

Lecture 2: Wetting and dewetting of solids and liquids

Olivier Pierre-Louis

ILM-Lyon, France

28th May 2017

- 1 Static Wetting of liquids and Solids
 - Introduction
 - Wulff-Kaishew construction
 - Thin Films
 - Elastic effects
- 2 Dynamics of solid wetting
 - Dewetting dynamics
 - Surface diffusion model with wetting potential
 - Derivation of the TL Boundary Condition
 - Spinodal dewetting and Accelerated mass shedding
 - Elastic dewetting /ATG
 - KMC study of magic heights
 - Dewetting without a rim
 - Non-conservation of the mass: evaporation and reaction
- 3 Islands on nano-patterns
 - Patterns larger than islands
 - Patterns smaller than islands
 - Islands on nano-pillars
 - Solid imbibition in nano-pillars
- 4 Conclusions

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3 Islands on nano-patterns

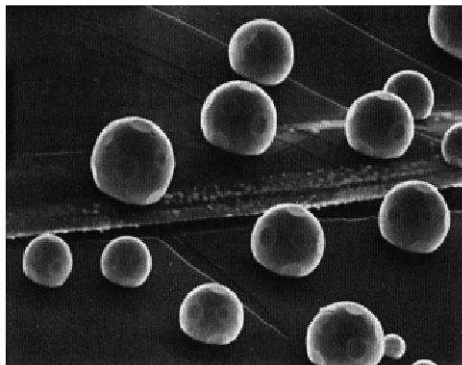
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4 Conclusions

Some examples



J.-J. Métois, Au/Graphite



Differences between liquids and solids

	Simple Liquids	Crystalline solids
Structure	Isotropic	Anisotropic
Energy	Surface & Interface	Surface & Interface + Elastic
Mass Transport	Bulk hydrodynamics	Surface diffusion

Other cases: Liquid crystals, Non-Newtonian Fluids, amorphous solids, etc.

→ Similar or different behaviors?

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Equilibrium equations

Free energy

$$\mathcal{F} = \int_{VS} ds \gamma_{VS}(\theta) + \int_{SA} ds \gamma_{SA}(\theta) + \int_{AV} ds \gamma(\theta)$$

Total number of atoms

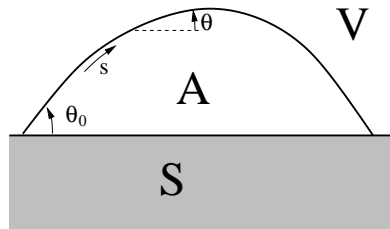
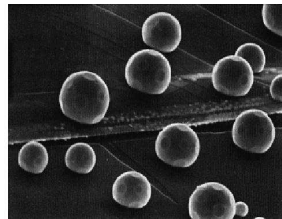
$$\mathcal{N} = \Omega^{-1} \int \int_A d^2\mathbf{r}$$

Vanishing variation

$$\delta(\mathcal{F} - \mu\mathcal{N}) = 0$$

→ Equilibrium equations

J.-J. Métois, Au/Graphite



Spreading or not spreading

Spreading coefficient $\mathcal{S} = \gamma_{SV} - \gamma_{SA} - \gamma(0)$

Complete dewetting

$$\gamma_{SV} + \gamma(0) < \gamma_{SA}$$

$$\mathcal{S} < -2\gamma(0)$$

Partial Wetting

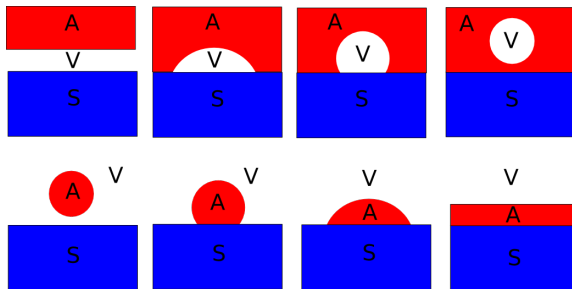
$$-\gamma(0) < \gamma_{SV} - \gamma_{SA} < \gamma(0)$$

$$-2\gamma(0) < \mathcal{S} < 0$$

Total Wetting

$$\gamma_{SV} > \gamma_{SA} + \gamma(0)$$

$$\mathcal{S} > 0$$



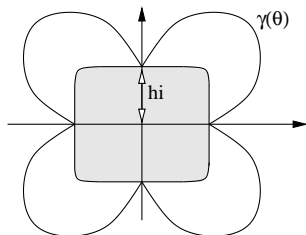
Facets

Roughening temperature T_r

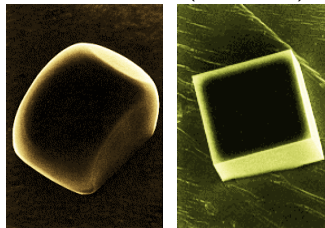
$T < T_r$



$T > T_r$



NaCl, Métois et al (620-710°C)



For usual crystals $T_r \sim T_M$

Equilibrium shape, Wulff 1901

Away from the substrate: Wulff Shape

- Discrete with facets

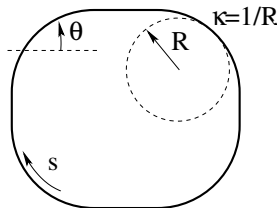
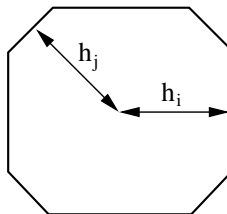
$$h_i = \frac{\Omega \gamma_i}{\mu}$$

Facet free energy γ_i

- Continuum

$$\mu = \Omega \tilde{\gamma}(\theta) \kappa$$

Stiffness $\tilde{\gamma}(\theta) = \gamma(\theta) + \gamma''(\theta)$



Remarks:

- Wulff construction
- Equivalence discrete - continuum
- Possible coexistence of smooth and facetted parts

Wetting equil. shape / flat substrate: Kaishew 1950, Winterbottom 1967

Main idea: flat substrate \leftrightarrow facet

- Global condition: Truncation

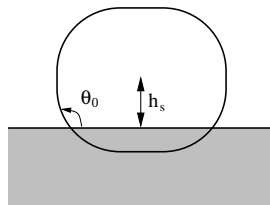
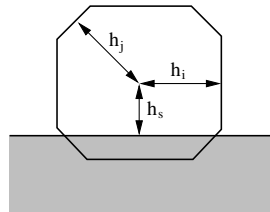
$$h_s = - \frac{\Omega(\gamma_{VS} - \gamma_{SA})}{\mu}$$

OR

- At the triple line if no facet: Young equation

$$\gamma_{VS} - \gamma_{SA} = \gamma(\theta_0) \cos(\theta_0) - \gamma'(\theta_0) \sin(\theta_0)$$

Contact angle not a good parameter for faceted crystals!

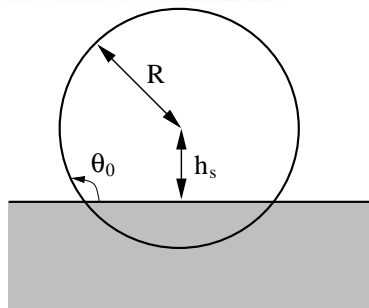
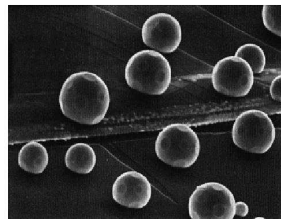


Isotropic

Isotropic solid or liquid: $\gamma(\theta) = \bar{\gamma}$

$$\mu = \Omega \bar{\gamma} \kappa \Leftrightarrow R = \frac{\Omega \bar{\gamma}}{\mu}$$

$$\bar{\gamma} \cos(\theta_0) = \gamma_{VS} - \gamma_{SA} \Leftrightarrow h_s = -\frac{\Omega(\gamma_{VS} - \gamma_{SA})}{\mu}$$



Finite size effects

Expansion of the thermodynamic energy in 3D

$$\mathcal{E} \sim \gamma_3 \mathcal{N} + \gamma_2 \mathcal{N}^{2/3} + \gamma_1 \mathcal{N}^{1/3} + \dots$$

- $\gamma_3 \sim$ chemical potential $\mathcal{N} \sim L^3$
- $\gamma_2 \sim$ surface energy $\mathcal{N}^{2/3} \sim L^2$
- $\gamma_1 \sim$ line energy $\mathcal{N}^{1/3} \sim L$

higher orders are non-trivial!

Perstipino, Laoi, Tosatti PRL2012, J.Chem.Phys. 2013

Edges between facets or Triple line $\sim L \sim \mathcal{N}^{1/3}$

\Rightarrow corrections to the equilibrium shape.

Contact angle influenced by triple line tension

γ_{TL} positive or negative

3D isotropic with line tension

$$\mathcal{G} = \bar{\gamma}\mathcal{A} + (\gamma_{AS} - \gamma_{SV})\mathcal{A}_S + \gamma_{TL}\mathcal{L}_{TL} - \mu\mathcal{N}$$

Spherical cap

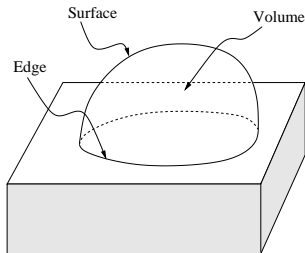
$$R = \frac{\Omega\bar{\gamma}}{\mu}$$

Modified truncation

$$\bar{\gamma} \frac{h_s}{R} = \gamma_{AS} - \gamma_{SV} + \frac{\gamma_{TL}}{(R^2 - h_s^2)^{1/2}}$$

Modified contact angle

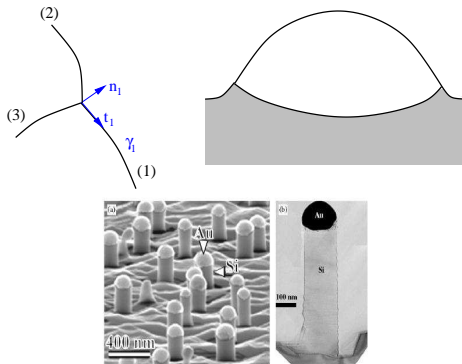
$$\bar{\gamma} \cos \theta = \gamma_{SV} - \gamma_{AS} - \frac{\gamma_{TL}}{R \sin \theta}$$



Non-frozen substrate

C. Herring (1951): Triple-point (triple-line):

$$\sum_{i=1}^3 (\gamma_i \mathbf{t}_i + \gamma'_i \mathbf{n}_i) = 0$$



Zakharov et al Physica E (2007)

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Thin film Wetting potential

Flat film thickness h

free energy $f(h)$

- $f(h = 0) = \gamma_{SV}$
- $f(h \rightarrow +\infty) = \gamma_{SA} + \gamma(\theta = 0)$

Relation $f \leftrightarrow W$

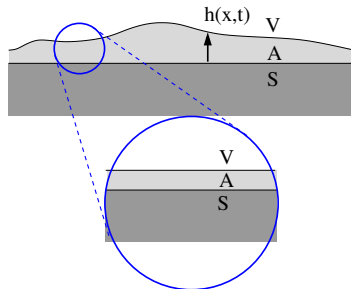
$$f(h) = \gamma_{SA} + \gamma(0) + W(h)$$

wetting potential $W(h)$

- $W(0) = \mathcal{S}$
- $W(+\infty) = 0$

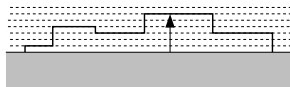
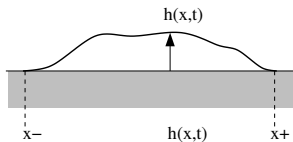
Disjoining Pressure

$$\Pi = -W'(h)$$



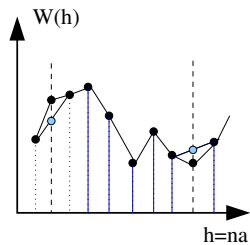
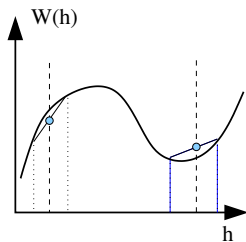
Thin film Wetting potential

Stability



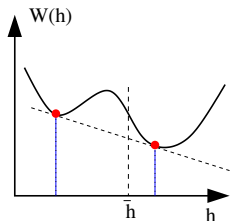
$$W''(h) > 0$$

$$W_{n+1} - 2W_n + W_{n-1} > 0$$



Thin film Wetting potential

Equilibrium: Double tangent construction

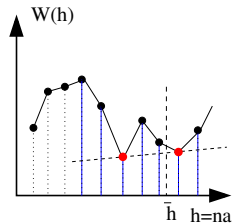


Film Tension

$$\gamma_{film}^{flat} = f(h) - hf'(h)$$

Equilibrium with substrate

$$\gamma_{film}^{flat} = \gamma_{SV}$$



Film Tension

$$\gamma_{film}^{+} = f_n - n(f_{n+1} - f_n)$$

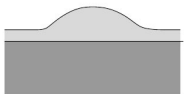
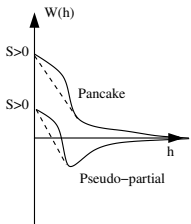
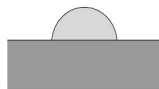
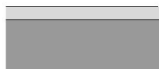
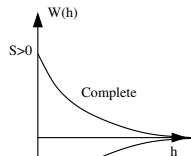
$$\gamma_{film}^{-} = f_n - n(f_n - f_{n-1})$$

Equilibrium with substrate

$$\gamma_{film}^{+} < \gamma_{SV} < \gamma_{film}^{-}$$

Thin film Wetting potential

Wetting Regimes



Small slope free energy

$$f(h) = \gamma_{SA} + \gamma(0) + W(h) + \frac{\Gamma(h)}{2}(\partial_x h)^2,$$

$$\Gamma(h) \rightarrow \tilde{\gamma}(0) \text{ when } h \rightarrow \infty$$

Macroscopic contact angle

$$\tilde{\gamma}(0) \frac{\theta_0^2}{2} = W(\infty) - W(0) = -S$$

Line tension

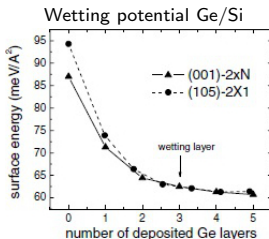
$$\gamma_{TL} = \int_0^\infty dh \left\{ \left[2\Gamma(h)(W(h) - S) \right]^{1/2} - \left[2\tilde{\gamma}(0)(-S) \right]^{1/2} \right\}$$

...Small slope model → lecture notes OPL

Thin film Wetting potential

Bonds and structural effects

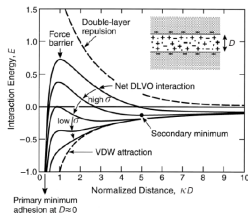
Type	form	prefactor	range
Chemical bonds	$W_0 e^{-h/d_0}$	$W_0 \sim J/a^2$	$d_0 \sim a$
Layering of Liquids and Polymers	$W_0 \cos(2\pi h/a_0) e^{-h/d_0}$	$W_0 \sim k_B T/a^2$	$d_0 \sim a$
Structural effects solids $T < T_R$	$W_0 \cos(2\pi h/a_0)$	$W_0 \sim J/a^2$, $k_B T \ll J$	$(a_0 = a)$



Thin film Wetting potential

DLVO-like contributions

Type	form	prefactor	range
Electrostatic effects	$W_0 e^{-h/\lambda_D}$	$W_0 = 2 \frac{\sigma^2 \lambda_D}{\epsilon_0 \epsilon}$	λ_D
Van der Waals Interactions	$-\frac{A}{12\pi h^2}$	$A \sim 10^{-20} - 10^{-19} \text{ J}$	—



Israelachvili, Intermolecular and surface Forces (1985)

Polymers Layering J. Krawczyk et al EPL 70 726 (2005)

Liquids Layering: Hansen and McDonald, Theory of Simple Liquids (2006)

Thin film Wetting potential

... and many other possible contributions!

Type	form	prefactor	range
Electronic confinement	$\frac{E_{fb}}{h^2} \cos(2k_{fb}h + \phi)$	$E_{fb} = 5.55\text{eV (Ag)}$	osc. $\lambda_f/2$

Z. Zhang et al, Phys.Rev.Lett.1998,1999

B. Wu and Z. Zhang, Phys. Rev. B 77, 035410 (2008)

Yong Han and Da-Jiang Liu PRE 80 155405 (2010)

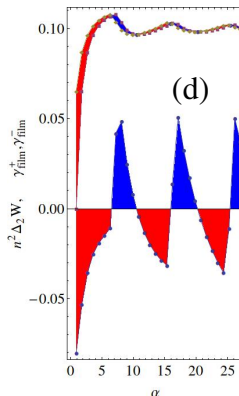
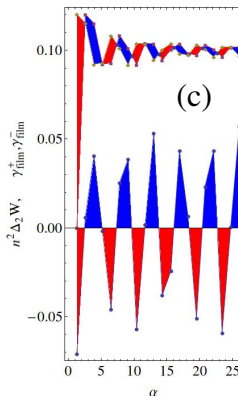
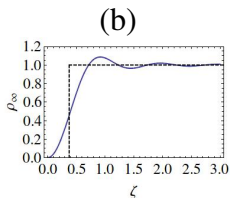
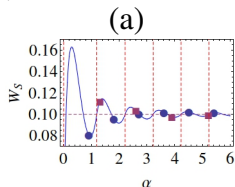
Debate in the literature: $1/h$ or $1/h^2$?

Electronic Quantum confinement

Free electron model

$$W_{EC}(h) \approx -\frac{E_{fb}}{(h+2b)^2} \frac{\pi}{36\sqrt{3}} \cos(2k_{fb}h)$$

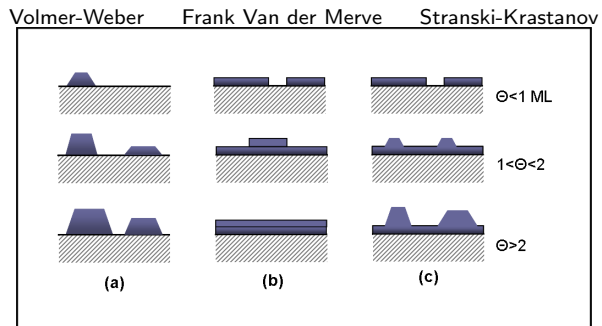
E_{fb} , k_{fb} Fermi energy and wavevect,
 $b = 3\pi k_{fb}/8$



(a) Al(111) (purple squares), Ag(111) (blue circles)

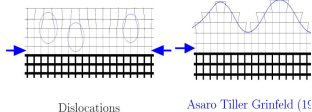
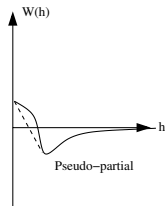
(c) Al(111) , (d) Ag(111) blue-Stable, red-Unstable

Growth modes

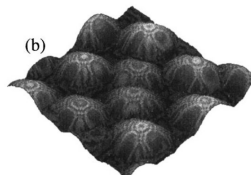
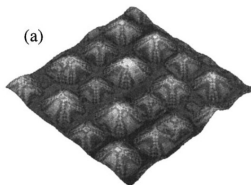
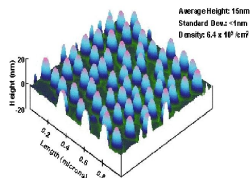


Pseudo-partial wetting vs ATG

Stranski-Krastanov Pseudo-partial wetting vs ATG



Fils quantiques
Boîtes quantiques



SiGe MBE growth

Floro et al 1999

recent developments ...

Aqua, Frisch, Berbezier, et al PRB (2010) PRL (2013)

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ATG instability

Hetero-epitaxial strain $\epsilon_0 = (a_f - a_s)/a_s$

In plane strain $u_{xx} = u_{yy} = \epsilon_0$

Stress $\sigma_0 = -Y\epsilon_0/(1 - \sigma)$

Flat film energy

$$\mathcal{E}_{el} = -h\epsilon_0\sigma_0 = \frac{Y}{1 - \sigma} h\epsilon_0^2$$

Periodic perturbation $\delta h, \ell$

$$\delta\mathcal{E}_{el} \sim -\delta h\epsilon_0\sigma_0 + C\epsilon^2\ell$$

Minimize $\epsilon \sim \delta h\sigma_0/C\ell$

Total perturbation energy

$$\delta\mathcal{E} = \frac{\gamma}{2} q^2 \delta h^2 - C\epsilon_0^2 \delta h^2 q$$

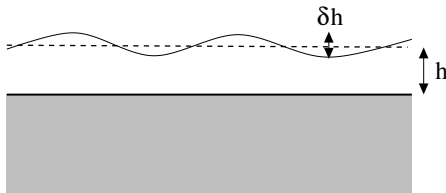
Wavelength

$$\ell_{ATG} \approx 2\pi \frac{\gamma}{C\epsilon_0^2}$$

$C \sim Y \sim 10^{11} \text{Pa}$, $\gamma \sim 1 \text{Jm}^{-2}$, and $\epsilon = n\%$

$\rightarrow \ell_{ATG} \sim n^{-2} \mu\text{m}$

($1 \mu\text{m}$ for 1% misfit to 10nm for 10% misfit)



ATG instability

Almost flat surface: 2D absorbate on flat surface

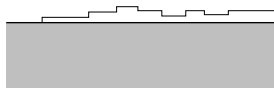
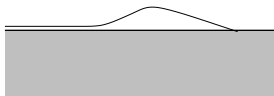
height $h \sim$ surface stress $\sigma = \sigma_0 + \alpha h$

Local surface forces \mathbf{f} and elastic energy \mathcal{F}_{elas}

$$\begin{aligned}\mathbf{f} &= -\nabla\sigma = -\nabla\sigma_0 - \alpha\nabla h \\ \mathcal{F}_{elas} &= \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \phi_{12} \\ \phi_{12} &= -\frac{1+\sigma}{\pi E} \left[(1-\sigma) \frac{\mathbf{f}_1 \cdot \mathbf{f}_2}{|\mathbf{r}_{12}|} + \sigma \frac{(\mathbf{f}_1 \cdot \mathbf{r}_{12})(\mathbf{f}_2 \cdot \mathbf{r}_{12})}{|\mathbf{r}_{12}|^3} \right]\end{aligned}$$

Edges and steps \rightarrow force lines

$$\mathbf{f}(\mathbf{r}) = \mathbf{f}_0(\mathbf{n}_0(s))\delta(\mathbf{r} - \mathbf{r}_0(s))$$



Islands

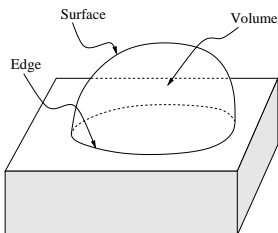
Contributions to the energy in 3D

Misfit $\epsilon = \Delta a/a$

$\mathcal{G}_{isl} = \mathcal{F}_{isl} - \mu \mathcal{N}$:

$$\begin{aligned} \mathcal{G}_{isl} = & +\Gamma_{surf} a^2 \mathcal{N}^{2/3} && \text{Surface} \\ & +\gamma_{e1} a \mathcal{N}^{1/3} && \text{Edge} \\ & -(\mu + f_1 \lambda \epsilon^2) a^3 \mathcal{N} && \text{Volume Elastic} \\ & -\gamma_{e2} f_2 a \mathcal{N}^{1/3} \ln[\mathcal{N}] && \text{Edge Elastic} \end{aligned}$$

$\Gamma_{surf}, \gamma_{e1}, \gamma_{e2}$ renormalized by ϵ



Schukin and Bimberg Rev Mod Phys 1999

Müller and Saúl Surf. Sci. Rep. 2004

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Liquid-state Dewetting

Polymer film (PDMS/Si)

G. Reiter et al PRL2000,2001, Fetzner et al

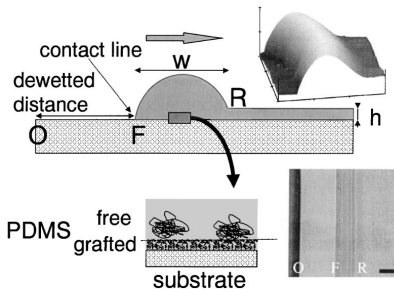
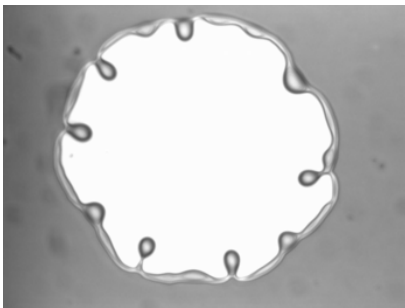


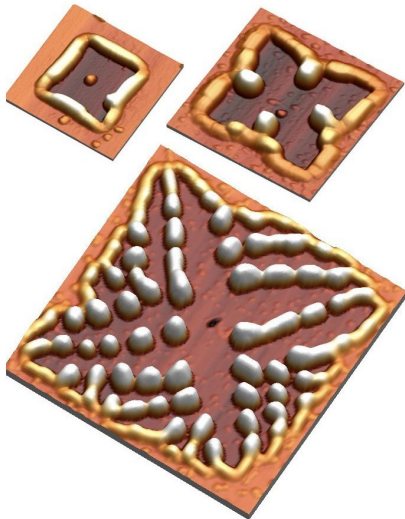
FIG. 1. Schematic representation of the experimental setup. A typical shape of the rim, as measured by atomic force microscopy, is shown in the upper right corner. The size of the image is $60 \times 60 \times 0.4 \mu\text{m}^3$. Note that the lateral scale is about a factor of 100 larger than the vertical scale. In the lower right corner we show an optical micrograph representing the top view corresponding to the scheme. The length of the bar equals $50 \mu\text{m}$.



Dewetting experiments: surface diffusion + anisotropy

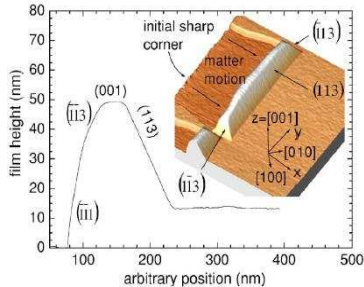
Experiments SOI: Si(100)/a-SiO₂

P. Müller et al Cinam Marseille



SOI (Si/SiO₂), AFM

Dornel Barbe Crecy Lacolle Eymeri PRB2006



Surface Diffusion Mullins' Model

Local chemical potential $\mu = \Omega \tilde{\gamma} \kappa$.

Mullins model:

$$j = -\frac{Dc}{k_B T} \partial_s \mu$$

$$v_n = -\Omega \partial_s j$$

Triple Line

Equilibrium contact angle $\theta = \theta_0$

$$v_n \sim \partial_{ss} \kappa$$

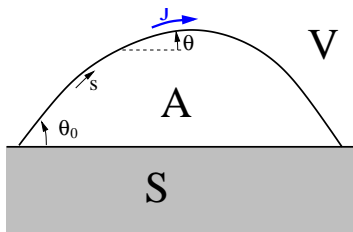
Relaxation time of island perturbations

$$t \sim L^4$$

Small slope limit

$$\partial_t h = -B \partial_{xxxx} h$$

Linear but free boundary



Liquids: viscosity and substrate friction

Viscous dissipation under shear $\dot{\gamma} = \partial_y v_x + \partial_x v_y$

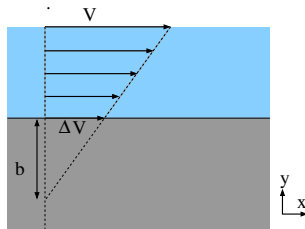
$$dQ \sim \eta \dot{\gamma}^2 dV$$

Continuity of tangential stress [Navier 1823](#)

$$\eta \partial_y v|_{\text{wall}} = \lambda \Delta v \rightarrow \Delta v = b \partial_y v|_{\text{wall}}$$

Slip length

$$\ell_s = \frac{\eta}{\lambda}$$



ℓ_s is usually small!

Link to wetting: hydrophobic \Rightarrow depletion $\Rightarrow b$ increases

$\ell_s \sim (1 + \cos \theta)^{-2}$ [D. M. Huang, et al Phys. Rev. Lett. 101, 226101 \(2008\)](#)

at max tens of nm for water on atomically flat hydrophobic surfaces

Hydrodynamics, lubrication Model

Local pressure variation $\Delta p = \tilde{\gamma}\kappa$.

Lubrication Model $\partial_x h \ll 1$, viscosity η , slip length ℓ_s

$$\begin{aligned} j &= -\frac{1}{\eta\Omega}(h^3/3 + \ell_s h^2)\partial_x \Delta p \\ \partial_t h &= -\Omega\partial_x j \\ \partial_t h &= -\frac{\gamma}{\eta}\partial_x[(h^3/3 + \ell_s h^2)\partial_{xxx} h] \end{aligned}$$

Triple Line

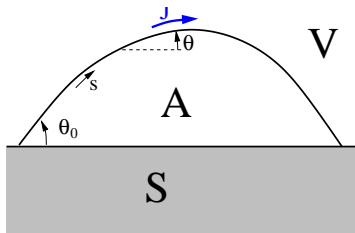
Equilibrium contact angle $\theta = \theta_0$

Linear perturbations $h = h_* + \delta h$

$\partial_t \delta h \sim \partial_{xxxx} \delta h$

Relaxation time of small perturbations

$t \sim L^4$



Generalized Model predictions 1D & small slopes

$$\partial_t h = \partial_x [h^n \partial_{xxx} h]$$

Scaling $\theta \ll 1$

$$\partial_{xx} h \sim \frac{1}{R} \quad h \sim R\theta^2 \quad x \sim R\theta$$

Triple line velocity

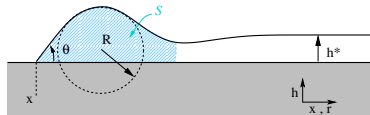
$$v = \frac{1}{\theta} \partial_t x_0 = \frac{1}{\theta} \partial_x [h^n \partial_x \frac{1}{R}] \sim \frac{\theta^{2n-3}}{R^{3-n}}$$

Mass conservation

$$\begin{aligned} \partial_t S = v h^* &\rightarrow \theta^3 \partial_t R^2 \sim \frac{\theta^{2n-3}}{R^{3-n}} h^* \\ S &\sim hL \sim R^2 \theta^3 \end{aligned}$$

Asymptotic scaling

$$\begin{aligned} R &\sim \theta^{-2(3-n)/(5-n)} h_*^{1/(5-n)} t^{1/(5-n)} \\ x_0 &\sim \theta^{(3+n)/(5-n)} h_*^{-(3-n)/(5-n)} t^{2/(5-n)} \end{aligned}$$



Multi-scale expansion / Example: $n = 0$, solid-state dewetting

Wong, Voorhees, Miskis, Davis (2000)

small slope limit $\partial_x h \ll 1$

Mullins model

$$\begin{aligned} \partial_t h &= -\partial_{xxx} h \\ h(x_0(t)) &= 0, \quad \partial_x h = \tan \theta = \alpha, \quad \partial_x^3 h(x_0(t)) = 0, \quad h(x \rightarrow \infty) = 1. \end{aligned}$$

normalized variables

$$X = \alpha(x - x_0(t)), \quad Y = h, \quad T = \alpha^4 t, \quad b = \alpha^{-3} \frac{dx_0}{dt}.$$

Boundary conditions

$$Y(X=0) = 0, \quad \partial_X Y(X=0) = 1, \quad \partial_X^3 Y(X=0) = 0, \quad Y(X \rightarrow \infty) = 1.$$

Slow dynamics $Y = Y_0 + Y_1 + Y_2 + \dots$, with $Y_{n+1} \ll Y_n$

$$\begin{aligned} \partial_X^4 Y_0 - b^3 \partial_X Y_0 &= 0 \\ \partial_X^4 Y_n - b^3 \partial_X Y_n &= -\partial_T Y_{n-1} \end{aligned}$$

Solve Y_n order by order and then impose no-flux condition

$$x_0(t) = \alpha \left(\frac{5t}{2\alpha} \right)^{2/5} - \frac{5}{4} \left(\frac{5t}{2\alpha} \right)^{1/5} + \dots$$

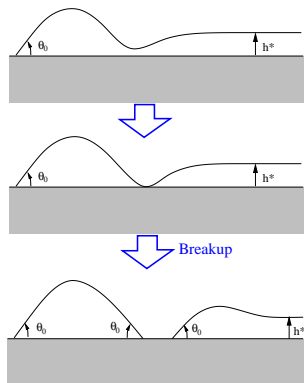
Example: $n = 0$, solid-state dewetting

Asymptotic scaling

$$R \sim \theta^{-6/5} h_*^{1/5} t^{1/5}$$

$$x_0 \sim \theta^{3/5} h_*^{-3/5} t^{2/5}$$

Mass shedding [Wong, Vorrhees, Miskis, Davis \(2000\)](#)



Example: $n = 2, 3$, liquid-state dewetting

Asymptotic scaling $n = 2$

$$R \sim t^{1/3}$$

$$x_0 \sim t^{2/3}$$

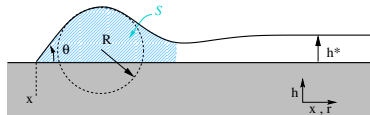
Asymptotic scaling $n = 3$

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

$$x_0 \sim t$$

No Mass shedding!

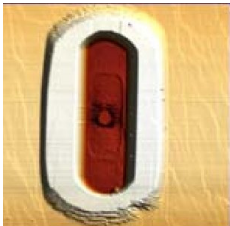
critical value $n = 3/2$



Evidences of facets on the rim

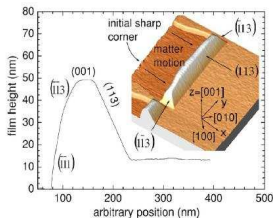
Ni(110)/MgO

J. Ye and C.V. Thompson, *Acta Materialia* 59, 582 (2011).



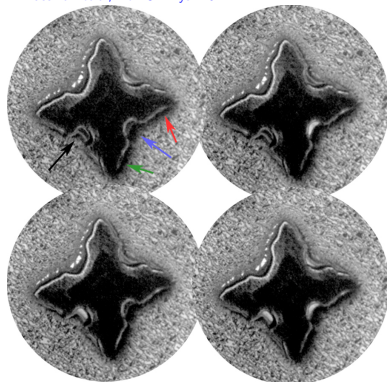
SOI (Si/SiO₂), AFM

Dornel Barbe Crecy Lacolle Eymery PRB2006



SOI (Si/SiO₂), LEEM

E. Bussman et al, *New J. Phys.* 2011



DEWETTING WITH FACETS?

Nucleation barrier

Dynamics limited by peeling or nucleation

Combe, Jensen, Pimpinelli, Phys Rev Lett 2000

Mullins and Rohrer, J. Am. Ceram. Soc. 2000

Cost: $2\pi\rho\gamma_{step}$

Gain: $\pi\rho^2\Delta\mu$ per atom, with $\Delta\mu = \Omega(-S)/h$

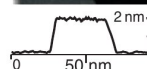
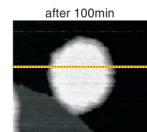
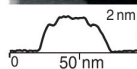
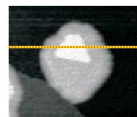
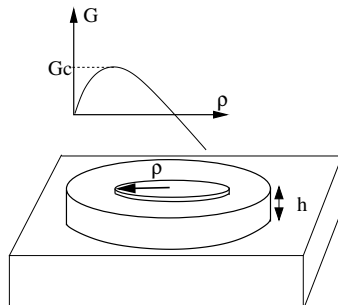
Total:

$$G = \gamma_{step}2\pi\rho - \frac{-S}{\Omega h}\pi\rho^2$$

$$G_c = \Omega\pi\frac{\gamma_{step}^2 h}{-S}$$

$$\mathcal{I} = \rho_0\Gamma_{+c} \left(\frac{-a^4\partial_{ss}G_c}{2\pi T} \right)^{1/2} e^{-G_c/T},$$

Slow relaxation time $t \sim e^{G_c/k_B T} \sim e^h$



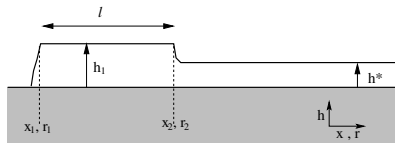
Experiments Ice/Pt(111)

Thurmer, Bartelt P.R.L. 2008

Facetted rim dynamics

Surface diffusion on top facet:

$$\begin{aligned}\Delta\mu &= \Omega \frac{-S}{h_1} \\ h_1 \partial_t x_1 &\sim \frac{\Delta\mu}{\ell} \\ \ell(h_1 - h^*) &= x_1 h^* \\ h_1 \gg h^* \Rightarrow x_1 &\sim t^{1/2} h_1^{-1/2}\end{aligned}$$



We recover the previous law:

$$\ell \sim h_1 \Rightarrow h_1^2 \sim x_1 \Rightarrow x_1 \sim t^{2/5}$$

Facetted rim

$$\begin{aligned}\partial_t h_1 \sim e^{-G_c} &\sim e^{-\Omega\pi\gamma_{step}^2 h_1 / (-S)} \\ \Rightarrow h_1 &\sim \ln t \\ \Rightarrow x_1 &\sim t^{1/2} (\ln t)^{-1/2}\end{aligned}$$

OPL, A. Chame, Y. Saito, PRL 2009

Distinguish $\ln t$ from $t^{1/5}$ in experiments??

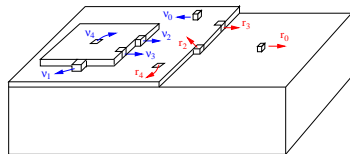
Si/SiO₂ Leroy et al $x \sim t^{1/3}$??

Metal GH Kim et al $x \sim t^{2/5}$.

SOS KMC model

KMC simulations SOS Hopping rates

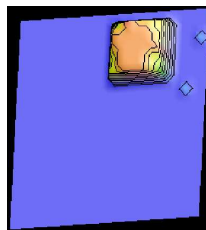
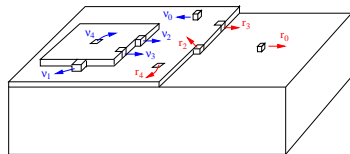
- $A/S: r_n = \nu_0 e^{-nJ/T + E_S/T}$
- $A/A: \nu_n = \nu_0 e^{-nJ/T}$
- J bond energy; E_S substrate contact energy



SOS KMC model

KMC simulations SOS Hopping rates

- A/S: $r_n = \nu_0 e^{-nJ/T + E_S/T}$
- A/A: $\nu_n = \nu_0 e^{-nJ/T}$
- J bond energy; E_S substrate contact energy



Equilibrium shape Low temperatures:

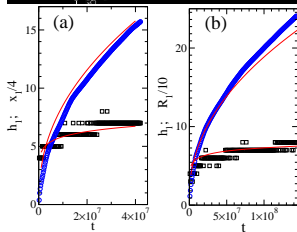
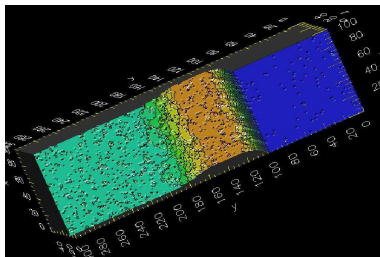
- $h = E_S^{2/3} J^{-2/3} N^{1/3}$; $h/L = E_S/J$
 $E_S = 1$, $N = 900$, $\rightarrow h = 8.7$, simul at $T/J = 0.35$

- Link $T \rightarrow O$:

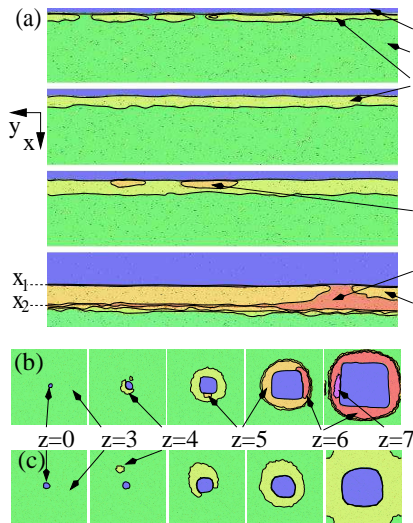
$$\gamma(0) = J/2$$

$$S = -E_S$$

Facetted rim



OPL, A. Chame, Y. Saito, PRL 2009



Rim instability

$$\partial_t h = \nabla \cdot [h^n \nabla \Delta h]$$

Transversal direction y , perturbation $q = 2\pi/\lambda$

Assuming $y \sim x$

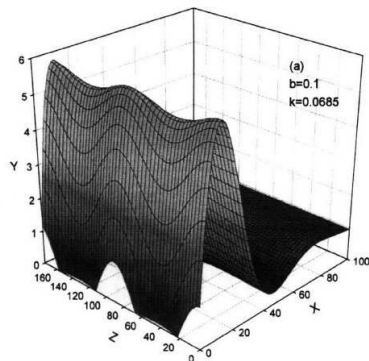
$$\rightarrow q \sim \frac{1}{\theta R} \sim \frac{1}{\theta^{(n-1)/(5-n)} h_*^{1/(5-n)} t^{1/(5-n)}}$$

$$n = 0 \rightarrow \lambda \sim t^{1/5}$$

$$n = 2 \rightarrow \lambda \sim t^{1/3}$$

$$n = 3 \rightarrow \lambda \sim t^{1/2}$$

OPL 2013, Münch-Wagner 2014

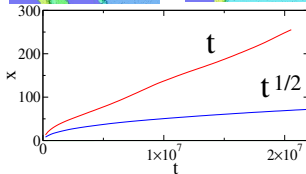
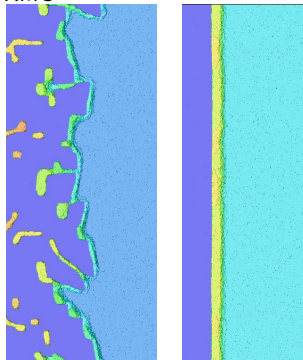


Final finger wavelength?

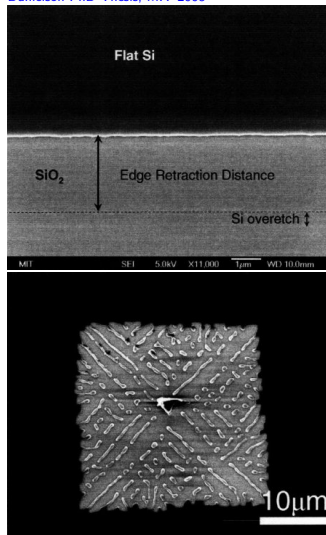
Kan, Wong J.Appl. Phys. 2005

10 fronts: Metastability?

KMC



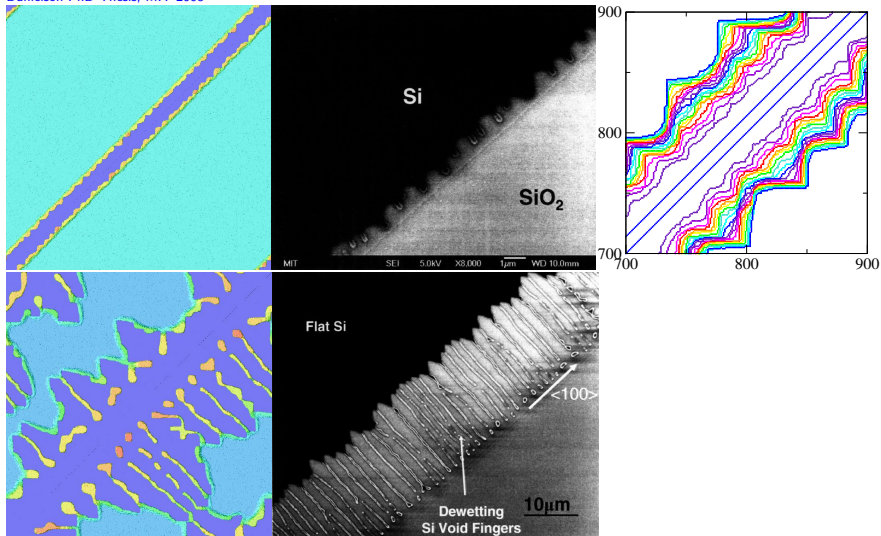
Danielson PhD Thesis, MIT 2008



11 fronts

$$h = 3, h_1 = 9, T = 0.5, E_S = 1.5,$$

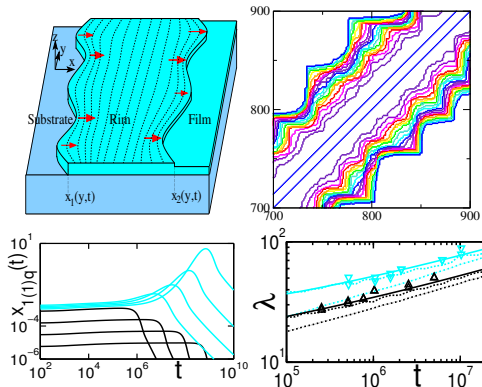
Danielson PhD Thesis, MIT 2008



Instability of a faceted rim: Linear Coarsening

Instability on a - **non-steady-state**:

- (110) -rough orientation $\tilde{\gamma}_1 \approx \gamma$ constant
 Coarsening: $\lambda \sim t^{1/4}(\ln t)^{-1/2}$
 Numerical power-law fit $\lambda \sim t^{0.2}$

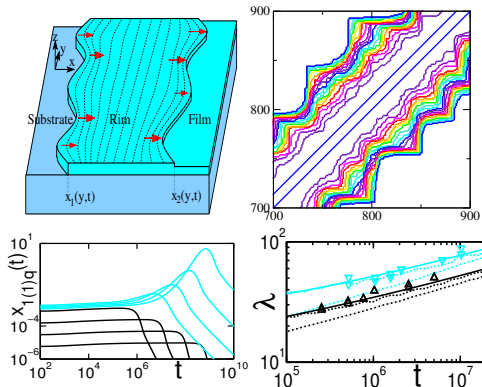


M. Dufay, OPL, PRL 2011

Instability of a faceted rim: Linear Coarsening

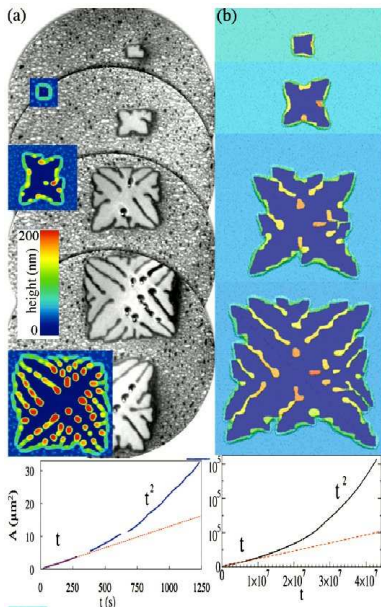
Instability on a - **non-steady-state**:

- (110) -rough orientation $\tilde{\gamma}_1 \approx \gamma$ constant
Coarsening: $\lambda \sim t^{1/4}(\ln t)^{-1/2}$
Numerical power-law fit $\lambda \sim t^{0.2}$
- (100) -vertical (100) facet
 $\tilde{\gamma}_1 = Ta/\beta^2 \approx (T/2a)e^{\gamma h_1/T}/h_1$
Stable

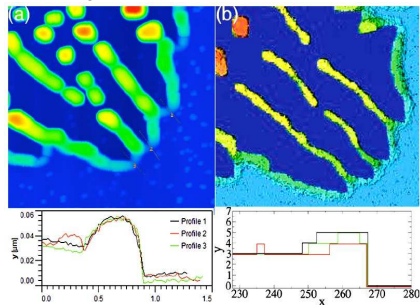


M. Dufay, OPL, PRL 2011

KMC vs SOI



$$h = 3, E_S = 1, T = 0.5$$



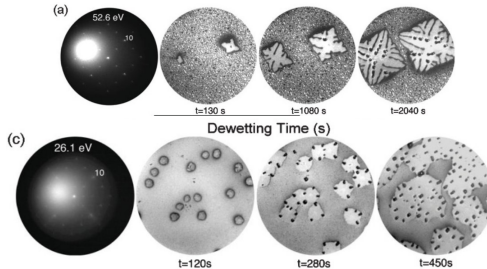
SOI system LEEM Experiments:

E. Bussman, F. Leroy, F. Cheynis, P. Müller, OPL NJP(2011)

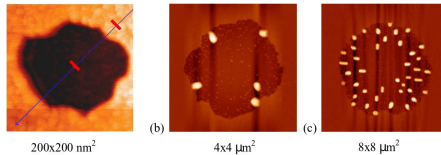
Isotropic

More or less isotropic?

Müller et al LP2MC Marseille



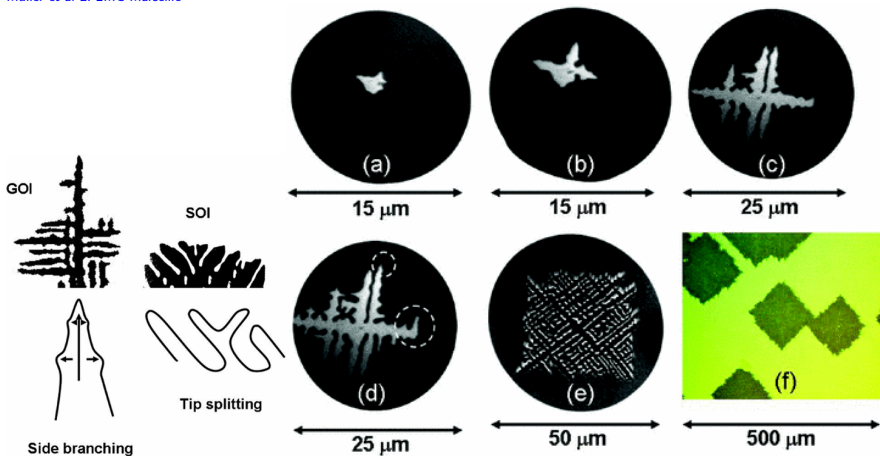
Berbezier et al LP2MC Marseille



Dendritic shapes

More or less dendritic shapes?

Müller et al LP2MC Marseille



Dewetting hole of shapes NNN KMC

- Seaweed

Isotropic

Example: dirty SOI??



- Anisotropic Ramified

Simple 4-fold

Example: SOI



- Dendritic

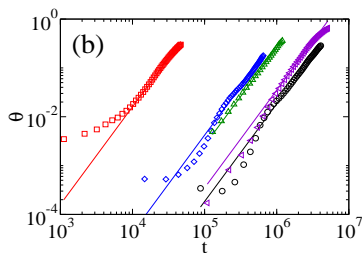
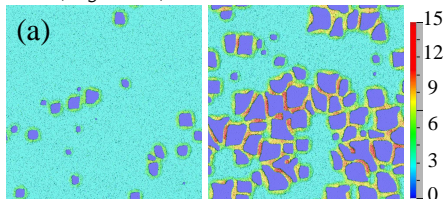
4-fold with secondary facet

Example: GOI



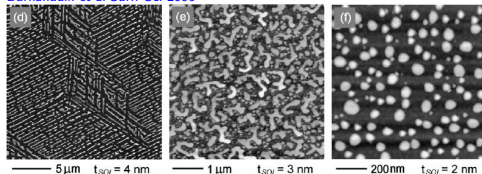
Dewetting of a complete film / Hole nucleation and growth

$h = 3$, $E_S = 0.7$, $T = 0.5$



hole radius $R \sim t^{1/2}$
 hole area $A \sim R^2 \sim t$
 uncoverage $\theta \sim t^2$

Burhanudin et al Surf. Sci 2006



1 Static Wetting of liquids and Solids

- Introduction
- Wulff-Kaisew construction
- Thin Films
- Elastic effects

2 Dynamics of solid wetting

- Dewetting dynamics
- **Surface diffusion model with wetting potential**
- Derivation of the TL Boundary Condition
- Spinodal dewetting and Accelerated mass shedding
- Elastic dewetting /ATG
- KMC study of magic heights
- Dewetting without a rim
- Non-conservation of the mass: evaporation and reaction

3 Islands on nano-patterns

- Patterns larger than islands
- Patterns smaller than islands
- Islands on nano-pillars
- Solid imbibition in nano-pillars

4 Conclusions

Continuum model with Wetting potential

Substrate at $h = 0$

Free energy per unit area :

$$\gamma(h) = \gamma_\infty + \mathcal{W}(h)$$

Wetting potential $\mathcal{W}(h) \rightarrow 0$ as $h \rightarrow \infty$

$$\mu(x) = -\gamma_\infty \partial_{xx} h + \gamma'(h)$$

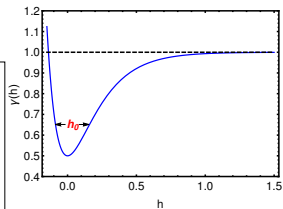
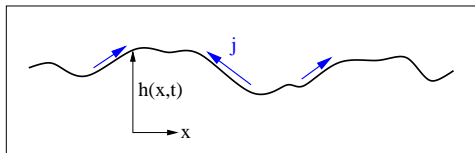
$$\mathbf{j} = -\mathcal{M}(h) \nabla \mu$$

$$\partial_t h = -\nabla \cdot \mathbf{j}$$

Far from the substrate: $h \rightarrow \infty$

$$\mathcal{M}(h) \rightarrow \mathcal{M}_\infty$$

$$\gamma(h) \rightarrow \gamma_\infty$$



1 Static Wetting of liquids and Solids

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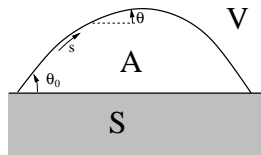
4 Conclusions

Non-equilibrium boundary condition

Equilibrium condition at Triple Line

Young-Dupré

$$\gamma \cos \theta_{eq} + \gamma_{int} = \gamma_{sub}$$



Liquids

P.G. de Gennes

Grain Boundaries

U. Czubyko et al, Acta Mater. (1998); M. Upmanyu et al Acta Mater. (2002).

Solid-state wetting

Wang, Jiang, Bao, Srolovitz (2015)

$$v = K(\cos \theta - \cos \theta_{eq})$$

Microscopic origin of the kinetic coefficients:

- Wetting potential?
- Microscopic Kinetic coefficients affected by the vicinity of substrate?

Is this the correct triple line BC?

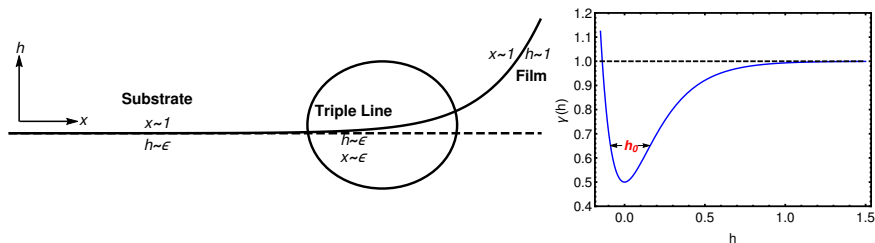
Derive K from mesoscopic model?

Matched asymptotic Expansion

- Expand in small parameter $\epsilon \sim h_0$

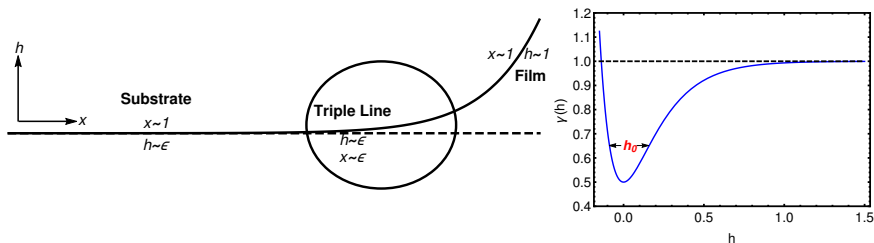
Matched asymptotic Expansion

- Expand in small parameter $\epsilon \sim h_0$



Matched asymptotic Expansion

- Expand in small parameter $\epsilon \sim h_0$



- (a) Film region $\begin{cases} h \sim O(1) \\ x \sim O(1) \end{cases}$
 - (b) TL region $\begin{cases} h = \epsilon H(X, t) \\ x = x_{TL} + \epsilon X \end{cases}$

- (c) Substrate region $\begin{cases} h(x, t) = \epsilon \mathcal{H}(\chi, t) \\ \chi = x \end{cases}$

Kinetic Boundary Conditions

To 0th order, Young & no-flux

$$\theta = \theta_{eq} \quad \frac{\gamma_{\infty}}{2} \theta_{eq}^2 = \gamma_{\infty} - \gamma_{min} \quad J = 0$$

... To 3rd order, KBC (Linear / Onsager)

$$\mathcal{L} \begin{bmatrix} v \\ J \end{bmatrix} = \begin{bmatrix} [U] \\ -[\mu] \end{bmatrix}$$

Kinetic Boundary Conditions

To 0th order, Young & no-flux

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- **Thermodynamic Fluxes :**
 v : velocity of triple line
 J : mass flux through triple line

Kinetic Boundary Conditions

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- Local Thermodynamic Potentials :

$$U = -\frac{\gamma_{\infty}}{2} (\partial_x h)^2 + \gamma(h).$$

$$\mu = -\gamma_{\infty} \partial_{xx} h + \gamma'(h),$$

- Thermodynamic Fluxes :

v : velocity of triple line

J : mass flux through triple line

- Thermodynamic Forces :

$$[U] = (U_+ - U_-) = \gamma_{\infty} (\cos \theta - \cos \theta_{eq})$$

$$[\mu] = (\mu_+ - \mu_-) \propto \gamma_{\infty} \kappa - h \gamma''_{min}$$

Kinetic Boundary Conditions

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- Kinetic Coefficients :

$$\mathcal{L} = \begin{bmatrix} \mathcal{L}_{2v} & \mathcal{L}_{1v} \\ \mathcal{L}_{1v} & \mathcal{L}_{1J} \end{bmatrix}$$

Kinetic Coefficients

$$\mathcal{L} \begin{bmatrix} v \\ J \end{bmatrix} = \begin{bmatrix} [U] \\ -[\mu] \end{bmatrix}$$

Kinetic coefficients

$$\mathcal{L}_{1J} = \int_{-\infty}^{\infty} dX \left(\frac{1}{M(H_0)} - \frac{\Theta(X)}{M(\infty)} - \frac{\Theta(-X)}{M(0)} \right) \sim \frac{\epsilon}{M}$$

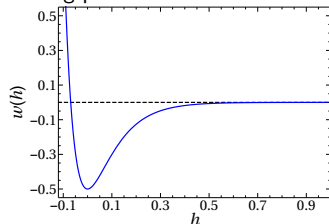
$$\mathcal{L}_{1v} = \int_{-\infty}^{\infty} dX \left(\frac{H_0}{M(H_0)} - \Theta(X) \frac{X \partial_x h_0(x_{TL})}{M(\infty)} \right) \sim \frac{\epsilon^2}{M}$$

$$\mathcal{L}_{2v} = \int_{-\infty}^{\infty} dX \left[\frac{H_0^2}{M(H_0)} - \frac{\Theta(X)}{M(\infty)} (X \partial_x h_0(x_{TL}))^2 \right] \sim \frac{\epsilon^3}{M}$$

In most cases $\theta \sim \theta_{eq}$?

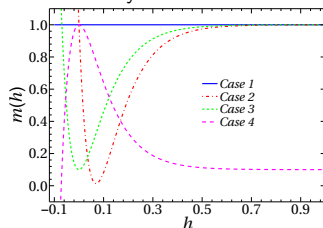
Numerical simulations

Wetting potential

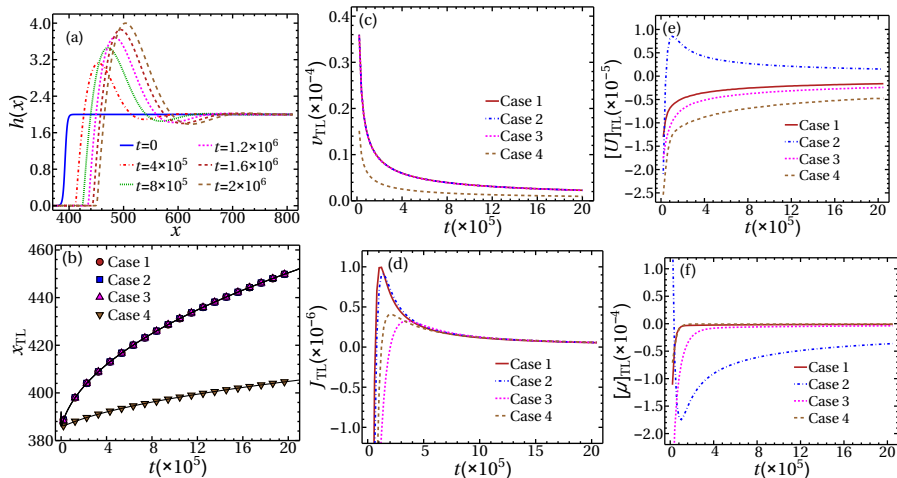


Mobility

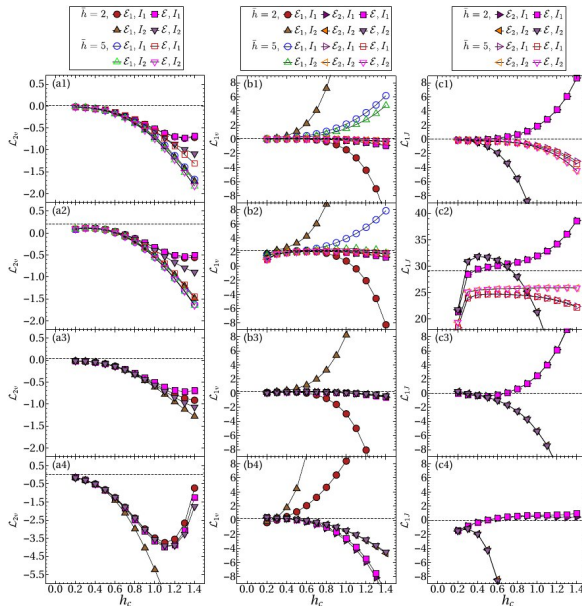
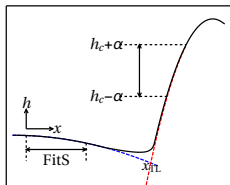
- case 1 constant mobility
- case 2 reduced mobility in the triple line region
- case 3 asymmetric: lower mobility in the substrate
- case 4 asymmetric: lower mobility in the film



Numerical simulations



Numerical simulations

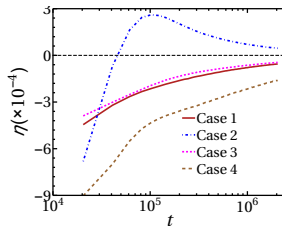
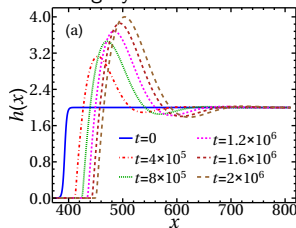


Numerical simulations

Dynamic contact angle θ_D

$$\eta = \frac{\theta_{eq} - \theta_D}{\theta_{eq}}$$

Dewetting dynamics



Summary on Kinetic Boundary Condition

- 2 Kinetic Boundary Conditions for v and J
- Numerical validation
- Convergence of kinetic coefficients.
 $W(h) - W(\infty) \sim h^{-n}$, with $n > 3$
 $M(h) - M(\infty) \sim h^{-m}$, with $m > 3$
Van der Waals $n = 2$??

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Small thicknesses: spinodal dewetting

Linear stability analysis : $h = \bar{h} + \delta h$

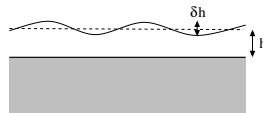
$$\delta h \sim e^{i\omega t + iqx}$$

$$i\omega = \mathcal{M}(\bar{h}) q^2 [-\gamma_\infty q^2 + W''(\bar{h})]$$

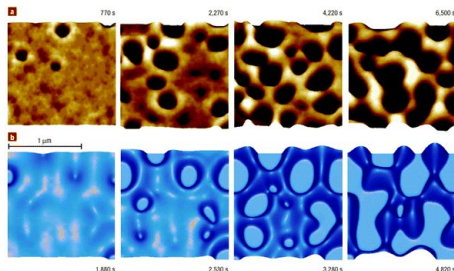
Spinodal Instability if $W''(\bar{h}) \leq 0$

$$\lambda_{LS} = \frac{2^{3/2} \pi \bar{\gamma}^{1/2}}{W''(\bar{h})^{1/2}}$$

$$T_{LS} = \frac{4\bar{\gamma}}{\mathcal{M} W''(\bar{h})^2}$$



Liquids



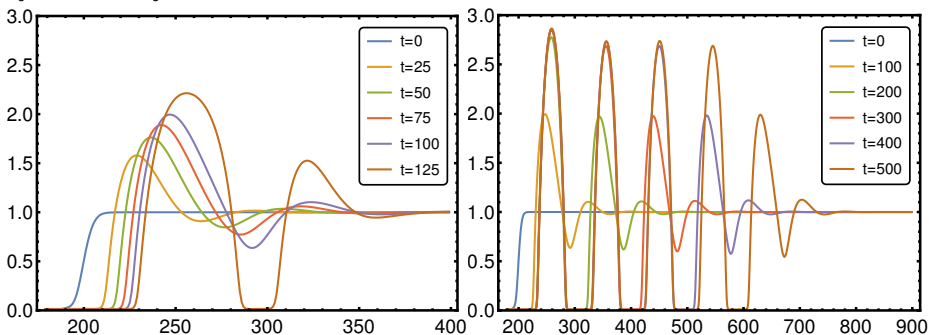
Embedded Animation

Aswani Tripathi, ILM-Lyon

Mass Shedding

Periodic Mass shedding

$\theta_0 = 60^\circ$ and $h_0 = 0.1$



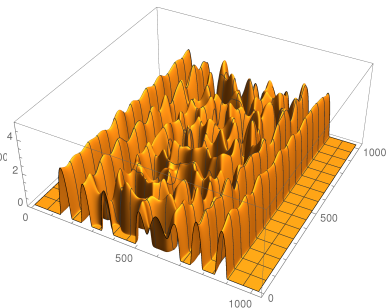
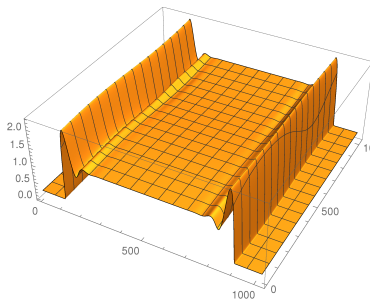
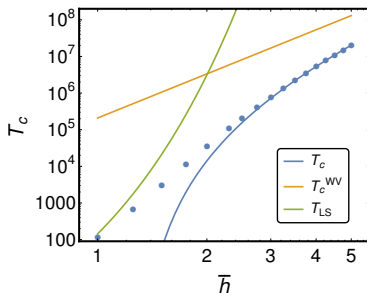
Small thicknesses: spinodal dewetting

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Spinodal Instability if $W'''(\bar{h}) \leq 0$

$$T_c^{WV} = \frac{\bar{h}^4}{\bar{\mathcal{M}}\bar{\gamma}\theta_0^4}$$

$$T_{LS} = \frac{4\bar{\gamma}}{\bar{\mathcal{M}}W'''(\bar{h})^2}$$



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Continuum model with Wetting potential

Substrate at $h = 0$

Free energy per unit area :

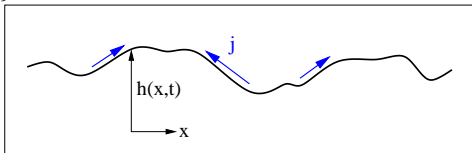
$$\gamma(h) = \gamma_\infty + \mathcal{W}(h) + \mathcal{E}_{el}$$

$$\mu(x) = -\gamma_\infty \partial_{xx} h + \gamma'(h) + C\epsilon_0^2 \mathcal{H}(\partial_x h)$$

$$\mathbf{j} = -\mathcal{M} \nabla \mu$$

$$\partial_t h = -\nabla \cdot \mathbf{j}$$

$$\mathcal{H}[\partial_x h] = \mathcal{F}^{-1}\{|q| \mathcal{F}[h]\}$$



Schifani, Frisch, Argentina, Aqua, PRE 20016

Continuum model with Wetting potential

Stabilizing exponential $W(h)$ and Anisotropy

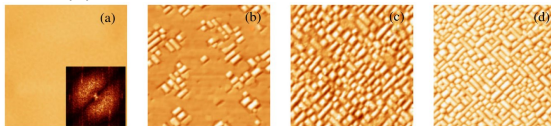


FIG. 1 (color online). AFM images of a 5-nm-thin $\text{Si}_{0.70}\text{Ge}_{0.30}$ layer (a) as grown (Fourier transform in inset), (b) after 18-h annealing, and (c) after 54-h annealing at 550 °C. (d) Image of a 8-nm film after 18-h annealing. The [110] direction is horizontal. (The scan area is $3 \times 3 \mu\text{m}^2$, and the vertical scale is 32 nm.)

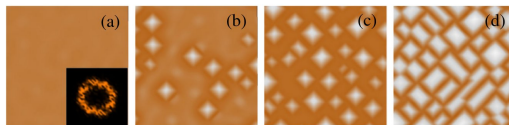


FIG. 2 (color online). Numerical resolution of the diffusion equation (1) for a strained anisotropic film for (a) a 5-nm film and $t = 0$ (Fourier transform in inset), (b) 18 h ($240t_0$), (c) 54 h ($720t_0$), and (d) an 8-nm film and $t = 18$ h ($240t_0$). [The scan area is $1.2 \times 1.2 \mu\text{m}^2 (= \sqrt{2}64l_0)$, and the vertical scale is 31 nm.]

[Aqua, Gouye, Ronda, Frisch, Berbezier, PRL 2013](#)

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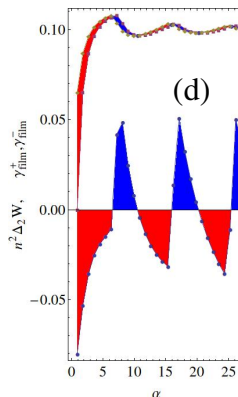
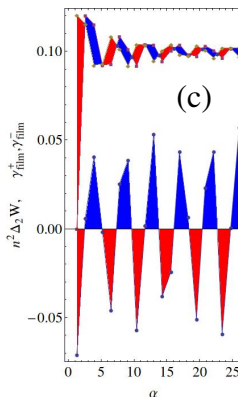
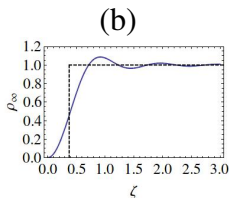
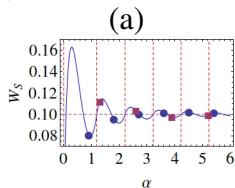
4 Conclusions

Electronic Quantum confinement

Free electron model

$$W_{EC}(h) \approx -\frac{E_{fb}}{(h+2b)^2} \frac{\pi}{36\sqrt{3}} \cos(2k_{fb}h)$$

E_{fb} , k_{fb} Fermi energy and wavevect,
 $b = 3\pi k_{fb}/8$



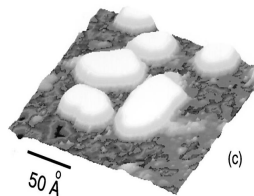
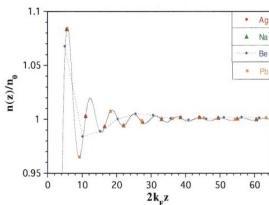
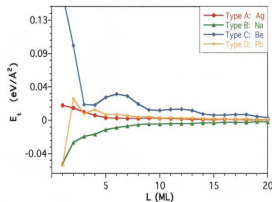
(a) Al(111) (purple squares), Ag(111) (blue circles)

(c) Al(111) , (d) Ag(111) blue-Stable, red-Unstable

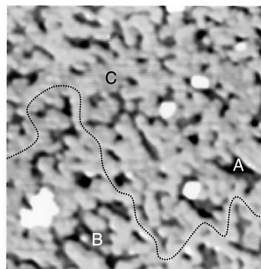
Magic heights and labyrinthine patterns

Metals/ semicon or insulator: Electronic confinement \rightarrow Magic thickness

Z. Zhang et al, Phys.Rev.Lett.1998,1999



Experiments Ag/Si(111)



SOS KMC model with magic height

KMC simulations SOS

$$z \neq 1 \text{ and } z \neq h_*$$

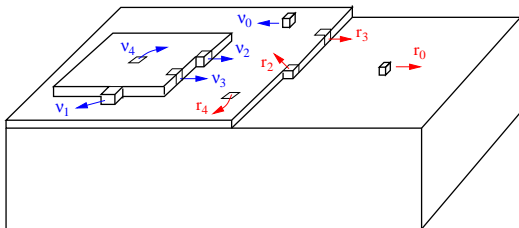
$$\nu_n = \nu e^{-(nJ+J_0)/T}$$

$$z = 1$$

$$r_n = \nu e^{-(nJ+J_0-E_S)/T}$$

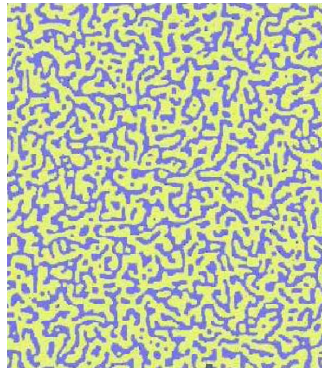
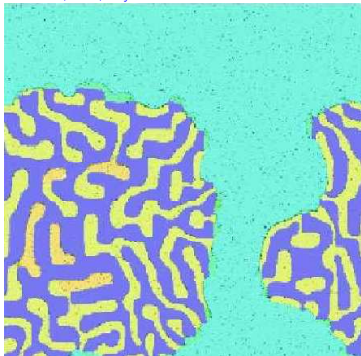
$$z = h_*$$

$$r_n^* = \nu e^{-(nJ+J_0-E_*)/T}$$



KMC simulations with magic height

A. Chame, OPL, Phys Rev B 2014



$\lambda \sim 30\text{nm}$

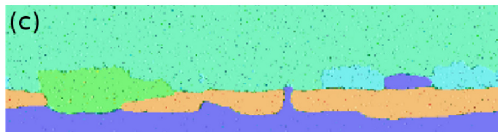
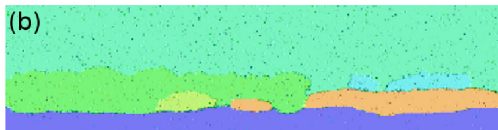
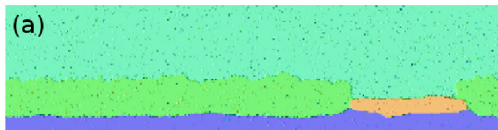
Semi-quantitative agreement with experiments

Magic-height rim

800×800 , $T = 0.4$, $h = 3$, $E_S = 0.4$, $h_* = 7$, $E = -0.5$

Induced nucleation and incomplete closure

A. Chame, OPL, Phys Rev B 2014



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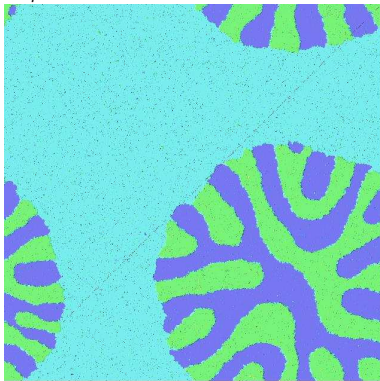
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Monolayer \rightarrow no rim

$$V_{zip} \sim V_{front}$$



OPL, A. Chame, Y. Saito, PRL 2007

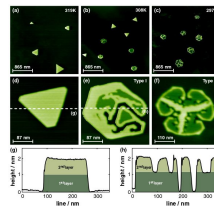


FIG. 1 (color online). (a)–(c) NC-AFM images of C_{60} islands on $CaF_2(111)$ at three different growth temperatures. (d)–(f) Magnified images of single islands: a compact triangle (d), and hexagonal islands with morphologies I (e) and II (f). (g). (h) Height profiles along lines scans shown in (d),(e).

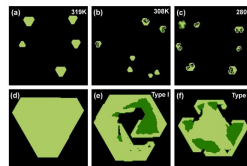


FIG. 2 (color online). (a)–(c) Simulated configurations of the growth model at different temperatures. (d)–(f) Magnified single island structures from the simulations resemble the same morphologies as found in experiments [Figs. 1(d)–1(f)].

P. Maas et al, PRL 2011

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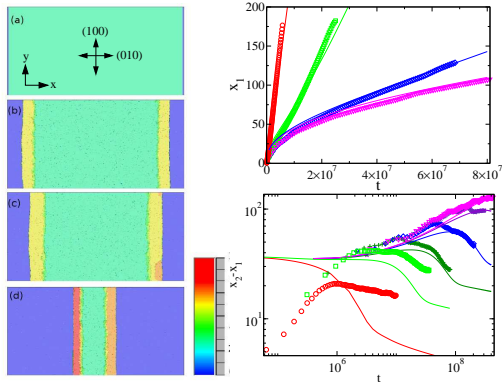
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Dewetting with substrate mediated evaporation

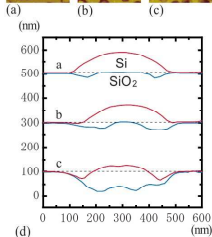
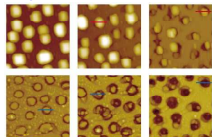
- Constant velocity
- Non-monotonous rim width



A. Chame, OPL, PRE 2013

Interface Reaction in SOI systems: substrate profile

Experiments



Sudoh, Naito, JAP 2010.

($2\mu\text{m} \times 2\mu\text{m}$, 1050°).

OPL, P. Müller et al PRB (2014), APL (2015)

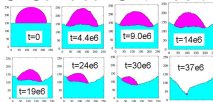
Kinetic Monte Carlo

Interface: $\text{Si} + \text{SiO}_2 \leftrightarrow 2\text{Si} + 2\text{O}$

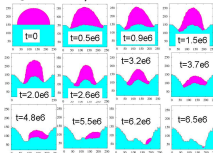
Interface: O diffusion

Triple Line: $\text{Si} + \text{O} \rightarrow \text{SiO}(\text{evap})$

Si Surface: Si diffusion



$$\nu_O = 10/\tau_A, \nu_E = 0.01/\tau_A.$$



$$\nu_O = 10/\tau_A, \nu_E = 0.1/\tau_A.$$

Analytic

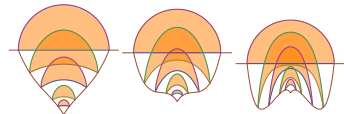
Reaction-Diffusion

$$\partial_t C_O = D \partial_{xx} C_O + K_0 - K_1 C_O^2$$

$$\partial_t h_I = K_0 - K_1 C_O^2$$

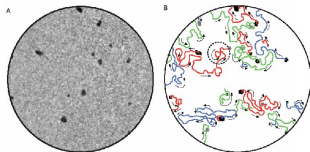
$$\theta_{TL} = \theta_{eq}$$

$$h = -\pi \frac{D_O^{1/2} K_0^{3/4}}{2^{1/2} K_1^{1/4}} \cosh \frac{x}{x_s} \int_{R_0/x_s}^{x/x_s} \frac{udu}{\sinh u}$$

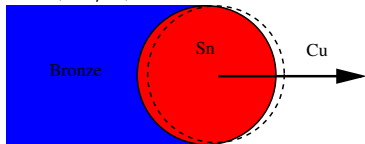


Interface Reaction: running droplets

Running sild-clusers Sn/Cu(111)

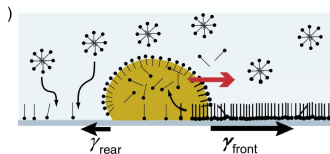
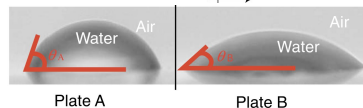
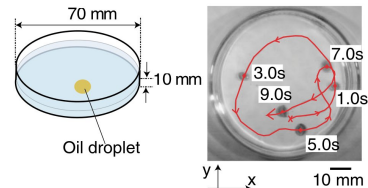


LEEM, $1.5\mu\text{m}$, 290K



Schmid, Bartelt, Hwang, Science Reports (2000).

Liquid Running oil Droplet



Sumino, Magome, Hamada, Yshikawa PRL2005

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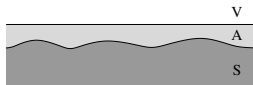
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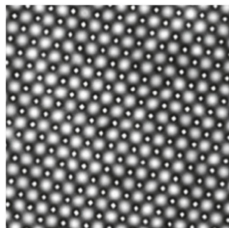
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Guided Self-Organisation vs Healing



Healing length

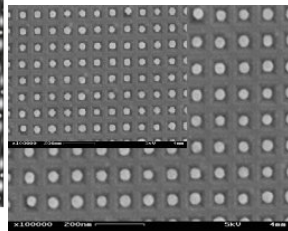
$$\xi_{heal} = \left(\frac{\gamma(\bar{h})}{W''(\bar{h})} \right)^{1/2}$$



Ge/Si, $5 \times 5 \mu\text{m}$

Zhong et al PRL 2007

Aqua and Xu PRE 2014



Au/Si

C.V. Thompson

Guided self-organization

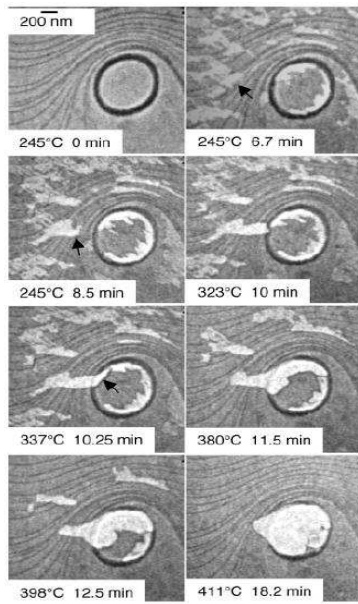
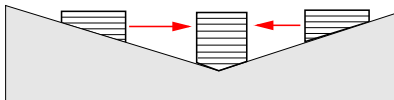
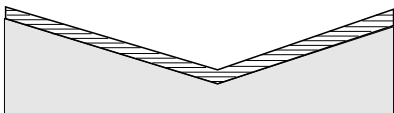
$$\xi_{heal} = \left(\frac{\gamma(\bar{h})}{-W''(\bar{h})} \right)^{1/2}$$

Guided Self-Organisation: Drift Experiments

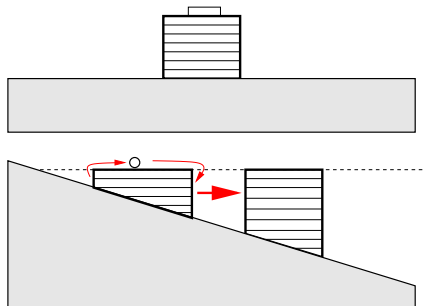
Controlled positionning of mass in holes

Ling *et al* Surf. Sci 2006

McCarty NanoLetters 2006 Ag/W(110)



Nucleationless motion

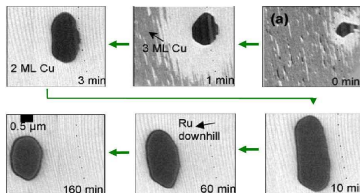


Going back to equilibrium height
without nucleation on top??

island position $\sim t^{1/4}$

M. Dufay, OPL, Phys Rev B, 2010

De-wetting on a vicinal surface



W. L. Ling et al. Surf. Sci. Lett. (2004)

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- Introduction
- Wulff-Kaisew construction
- Thin Films
- Elastic effects

2 Dynamics of solid wetting

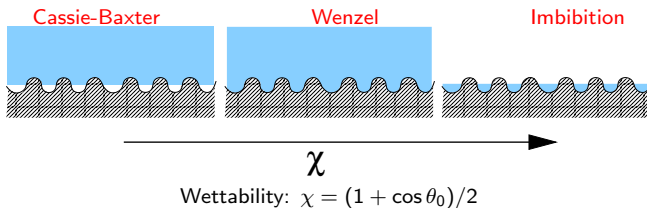
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4 Conclusions

Three wetting states for liquids on patterns



Bico, Marzolin, Quéré (1999)

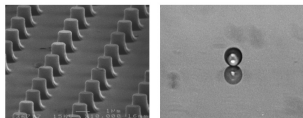
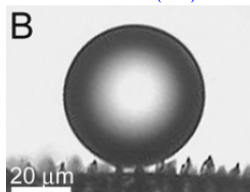


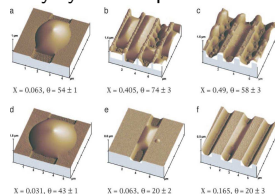
Figure 12. Substrate decorated with posts (the bar indicates 1 μm). If coated with a monolayer of fluorinated silanes, this substrate is found to be super-hydrophobic [37].

Watson et al PLoS ONE (2011)



Seeman et al (2005)

Polystyrene drops on Silicon



3D KMC Model

3D KMC

Hopping along the surface

$$\nu = \nu_0 e^{-(n_1 J_1 + n_2 J_2 + n_{s1} J_{s1} + n_{s2} J_{s2}) / T}$$

J bond energy, n_i nb neighbors

$i = 1, 2$ NN, NNN adsorbate

$i = s1, s2$ NN, NNN substrate

Moves to NN

Allowed when there is NN or NNN

Shape controlled by

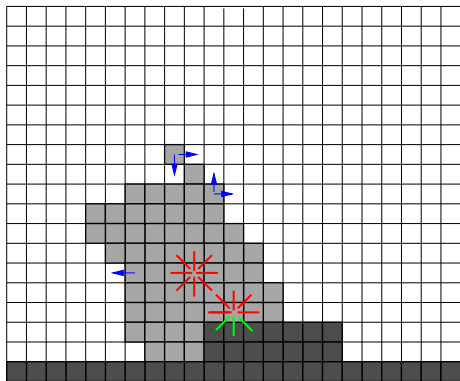
$$\zeta = \frac{J_2}{J_1} = \frac{J_{s2}}{J_{s1}}$$

Wetting controlled by

$$\chi = \frac{J_{s1}}{J_1}$$

Link $T \rightarrow 0$:

$$1 - \chi = \frac{-S}{2\gamma(0)}$$



$\chi \rightarrow 0$: Complete de-wetting

$\chi \rightarrow 1$: Complete Wetting

ψ parameter

Contact angle not a good parameter for faceted crystals!

$$\psi = \frac{S_{AV}}{S_{AS}}$$

3D Isotropic crystal $\gamma(\theta) = \bar{\gamma}$

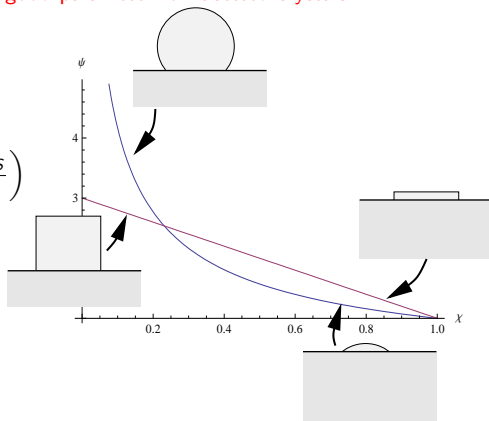
$$\chi = \frac{1}{2} (1 + \cos \theta_0) = \frac{1}{2} \left(1 + \frac{\gamma_{SV} - \gamma_{AS}}{\bar{\gamma}} \right)$$

$$\psi = \frac{1}{\chi}$$

3D Square crystal γ_0

$$\chi = \frac{1}{2} \left(1 + \frac{\gamma_{SV} - \gamma_{AS}}{\gamma_0} \right)$$

$$\psi = 5 - 4\chi$$



$\chi \rightarrow 0$: Complete de-wetting

$\chi \rightarrow 1$: Complete Wetting ($\psi = 1$)

Wetting on a flat substrate

Wetting control parameter

$$\chi = \frac{J_{s1}}{J_1}$$

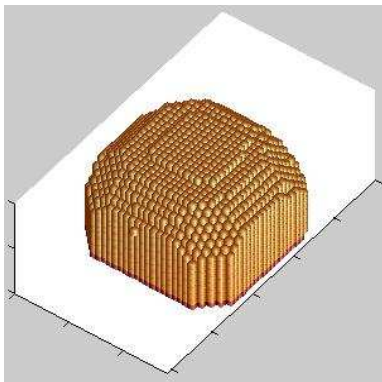
Cube $\zeta = 0$

$$\psi = 5 - 4\chi$$

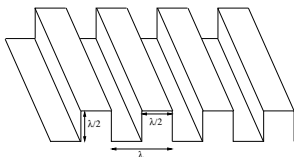
KMC:

$N = 11025$, $\zeta = 0.2$, $\chi = 0.4$, $T/J_1 = 0.5$

Error: Energy 1%; ψ 3%.



Parallel nano-grooves



$$N = 10^4$$

$$\lambda = 20$$

$$\zeta = 0.2$$

$$\chi = 0.4$$

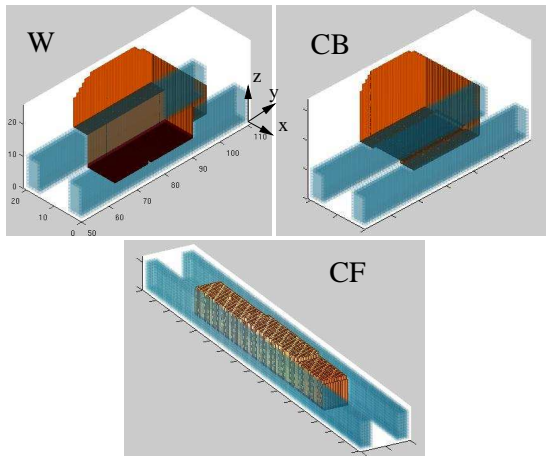
$$T/J_1 = 0.5$$

Parallel grooves:

Cassie-Baxter state (CB)

Wenzel state (W)

Capillary filling (CF)



ψ

Wetting parameter

$$\psi = \frac{S_{AV}}{S_{AS}}$$

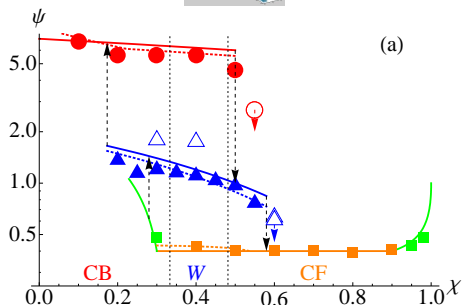
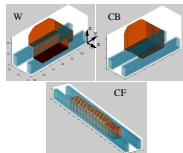
neglecting (110) and (111)

$$\psi_{CB} = 7 - 2\chi$$

$$\psi_W = 2 - 2\chi$$

$$\psi_{CF} = \frac{1}{3} + \frac{1}{12\nu}.$$

$$\nu = Na^3/\lambda^3$$



Hysteresis/Stability

Instability thresholds

$$\chi_{CB \rightarrow W} = \frac{1}{2}.$$

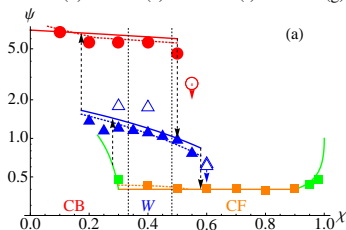
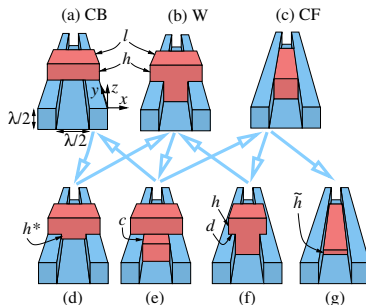
$$\chi_{W \rightarrow CB} = \frac{1}{3} - \frac{1}{36\nu} \left[1 + (1 + 30\nu)^{1/2} \right],$$

$$\chi_{W \rightarrow CF} = \frac{2}{3} - \frac{1}{36\nu} \left[1 + (1 + 6\nu)^{1/2} \right],$$

$$\chi_{CF \downarrow} = 1 - \frac{1}{8\nu}$$

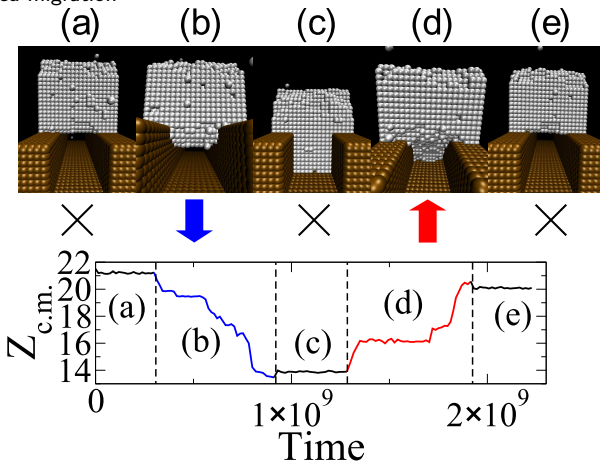
$$\chi_{CF \uparrow} = \frac{1}{3} - \frac{1}{24\nu}$$

Finite temperature effects $CF \rightarrow W$



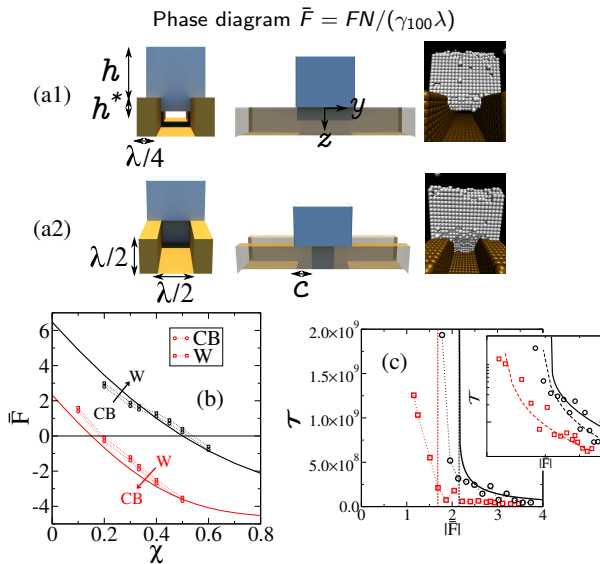
Migration-induced switching

Nanoswitch controlled by an electron beam
KMC with imposed migration

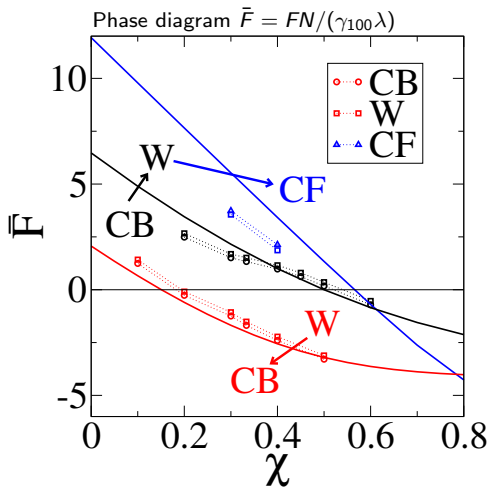


M. Ignacio, OPL, PRE (2015)

Migration-induced switching



Migration-induced switching

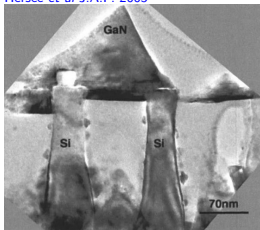


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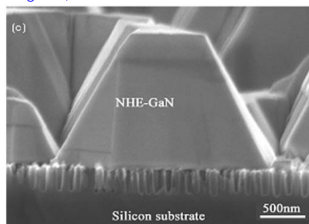
Nanocrystals in Cassie-Baxter state

Growth of GaN on Si nano-pillars

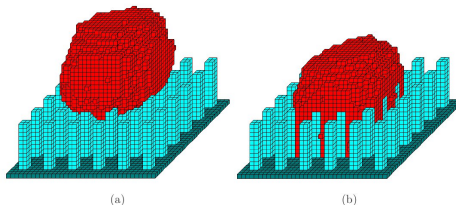
Hersee et al J.A.P. 2005



Zang et al, APL 2006

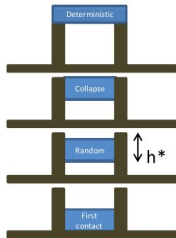
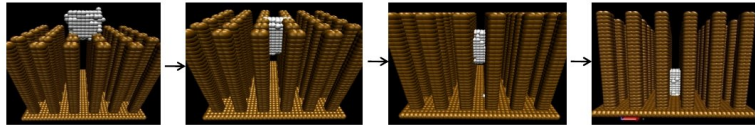


- Avoiding dislocations?
- Growing without collapse?
- Stability?

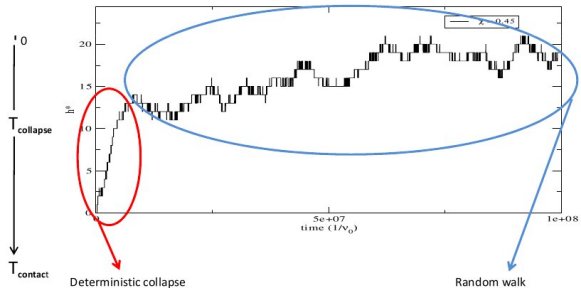


$$\chi = 0.390, \chi = 0.405$$

Dynamics of the island: 3 Stages



13/09/2011



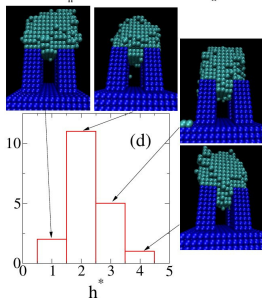
Maxime Ignacio

5

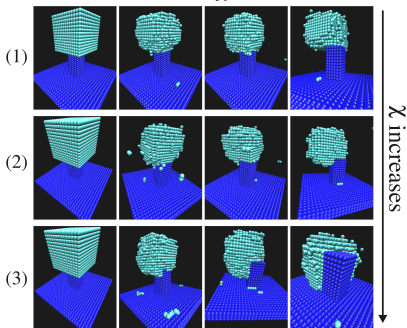
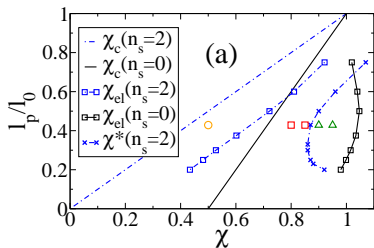
Elastic islands on nano-pillars

3D KMC with elastic effects

- Extended stability
- Asymmetric CB state
- Partially collapsed state



M. Ignacio, Y. Saito, P. Smereka, OPL, PRL 2014



(b)

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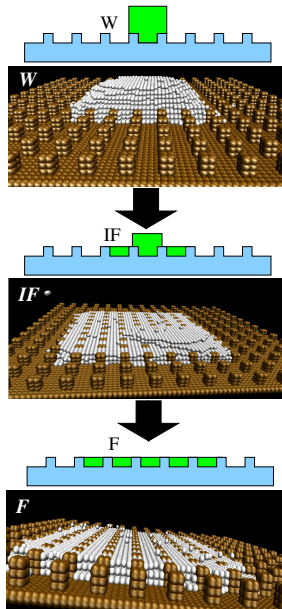
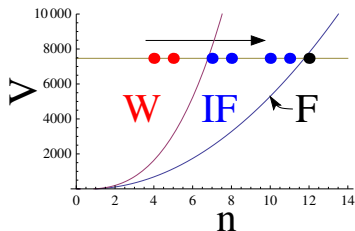
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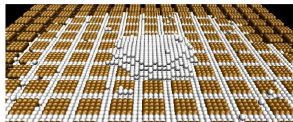
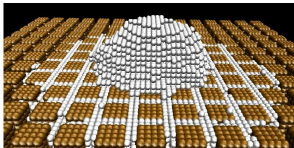
Imbibition criterion

$$1 > \chi > \chi_{imb} = \frac{1}{2} \left(1 + \frac{\ell_x^2 - \ell_p^2}{\ell_x^2 + 4h\ell_p - \ell_p^2} \right)$$



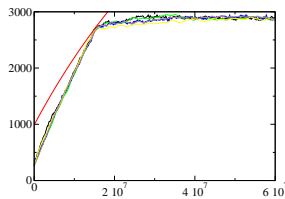
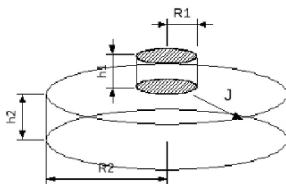
Diffusion-limited spreading

$$\chi = 0.8, \ell_x = 6, h = 3, \ell_p = 4$$



$L \sim t^{1/2}$, and $A \sim t$ with log corrections

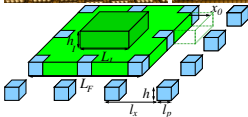
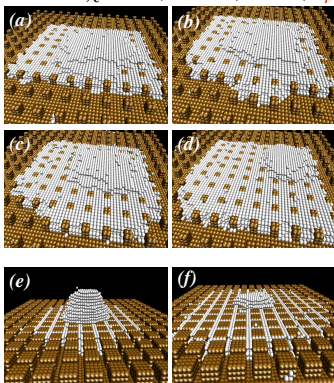
$$\begin{aligned} & (V - A_2 h(1 - \phi))(1 - \ln[(\frac{(1 - \phi)\pi h}{V})^{\frac{3}{2}} \frac{V - A_2 h(1 - \phi)}{\pi 2\phi(1 - \chi)}]) \\ &= \frac{3}{2} \pi \Omega^2 D C_{eq} \frac{\gamma}{k_b T} \frac{(t_0 - t)}{(1 - \phi)h} [\phi \rho(2\chi - 1) - 2(1 - \chi)(1 - \phi)] \end{aligned}$$



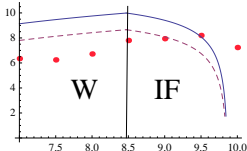
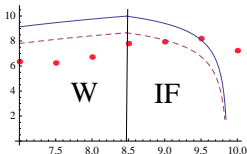
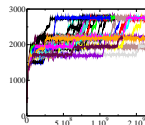
P. Gaillard, Y. Saito, OPL, Phys Rev Lett 2011

Nucleation-limited imbibition front motion

$$\chi = 0.8, \ell_x = 6, h = 3, \ell_p = 2$$



P. Gaillard, Y. Saito, OPL, Phys Rev Lett 2011



Summary

- Equilibrium and stability of islands and films
- Dewetting of solid films: Rim faceting, Instability Coarsening and Anisotropy
- Islands on nano-patterns: Multi-stability / Collapse / Elasticity
- Wetting of reactive islands

Other related issues and Perspectives

- Reactive wetting and nanowire growth
- Surface melting
- Non-equilibrium TL condition
- Link to complex fluids (polymers, etc)
- ... nucleation and growth