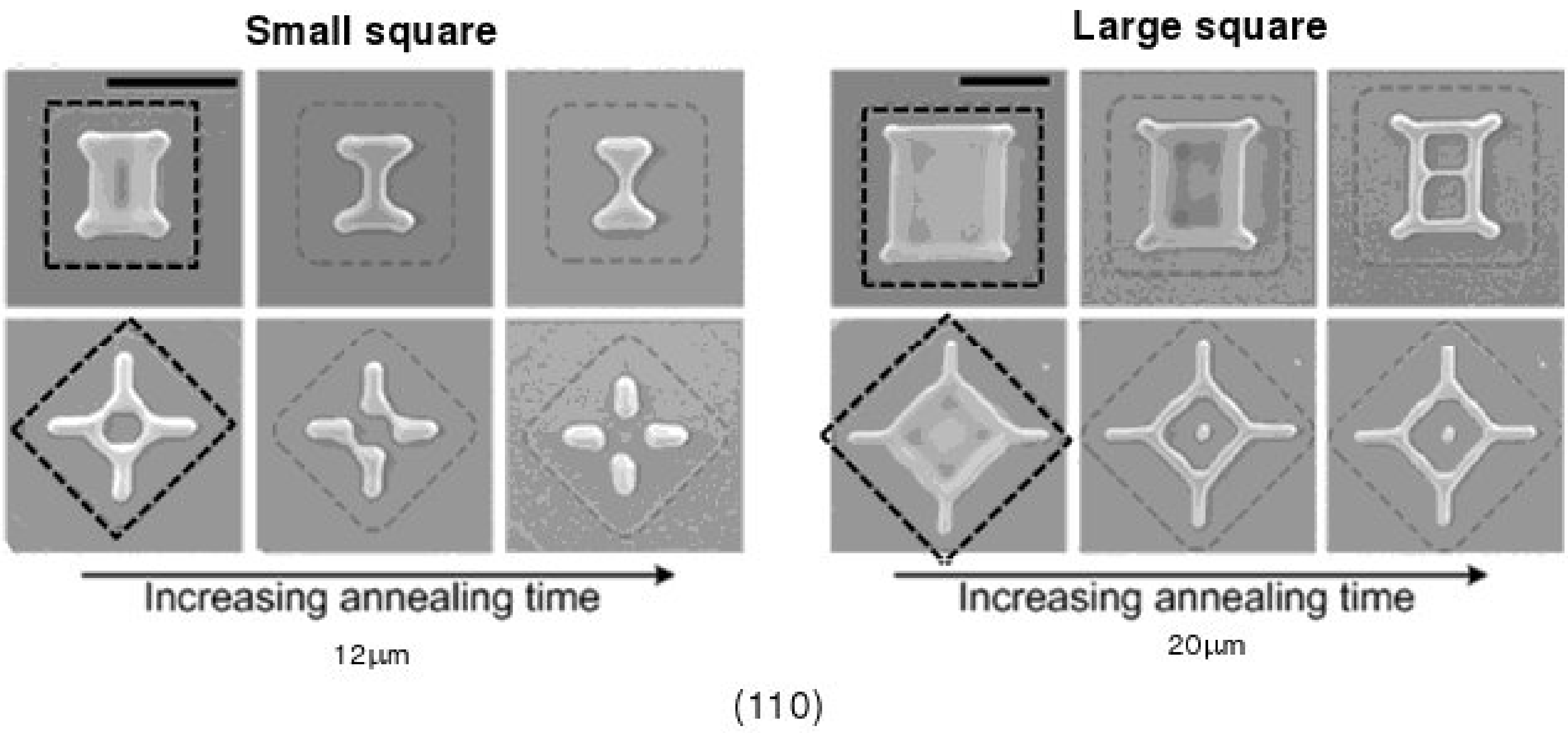


Dewetting Patterned Films



[1] J. Ye & C.V. Thompson, Phys. Rev. B, 82 (2010), 193408.

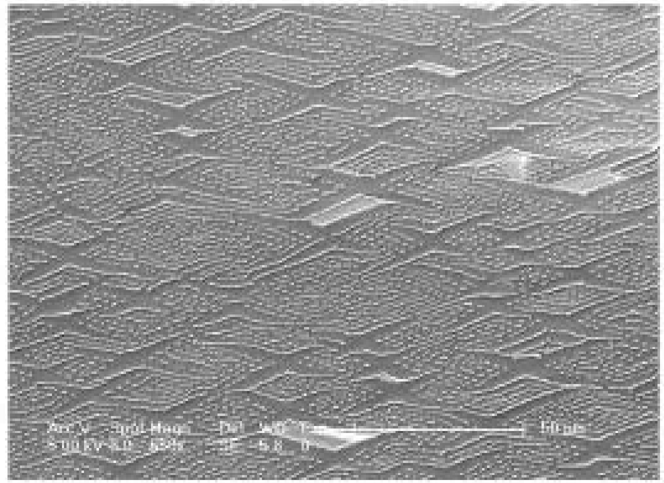
Effect of Size & Orientation of Pattern

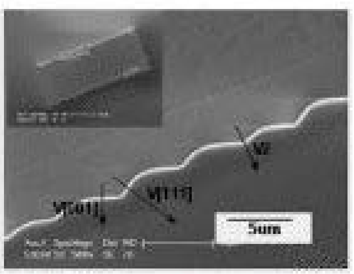


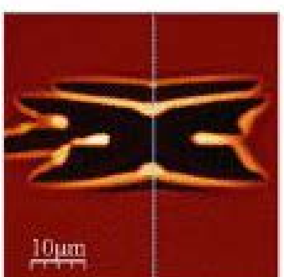
[1] J. Ye & C.V. Thompson, Adv. Mater., 23 (2011), 1567.

Dewetting of Patterned Single-Crystal Films

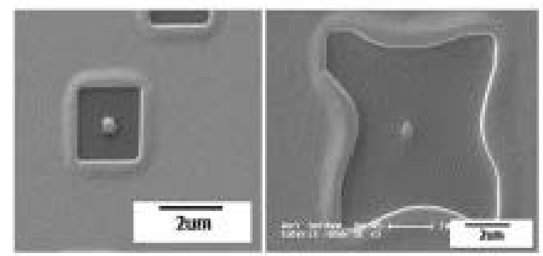
Complex pattern formation

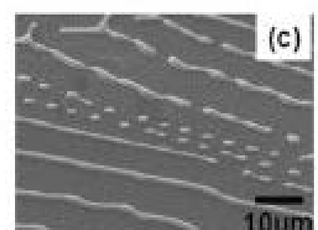






- Edge faceting
- Corner instability
- Mass shedding instability
- Rayleigh-like instability



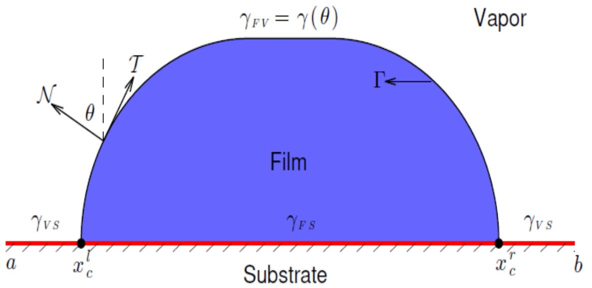


Models and Methods for Dynamical Evolution

- Sharp interface model
  - Isotropic case
    - Model & power law --- Srolovitz & Safran JAP 86'
    - Marker particle method ---- Wong, Voorheers & Miksis 00'; Du etc JCP 10'; ….
  - Anisotropic (weakly and strongly) case
    - Model via thermodynamical variation – Wang etc PRB 15'; Jiang etc 16', …
    - Parametric finite element method (PFEM) -- Bao, Jiang, Wang &Zhao, 16'
- Kinetic Monte Carlo method – Dufay & Pierre-Lious PRL 11'; Pierre-Louis etc, EPL&PRL 09
- Discrete surface chemical potential method –Dornel etc. PRB 06'; Klinger etc 12
- Phase field model ---Jiang, Bao Thompson & Srolovitz, Acta Mater. 12'
- Crystalline formulation method – Cahn & Taylor 94'; Cater etc 95'; Kim etc 13'; Zucker etc 13'; Roosen etc 94'&98'; …..

Sharp Interface Models (SIM)

$\Gamma: \quad \vec{X}(s,t) = (x(s,t), y(s,t)) \qquad s$ -- arclength



- Isotropic surface energy--dynamics:

$$\frac{\partial \vec{X}(s,t)}{\partial t} = V_n \vec{n} \qquad \text{with} \qquad V_n = B \Delta_s \kappa$$

- $\vec{X}(s,t) = (x(s,t), y(s,t))$: moving front curve in 2D(surface in 3D)
- $\vec{n}$: unit outward normal direction
- V_n : normal velocity of the moving interface
- B : material constant
- Δ_s : surface Laplacian or Laplace-Beltrami operator
- κ : mean curvature of the surface

$$V_n = B \frac{\partial^2 \kappa}{\partial s^2} \qquad \text{(in 2D)}$$

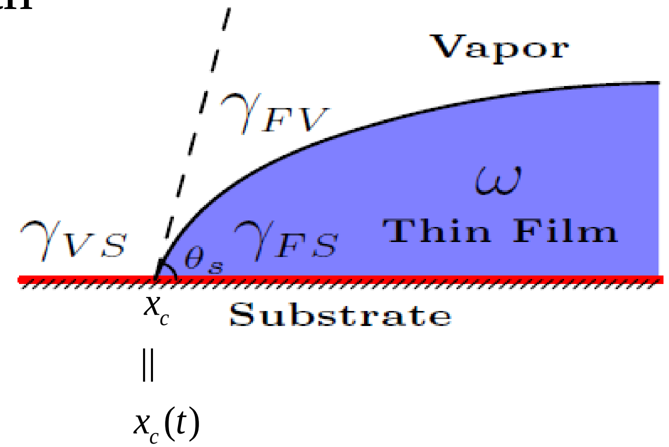
$$\kappa = -\frac{\partial^2 y}{\partial s^2}\frac{\partial x}{\partial s} + \frac{\partial^2 x}{\partial s^2}\frac{\partial y}{\partial s}$$

[1] D.J. Srolovitz & S.A. Safran, J. Appl. Phys., 60 (1986), 255.

[2] H. Wong et al., Acta Mater., 48 (2000), 1719.

SIM of Isotropic Surface Energy--Dynamics

$\Gamma: \quad \vec{X}(s,t) = (x(s,t), y(s,t)) \qquad s$ -- arclength



- **Boundary conditions (2D)**
  - Contact point condition (BC1)

$$y(x_c, t) = 0$$

  - Contact angle condition (BC2)

$$\frac{\frac{\partial y}{\partial s}(x_c,t)}{\frac{\partial x}{\partial s}(x_c,t)} = \tan\theta_i \qquad \theta_i \text{ -- prescribed isotropic Young angle}$$

$$\cos\theta_i = \frac{\gamma_{VS} - \gamma_{FS}}{\gamma_{FV}} := \sigma$$

  - Zero-mass flux condition (BC3)

$$\frac{\partial \kappa}{\partial s}(x_c, t) = 0$$

Total mass conservation of the film. No mass flux at the contact point-- no mass diffuses under the thin film at the film/substrate interface & any flux along the surface to the contact point simply moves the contact point along the substrate s.t. no flux remains

SIM for Isotropic Surface Energy –Equilibrium State

- Total interfacial free energy

$$W(\omega) = \gamma_{FV} |\Sigma_{FV}| + \underbrace{\gamma_{FS} |\Sigma_{FS}| + \gamma_{VS} |\Sigma_{VS}|}_{\text{Wall Energy}}$$

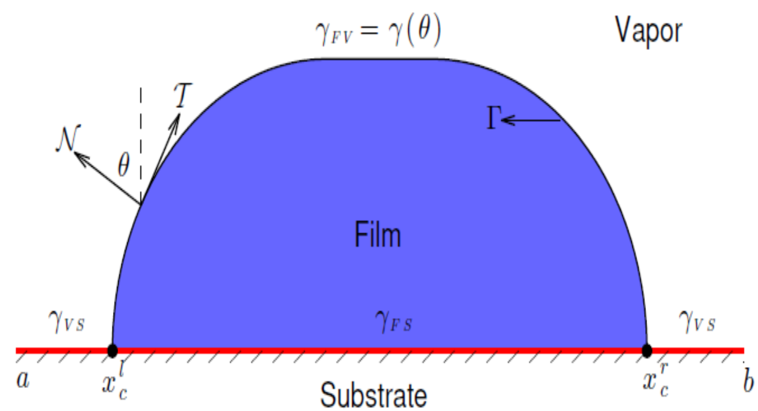
γ_{FV} -- interfacial energy (density)

$|\Sigma_{FV}|$ -- interface length (2D) or area (3D)

- Equilibrium configuration:

$$\min W(\omega)$$

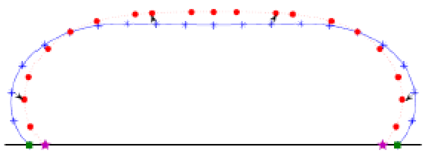
$$\text{subject to } \int_{\omega} d\omega = \text{constant}$$

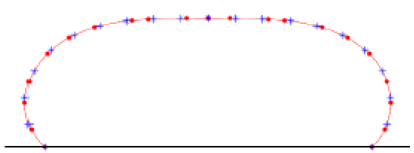


- Wulff construction & Winterbottom construction

Existing Results for SIM of Isotropic Surface Energy

- Asymptotic/mathematical results $x_c(t) \sim t^{2/5} \quad t \gg 1, \quad 0 \le \theta_i \ll 1$
  - For 3D linearized problem (small angle) — [1]:
  - For equilibrium static problem -- linearized stability analysis -- [2]
  - For dynamic nonlinear problem ????
- Front-track approaches (marker particle methods) [3]:
  - Results:
    - 2D with arclength – works well
    - 3D with marker particles – too tedious and low accuracy!!
  - Main difficulties
    - Fourth-order derivatives along the surfaces -- accuracy
    - Complex topological changes (pinch-off) – complexity



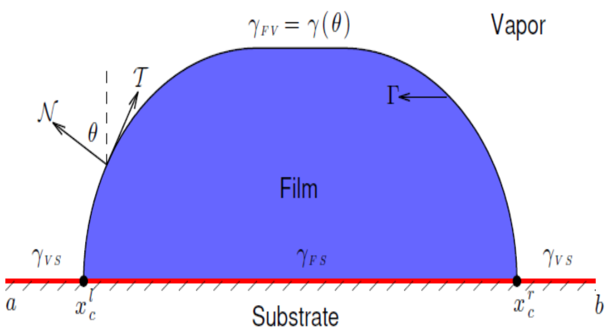


[1] D.J. Srolovitz & S.A. Safran, J. Appl. Phys., 60 (1986), 247; 60(1986), 255.
[2] H. Garcke, K. Ito & Y. Kohsaka, SIAM J. Math. Anal., 36 (2005), 1031-1056.
[3] H. Wong, PW Voorhees, MJ Miksis, SH Davis, Acta Mater, 48 (2000), 1719.

SIM for Anisotropic Surface Energy

(via thermodynamical variation)

$\Gamma: \quad \vec{X}(s,t) = (x(s,t), y(s,t)) \qquad s$ -- arclength



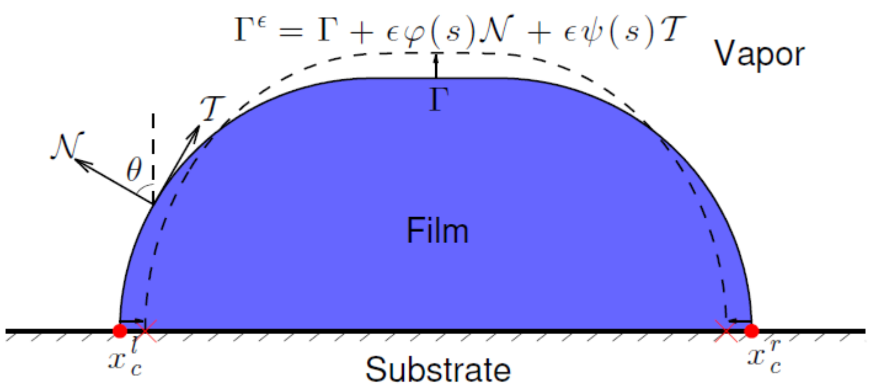
- Total interfacial free energy

$$W = \int_\Gamma \gamma_{FV}(\theta) d\Gamma + (\gamma_{FS} - \gamma_{VS})(x_c^r - x_c^l)$$

  – Anisotropic surface energy

$$\gamma_{FV} = \gamma(\theta) = \gamma_0[1 + \beta\cos(m\theta)], \qquad m = 2,3,4,6$$

- Thermo-dynamical variation: $\psi(s)$ is arbitrary & $\int_0^L \varphi(s) ds = 0$



$$\Gamma^\varepsilon(t) = (x^\varepsilon(s,t), y^\varepsilon(s,t))$$
$$= (x(s,t) + \varepsilon u(s,t), y(s,t) + \varepsilon v(s,t))$$

$$u(s,t) = x_s(s,t)\psi(s) - y_s(s,t)\varphi(s)$$
$$v(s,t) = x_s(s,t)\varphi(s) + y_s(s,t)\psi(s)$$
$$v(0,t) = v(L,t) = 0 \quad \& \quad |A(\Gamma^\varepsilon) - A(\Gamma)| \le C_0\,\varepsilon^2$$

SIM for Anisotropic Surface Energy

(via thermodynamical variation)

- Calculate first variation of the energy functional

$$W = \int_\Gamma \gamma_{FV}(\theta)d\Gamma + (\gamma_{FS} - \gamma_{VS})(x_c^r - x_c^l)$$

$$W^\varepsilon = \int_{\Gamma^\varepsilon} \gamma_{FV}(\theta^\varepsilon)d\Gamma + (\gamma_{FS} - \gamma_{VS})[(x_c^r + \varepsilon u(L,t)) - (x_c^l + \varepsilon u(0,t))]$$

$$\left.\frac{dW^\varepsilon}{d\varepsilon}\right|_{\varepsilon=0} = \lim_{\varepsilon\to 0}\frac{W^\varepsilon - W}{\varepsilon} = \int_0^L \big(\gamma(\theta) + \gamma''(\theta)\big)\kappa\varphi ds + f(\theta_c^r)u(L,t) - f(\theta_c^l)u(0,t)$$

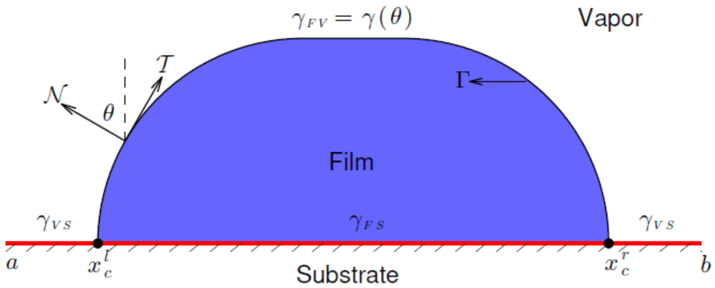
$$\mu := \frac{\delta W}{\delta\Gamma} = (\gamma(\theta) + \gamma''(\theta))\kappa, \quad \frac{\delta W}{\delta x_c^r} = f(\theta)\big|_{\theta=\theta_c^r}, \quad \frac{\delta W}{\delta x_c^l} = -f(\theta)\big|_{\theta=\theta_c^l}$$

$$f(\theta) := \gamma(\theta)\cos\theta - \gamma'(\theta)\sin\theta - \gamma_0\cos\theta_i, \quad \cos\theta_i = \sigma := \frac{\gamma_{VS} - \gamma_{FS}}{\gamma_0}$$

[1] Wang, Jiang, Bao & Srolovitz, Phys. Rev. B, 2015.

SIM for Weakly Anisotropic Surface Energy

$\Gamma: \quad \vec{X}(s,t) = (x(s,t), y(s,t)) \qquad s$ -- arclength



- The Model (Wang, Jiang, Bao, Srolovitz, PRB 15')

$$\frac{\partial \vec{X}(s,t)}{\partial t} = V_n \vec{n}, \qquad \text{with} \quad V_n = B\frac{\partial^2 \mu}{\partial s^2}$$

$$\mu(\theta) = B(\gamma(\theta) + \gamma''(\theta))\kappa$$

θ_c^r --Dynamical contact angle

θ_i----Isotropic Young contace angle

- Boundary conditions
  - Contact point condition (BC1): $y(x_c^r, t) = 0$
  - Relaxed contact angle condition (BC2)[1]: $\frac{dx_c^r(t)}{dt} = -\eta\frac{\delta W}{\delta x_c^r} = -\eta f(\theta_c^r),$
  - Zero-mass flux condition (BC3): $\partial_s \mu(x_c^r, t) = 0$
- Anisotropic Young equation $\eta \rightarrow \infty$

$$\gamma(\theta)\cos\theta - \gamma'(\theta)\sin\theta - \gamma_0\cos\theta_i = 0 \overset{\gamma(\theta)\equiv\gamma_0}{\Longrightarrow} \cos\theta = \cos\theta_i$$

[1] Ren, E, Phys. Fluid, 2007&2011; Ren, Hu & E, Phys Fluid, 2010.

Dynamical Properties

$$A(t) = \int_0^{L(t)} y\partial_s x \, ds \Rightarrow A(t) \equiv A(0)$$

- Area (Mass) conservation
- Energy dissipation

$$W(t) = \int_0^{L(t)} \gamma_{FV}(\theta)ds + (\gamma_{FS} - \gamma_{VS})(x_c^r - x_c^l) \Rightarrow W'(t) = -\int_0^{L(t)} (\partial_s \mu)^2 ds + \mu\partial_s\mu\Big|_{s=0}^{s=L(t)}$$

$$+\frac{dx_c^r(t)}{dt} f(\theta)\Big|_{\theta=\theta_c^r} - \frac{dx_c^l(t)}{dt} f(\theta)\Big|_{\theta=\theta_c^l} = -\int_0^{L(t)} (\mu_s)^2 ds - C\left[\left(\frac{dx_c^r(t)}{dt}\right)^2 + \left(\frac{dx_c^l(t)}{dt}\right)^2\right] \le 0$$

- Weakly anisotropic case:

$$\gamma(\theta) + \gamma''(\theta) > 0 \quad \Leftrightarrow \quad 0 \le \beta < \frac{1}{m^2 - 1}$$

Strongly Anisotropic Case

- Strongly anisotropic case
  - Case I: $\beta > \frac{1}{m^2 - 1} \Rightarrow \gamma(\theta) + \gamma''(\theta)$ change sign
    - ill-posedness
    - Multiple solution of the anisotropic Young equation

$$\gamma(\theta)\cos\theta - \gamma'(\theta)\sin\theta - \gamma_0 \cos\theta_i = 0$$

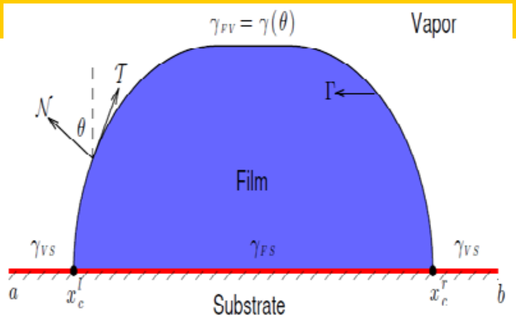
    - Regularize the total energy
  - Case II: Surface energy is not smooth $\gamma(\theta) \notin C^2 \Rightarrow \gamma_\varepsilon(\theta) \in \mathrm{C}^2$
    - A typical example

$$\gamma(\theta) = \sqrt{|\cos\theta| + |\sin\theta|} \Rightarrow \gamma_\varepsilon(\theta) = \sqrt{\left(\varepsilon + \cos^2\theta\right)^{1/2} + \left(\varepsilon + \sin^2\theta\right)^{1/2}}$$

    - Regularize (or smooth) the surface energy density

Strongly Anisotropic Surface Energy

$\Gamma: \quad \vec{X}(s,t) = (x(s,t), y(s,t)) \qquad s$ -- arclength



- Regularized interfacial free energy

$$W_\varepsilon = \int_\Gamma \gamma_{FV}(\theta)\, d\Gamma + (\gamma_{FS} - \gamma_{VS})(x_c^r - x_c^l) + \frac{\varepsilon^2}{2}\int_\Gamma \kappa^2\, d\Gamma$$

- Calculate first variation of the energy functional

$$\mu_\varepsilon := \frac{\delta W_\varepsilon}{\delta \Gamma} = (\gamma(\theta) + \gamma''(\theta))\kappa - \varepsilon^2\left[\partial_{ss}\kappa + \frac{\kappa^3}{2}\right],$$

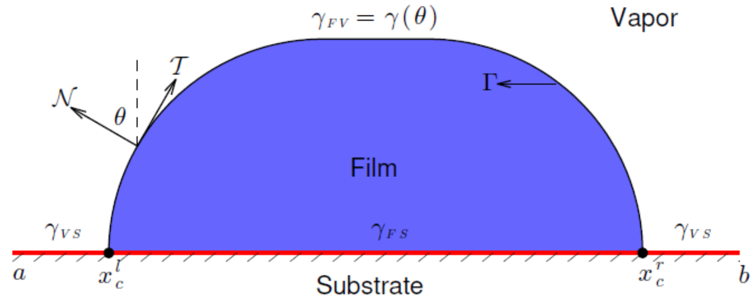
$$\frac{\delta W_\varepsilon}{\delta x_c^r} = f_\varepsilon(\theta)\Big|_{\theta=\theta_c^r}, \quad \frac{\delta W_\varepsilon}{\delta x_c^l} = -f_\varepsilon(\theta)\Big|_{\theta=\theta_c^l}, \qquad \cos\theta_i = \sigma := \frac{\gamma_{VS} - \gamma_{FS}}{\gamma_0}$$

$$f_\varepsilon(\theta) := \gamma(\theta)\cos\theta - \gamma'(\theta)\sin\theta - \gamma_0\cos\theta_i + \varepsilon^2\left[\frac{\kappa(\theta)^2}{2}\cos\theta - \partial_s\kappa(\theta)\sin\theta\right]$$

[1] J. Lowengrub, A. Voigt, ….
[2] Jiang, Wang, Zhao, Srolovitz & Bao, Script. Mater., 16'.

SIM for Strongly Anisotropic Surface Energy

$\Gamma: \quad \vec{X}(s,t) = (x(s,t), y(s,t))$ $\quad s$ -- arclength



- The Model (Jiang, Wang, Zhao, Srolovitz, Bao, 16')

$$\frac{\partial \vec{X}(s,t)}{\partial t} = V_n\, \vec{n}, \qquad \text{with} \qquad V_n = B\frac{\partial^2 \mu_\varepsilon}{\partial s^2}$$

$$\mu_\varepsilon(\theta) = B(\gamma(\theta) + \gamma''(\theta))\kappa - \varepsilon^2\left[\partial_{ss}\kappa + \frac{\kappa^3}{2}\right]$$

θ_c^r --Dynamical contact angle

θ_i----Isotropic Young contace angle

- Boundary conditions
  - Contact point condition (BC1): $y(x_c^r, t) = 0$
  - Relaxed contact angle condition (BC2): $\dfrac{dx_c^r(t)}{dt} = -\eta\dfrac{\delta W}{\delta x_c^r} = -\eta f_\varepsilon(\theta_c^r),$
  - Zero-curvature condition (BC3): $\kappa(x_c^r, t) = 0$
  - Zero-mass flux condition (BC4): $\partial_s \mu(x_c^r, t) = 0$

Parametric Finite Element Method (PFEM)

- Weakly anisotropic case
  - Mathematical model and variational form

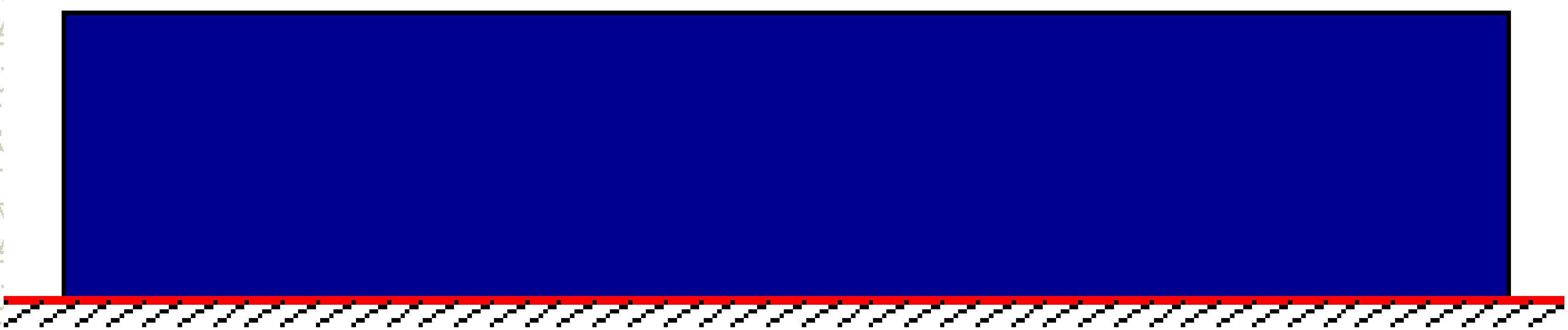
$$(\partial_t \vec{X}(s,t))\bullet\vec{n} = B\partial_{ss}\mu \qquad \int_C (\partial_t \vec{X}(s,t))\bullet\vec{n}\,\phi dp + \int_C B\partial_s\mu\,\partial_s\phi dp = 0, \quad \phi \in H_0^1$$

$$\mu(\theta) = (\gamma(\theta)+\gamma''(\theta))\kappa \Leftrightarrow \qquad \int_C [\mu(\theta) - (\gamma(\theta)+\gamma''(\theta))\kappa]\varphi dp = 0, \qquad \varphi \in H^1$$

$$\kappa\vec{n} = -\partial_{ss}\vec{X}(s,t) \qquad \int_C \kappa\vec{n}\bullet\vec{\eta} dp + \int_C \partial_s \vec{X}(s,t)\bullet\partial_s\vec{\eta} dp = 0, \qquad \vec{\eta} \in (H_0^1)^2$$

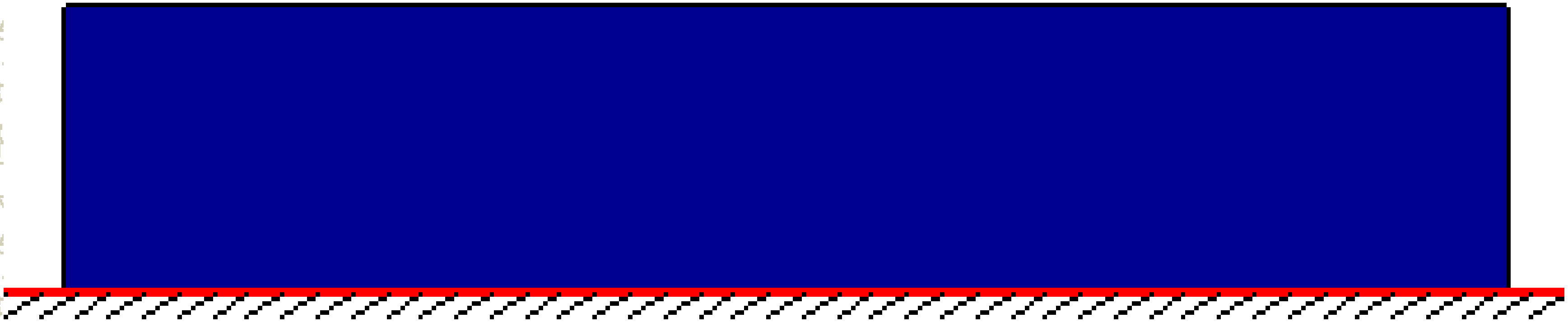
  - Boundary conditions $y(x_c^r, t) = 0, \qquad \frac{dx_c^r(t)}{dt} = -\eta f(\theta_c^r)$
  - Finite element discretization via piecewise polynomials
- Ref: [1] J.W. Barratt, H. Garcke & R. Nurnberg, J. Comput. Phys., 2007; SISC (2007); 2012.
  [2] W. Bao, W. Jiang & Q. Zhao, 2015.

$$L = 5, \beta = 0, \sigma = \cos(3\pi/4)$$



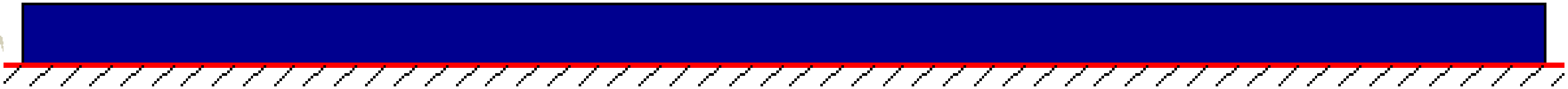
Isotropic surface energy and short

$$L = 5, m = 4, \beta = 0.06, \sigma = \cos(3\pi/4)$$



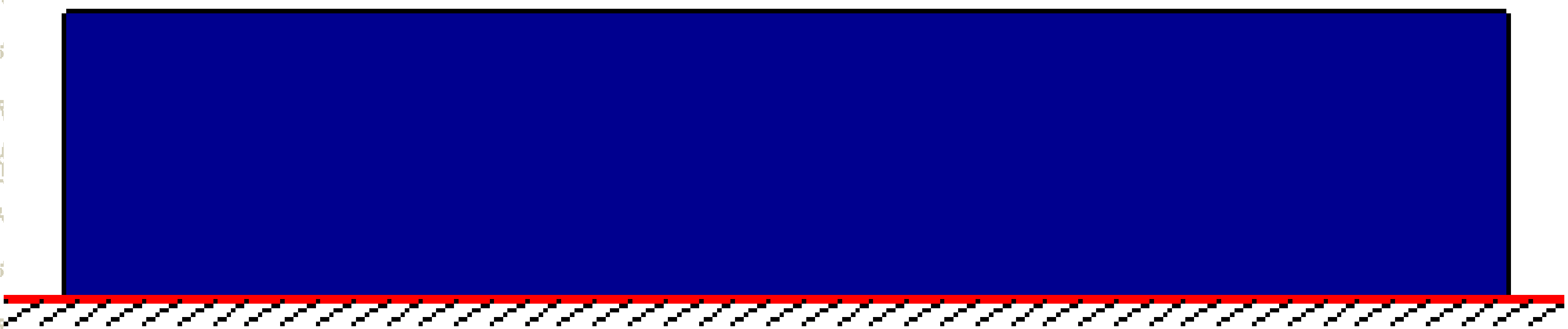
Weakly anisotropic surface energy & short

$$L = 60, m = 4, \beta = 0.06, \sigma = \cos(5\pi/6)$$



Weakly anisotropic surface energy & long for pinch-off

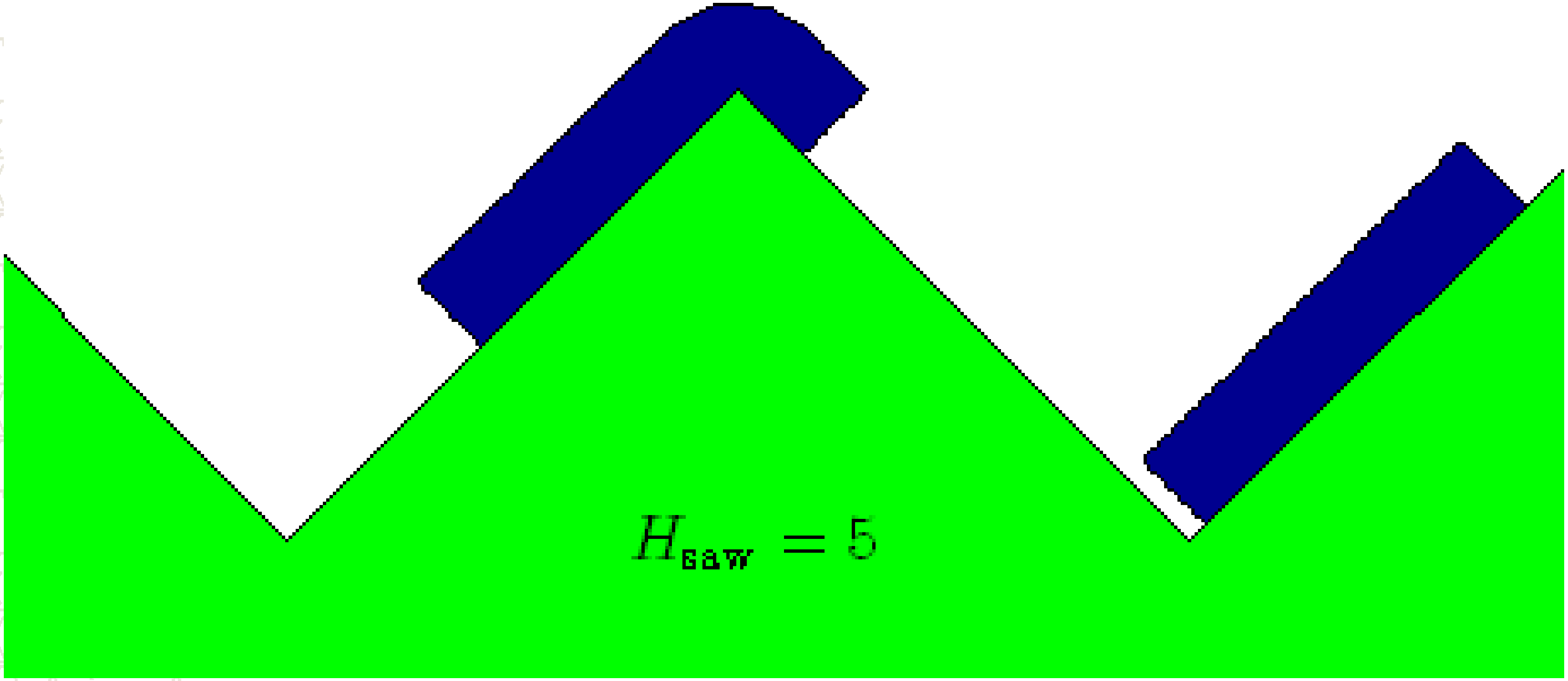
$$L = 5, m = 4, \beta = 0.2, \sigma = \cos(3\pi/4)$$



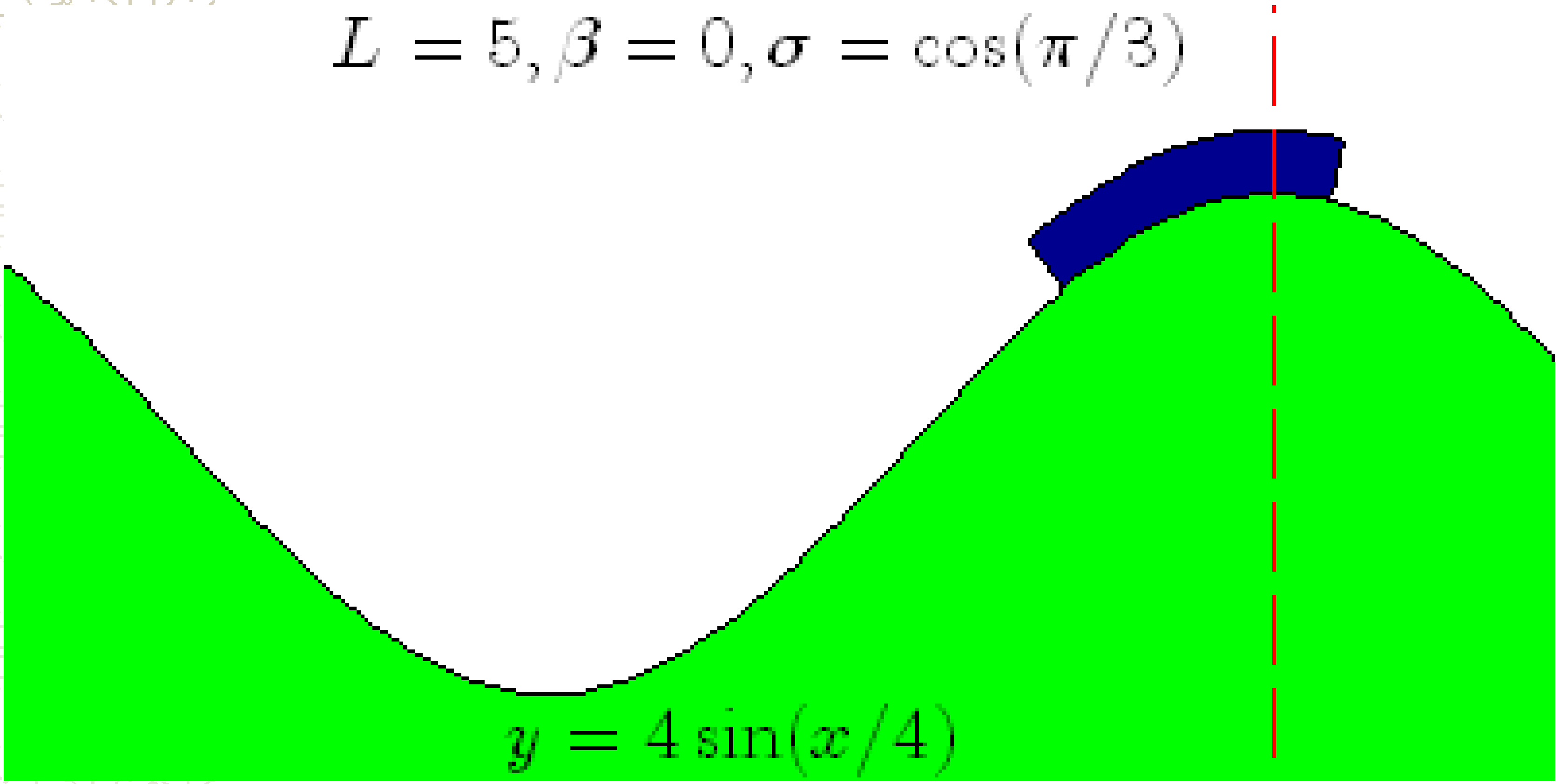
Strongly anisotropic surface energy & short

Extension to Curved Substrate

$$L = 5, \beta = 0, \sigma = \cos(\pi/3)$$

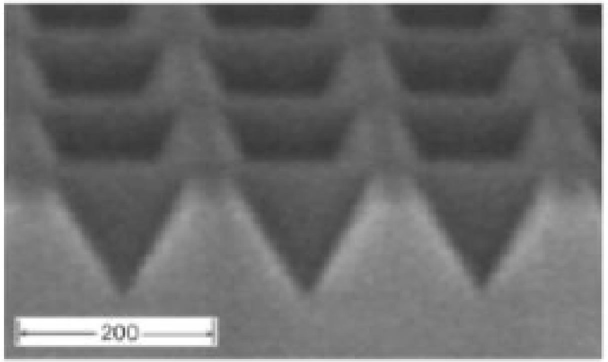


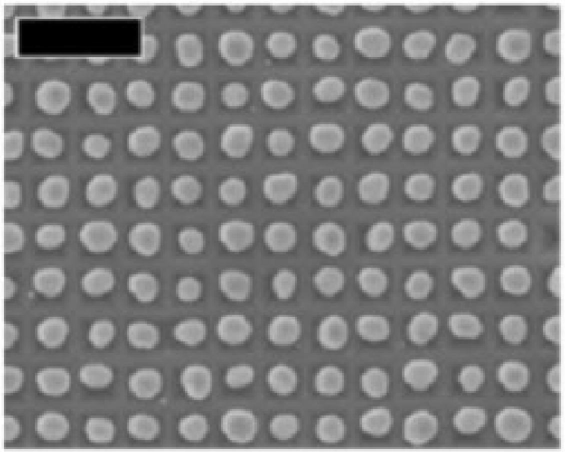
Extension to Curved Substrate



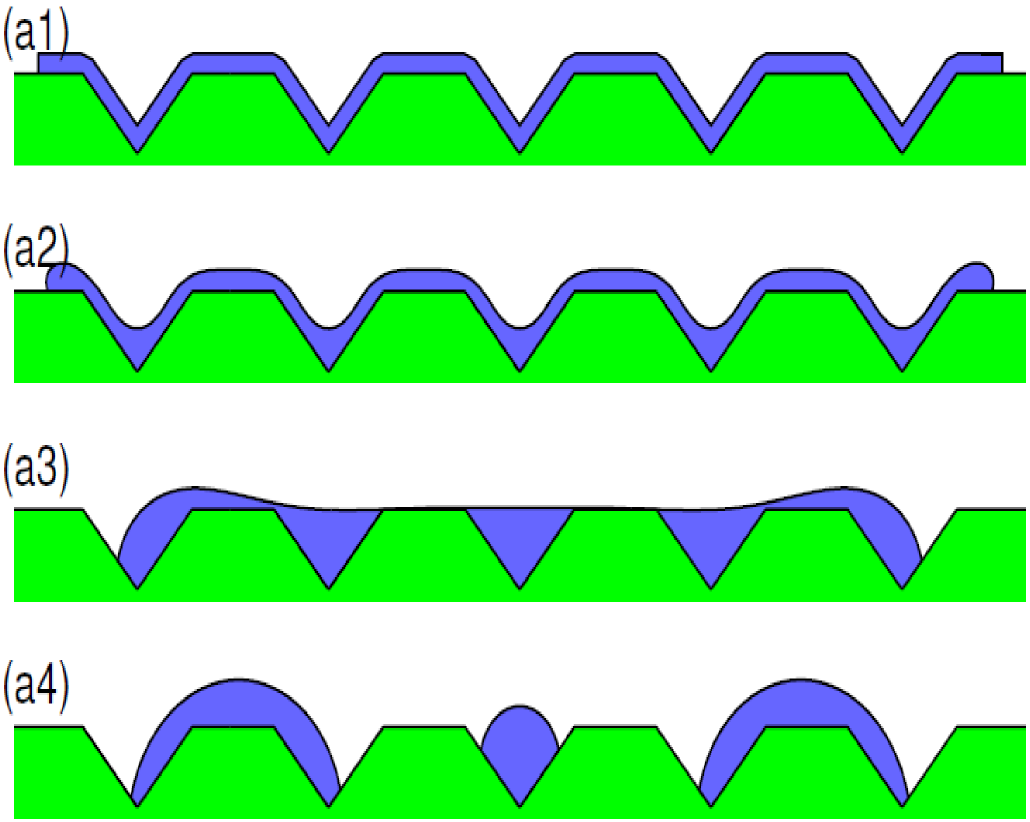
$$\Gamma(s) = (x(s), y(s)) \text{ with } \kappa := \kappa(s) \Rightarrow v(s) \propto C(\sigma)\kappa'(s)$$

Extension to Curved Substrate





Experiment (Ye, et. Al, PRB, 10')



Simulation

Phase Field/Diffuse Interface Model

- Phase field models --- S. Allen & J.W. Cahn (1975—79), J.W. Cahn & J. E. Hilliard (1958); G.J. Fix (1983), J.S. Langer (1986), L.Q. Chen (2002); C.M. Elliott, X.F. Chen, J. Shen, Q. Du, J. Lowengrub, A. Voigt, Q. Wang, G. Forest, XB Feng, PW Zhang, A.A. Lee A. Munch & E. Suli, …
  - Introduce a phase function& write down the energy
  - By variation – Allen-Cahn or Cahn-Hilliard equations
  - Applications in materials simulation: solidification; viscous fingering; fracture; solid-state nucleation; dislocation dynamics, …….
- Advantages
  - Interface/surface capturing method – Eulerian coordinates
  - Easy extension from 2D to 3D
  - Naturally capture complex topological changes

Problem Set-up

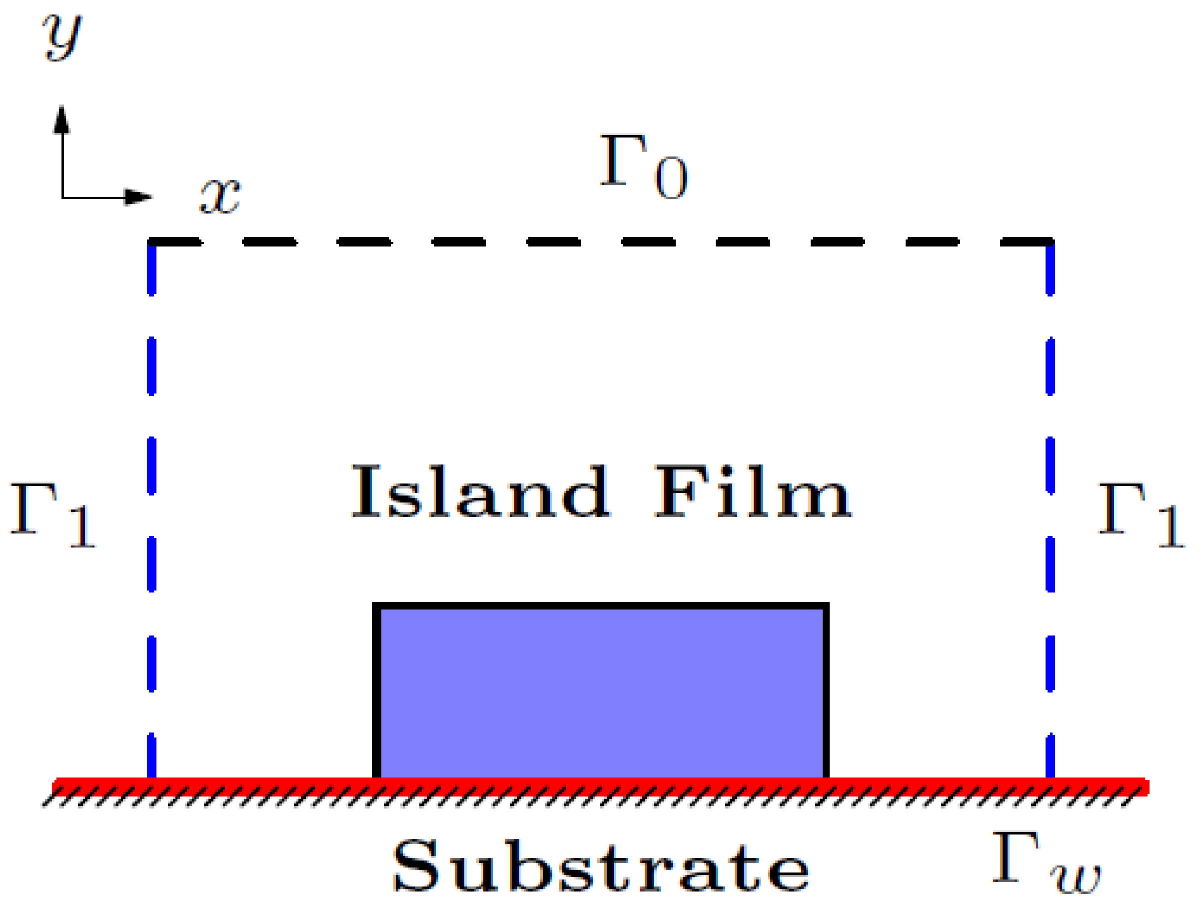


Figure: A schematical illustration of the problem set-up.

Phase Field Model

- Introduce the phase function $\phi := \phi^\varepsilon(\vec{x}, t) \in [-1,1]$

$$\phi = \begin{cases} \approx 1 \,\&\, \in (0,1] & \text{thin film phase} \\ \approx -1 \,\&\, \in [-1,0) & \text{vapor phase} \\ = 0 & \text{interface/surface} \end{cases}$$

ε --interface width

$\tanh\left(\dfrac{d_s(\vec{x},\Gamma)}{\varepsilon}\right)$

- Total free energy-- isotropic surface energy

$$W^\varepsilon = \underbrace{W_{FV}^\varepsilon}_{\text{Film-vapor phase energy}} + \underbrace{W_W^\varepsilon}_{\text{Wall energy}}$$

$$= \int_\Omega \underbrace{f_{FV}}_{\text{Film-vapor energy density}} d\Omega + \int_{\Gamma_W} \underbrace{f_W}_{\text{Wall energy density}} d\Gamma_W$$

- Energy minimization problem:

$$\min W^\varepsilon \qquad \text{subject to BCs}$$

Phase Field Model

- Film/vapor phase energy – Ginzburg-Landau free energy

$$f_{FV}(\phi,\nabla\phi) = \underbrace{\lambda}_{\text{mixing constant}} \left[\frac{\varepsilon}{2} \underbrace{|\nabla\phi|^2}_{\text{film/vapor energy}} + \frac{1}{\varepsilon} \underbrace{F(\phi)}_{\text{interface energy}} \right], \qquad F(\phi) = (\phi^2 - 1)^2$$

  - Convergence – L. Modica & S. Mortola, Boll. Un. Mat. Ital. A, 14 (1977), 526.

$$\text{If } \lambda = \frac{3\sqrt{2}}{4}\gamma_{FV} \quad \Rightarrow \quad W_{FV}^{\varepsilon} \to \gamma_{FV} |\Sigma_{FV}|$$

- Wall energy must satisfy
  - At homogeneous vapor phase $\phi = -1 \Rightarrow f_W(\phi) = \gamma_{VS}$ & $f_W'(\phi) = 0$
  - At homogeneous film phase $\phi = 1 \Rightarrow f_W(\phi) = \gamma_{FS}$ & $f_W'(\phi) = 0$

$$f_W(\phi) = \frac{\gamma_{VS} + \gamma_{FS}}{2} - \frac{\phi(3 - \phi^2)}{4}(\gamma_{VS} - \gamma_{FS})$$

Phase Field Model

- Cahn-Hilliard equation with function-dependent mobility

$$\begin{cases} \frac{\partial \phi}{\partial t} = \nabla \bullet (M \nabla \mu) \\ \mu = \phi^3 - \phi - \varepsilon^2 \Delta \phi \end{cases} \quad \text{in} \quad \Omega \qquad \text{with} \qquad M = (1-\phi^2)^2$$

- With BCs(Jiang, Bao, Thompson & Srolovitz, Acta Mater., 12')
  - On wall boundary Γ_W $\quad \varepsilon \frac{\partial \phi}{\partial \vec{n}} + \frac{f_W'(\phi)}{\lambda} = 0 \quad \& \quad \cos\theta_s = \frac{\gamma_{VS} - \gamma_{FS}}{\gamma_{FV}}$

$$\varepsilon \frac{\partial \phi}{\partial \vec{n}} + \frac{\sqrt{2}}{2}(\phi^2 - 1)\cos\theta_s = 0 \qquad \& \qquad \frac{\partial \mu}{\partial \vec{n}} = 0$$

  - On other boundaries $\Gamma_0 \cup \Gamma_1 = \partial\Omega \setminus \Gamma_W \; \frac{\partial \phi}{\partial \vec{n}} = 0 \quad \& \quad \frac{\partial \mu}{\partial \vec{n}} = 0$
- Recent debate on proper mobility for surface diffusion – A.A. Lee, A. Munch & E Suli, APL 15' & 16'; A. Voigt, APL 16', …..

Numerical Method

- Stabilized semi-implicit method

$$\frac{\phi^{n+1}-\phi^{n}}{\tau} = A\varepsilon^{2}\Delta^{2}(\phi^{n}-\phi^{n+1}) + S\Delta(\phi^{n+1}-\phi^{n}) + \nabla\bullet(M^{n}\nabla\mu^{n})$$

$$\mu^{n} = (\phi^{n})^{3} - \phi^{n} - \varepsilon^{2}\Delta\phi^{n}, \qquad M^{n} = 1-(\phi^{n})^{2}$$

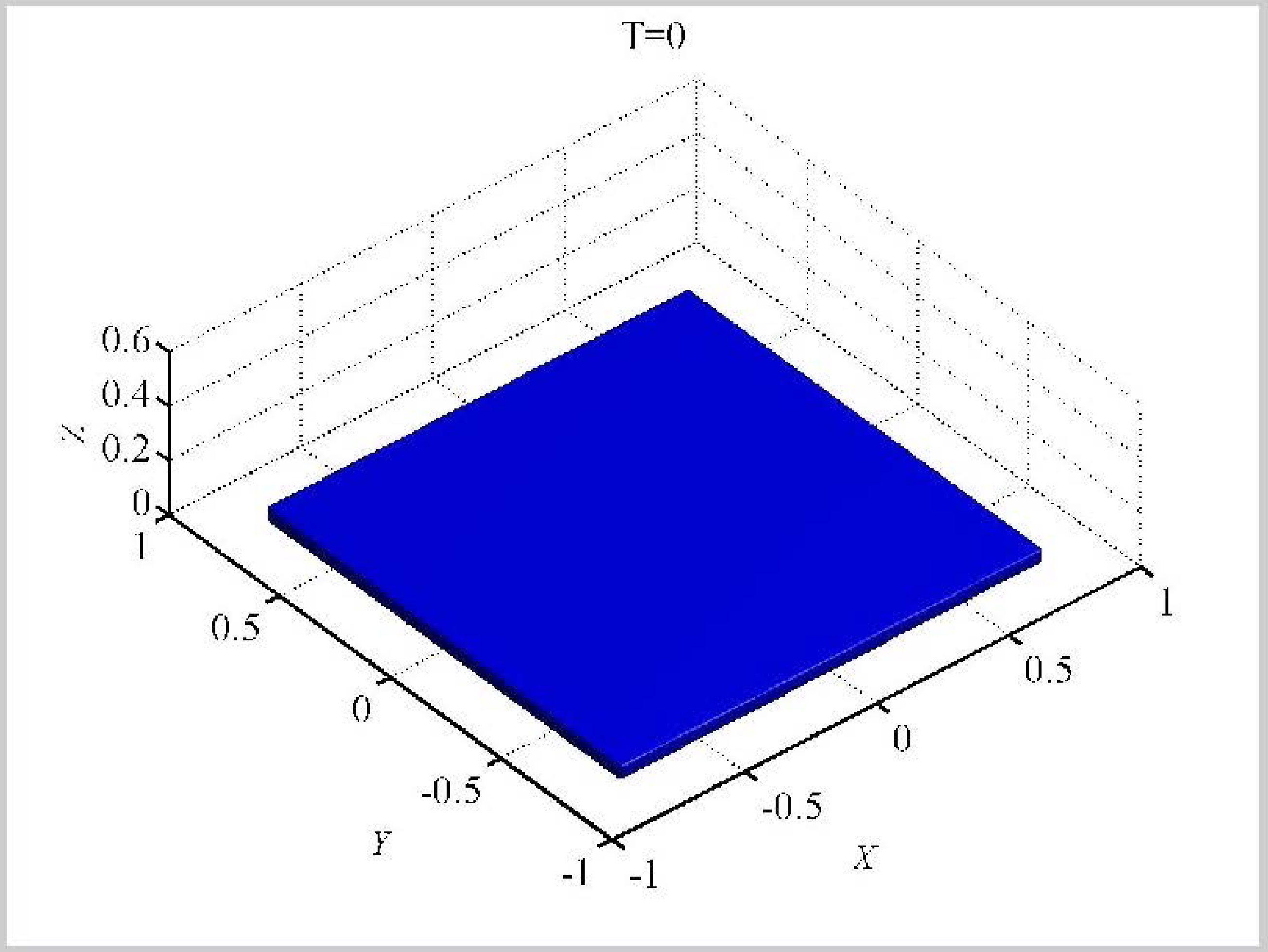
  - *A* and *S* are two stabilizing constants
  - *x*-direction by cosine pseudospectral method
  - *y*-direction by finite difference/finite element
  - 1st order in time & can be upgraded to 2nd
  - Can be solved efficiently at every step & Extension to 3D is easy

[1] W. Jiang, W. Bao, C.V. Thompson &D. J. Srolovitz, Acta Mater. 60(2012), 5578.

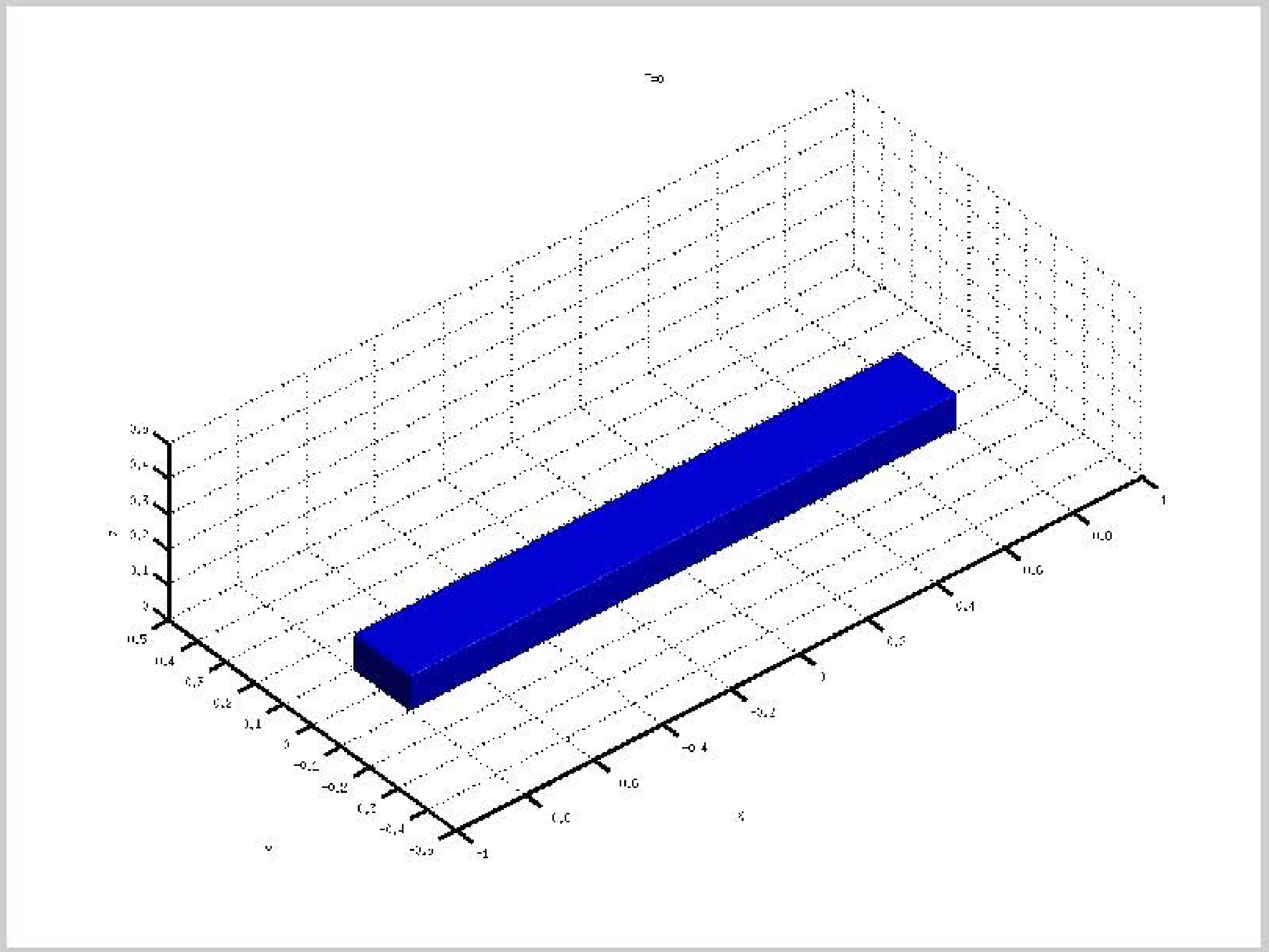
[2] J.Z. Zhu, L.Q. Chen, J Shen & V. Tikare, Phys. Rev. E, 60 (1999), 3564.

[2] J. Shen & X.F. Yang, SIAM J. Sci. Comput., 32 (2010), 1159.

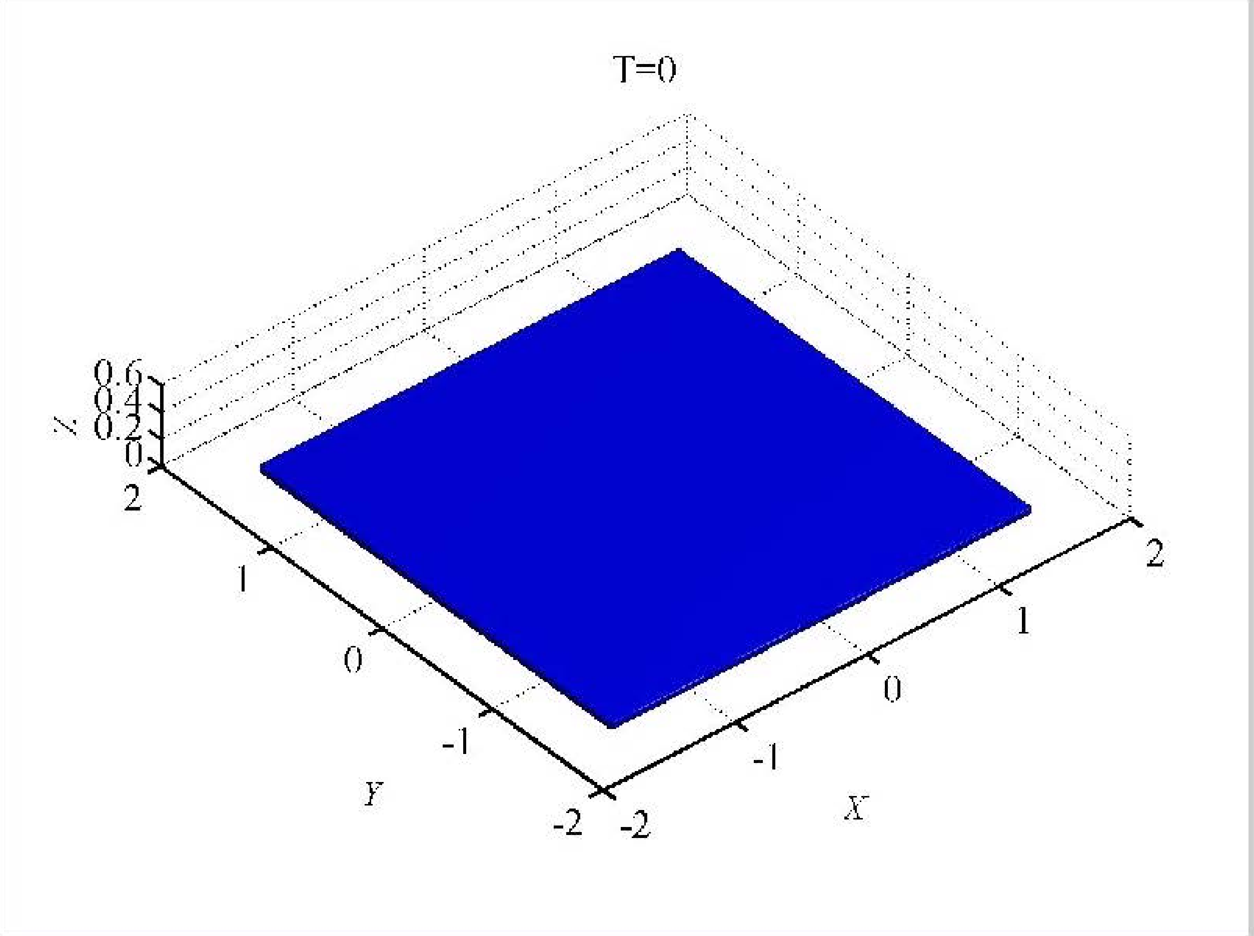
3D Results I -- Square $\theta_s = 5\pi/6$



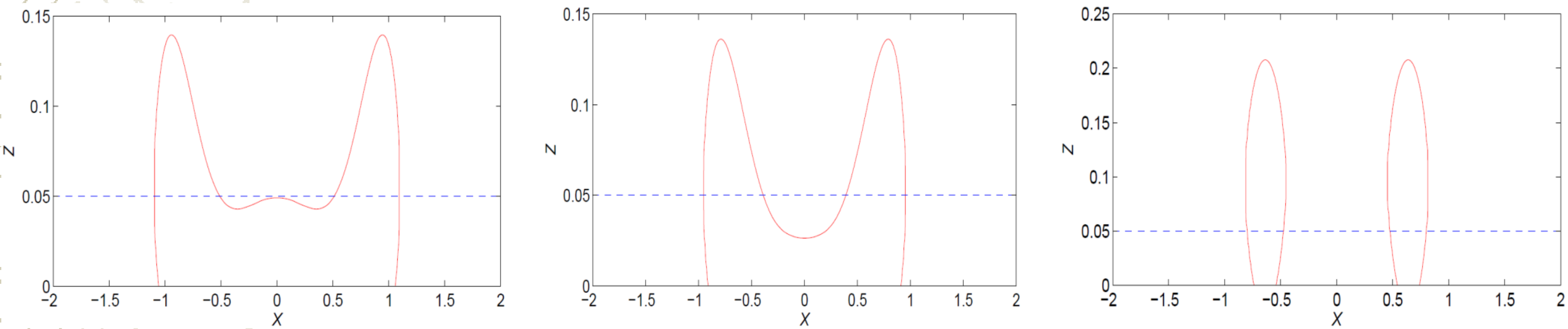
3D Results II – Pinch-off $\theta_s = 5\pi / 6$



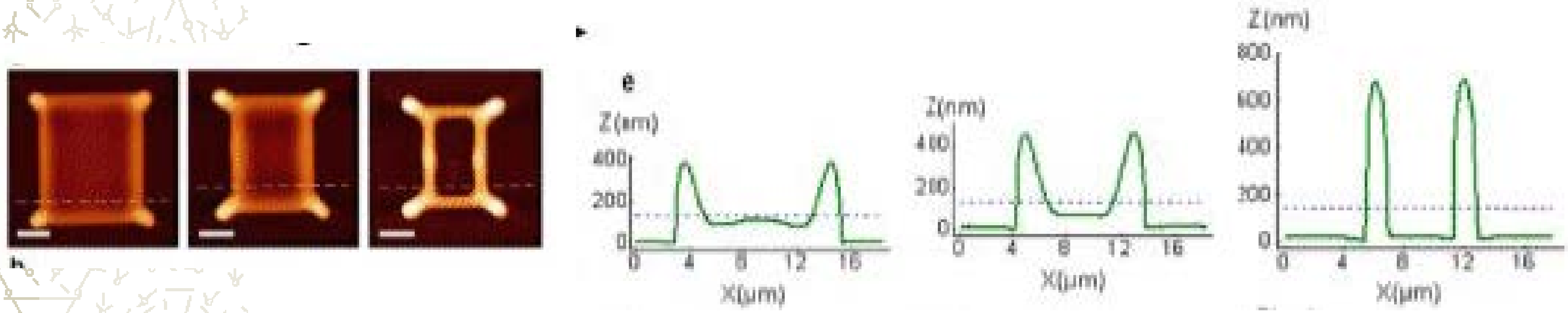
3D Results III – Large-Thin Square



3D Results – Comparison with Experiment



Computational Results



Experimental Results

Conclusion & Future Works

- Conclusion
  - Propose sharp interface model (SIM) for anisotropic surface energy
  - Propose phase field model – Cahn-Hilliard Eq. with function-dependent mobility
  - Design stable, efficient & accurate numerical methods
  - Test parameters regimes & simulate 2D & 3D results
  - Compare qualitatively with experimental / asymptotic results
- Future works
  - Phase field model with anisotropic surface energy
  - Sharp interface model in 3D and/or rough substrate
  - Investigate role of different surface energy anisotropy & regularization
  - Develop adaptive & parallel numerical method
  - Mathematical analysis of the models
  - Compare with experiments quantitatively & guide new experiments