Surface diffusion on stepped surfaces

Axel Voigt

based on joint work with Eberhard Bänsch, Frank Haußer, Omar Lakkis, Bo Li, Felix Otto, Patrick Penzler, Andreas Rätz, Tobias Rump

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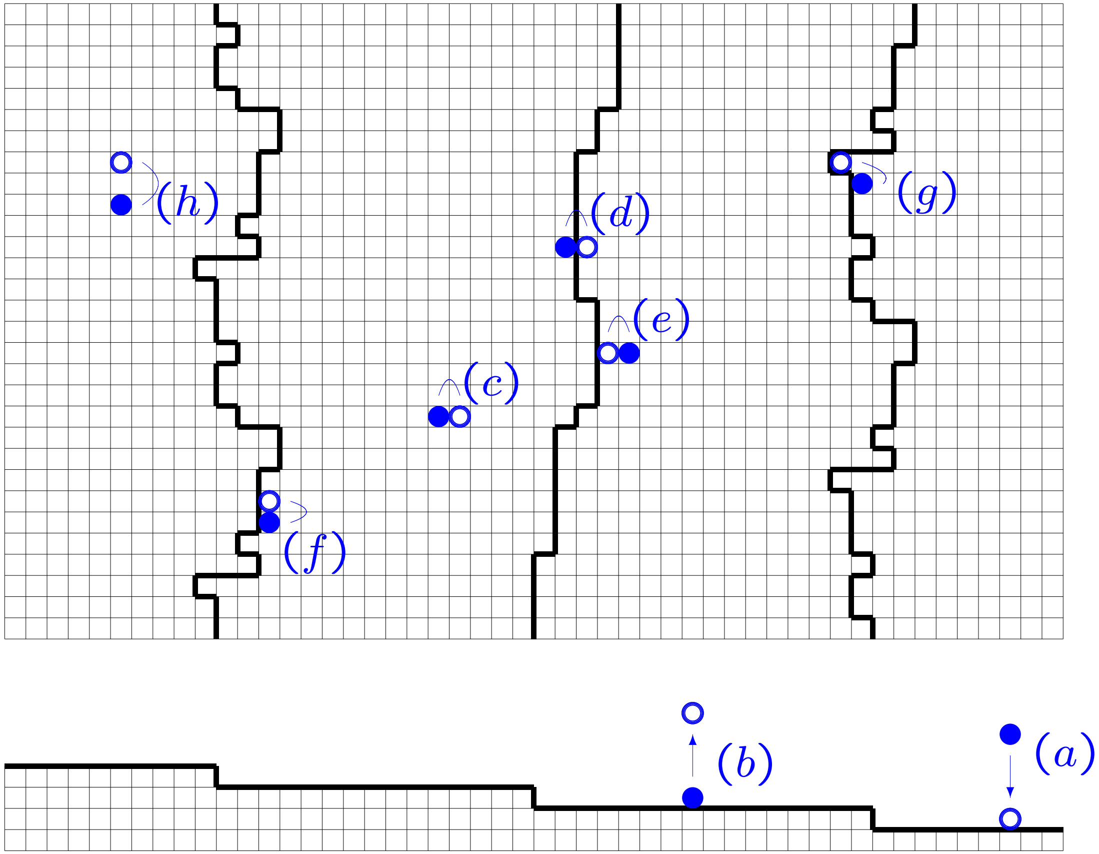
Stepped surfaces are common in epitaxial growth

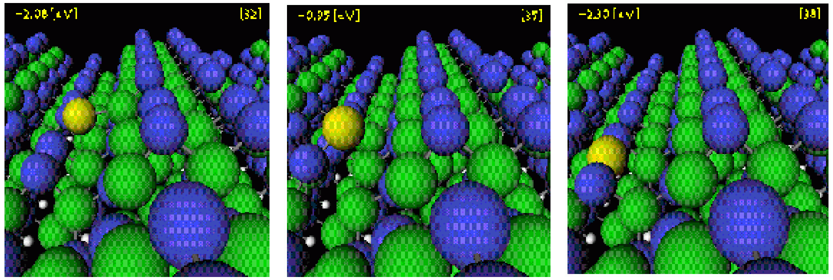
STM image of Si(110) steps on a Si(001) vicinal face, [Lagally et al. 1993]

Simplified atomic picture



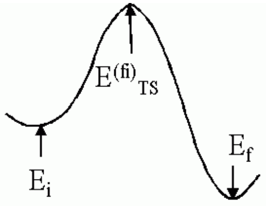
Molecular dynamics

identify single events



Transition State Theory

compute energy barriers



compute probabilities

Kinetic Monte Carlo

perform simulation

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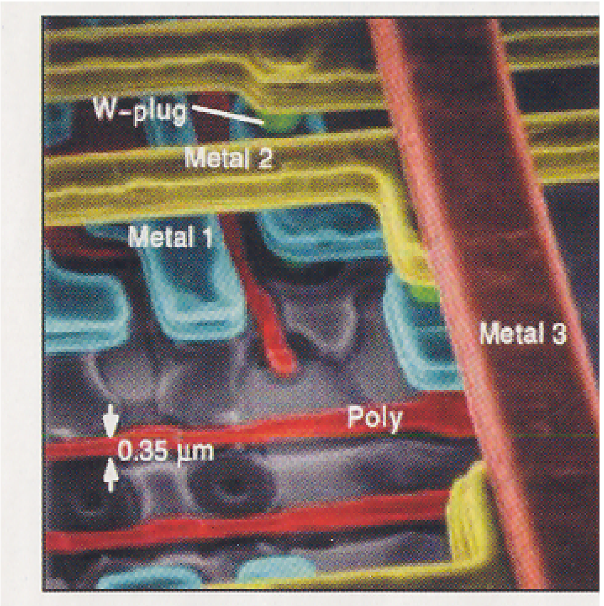
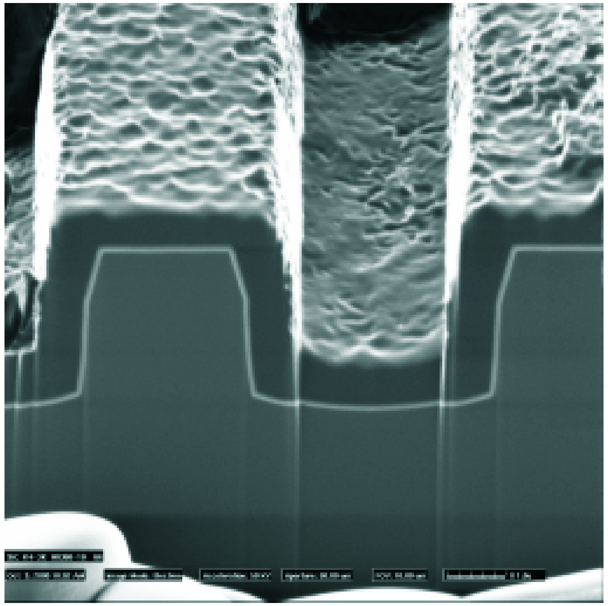
Limitations of KMC

time scale: $< \mu s$, length scale: $< nm$

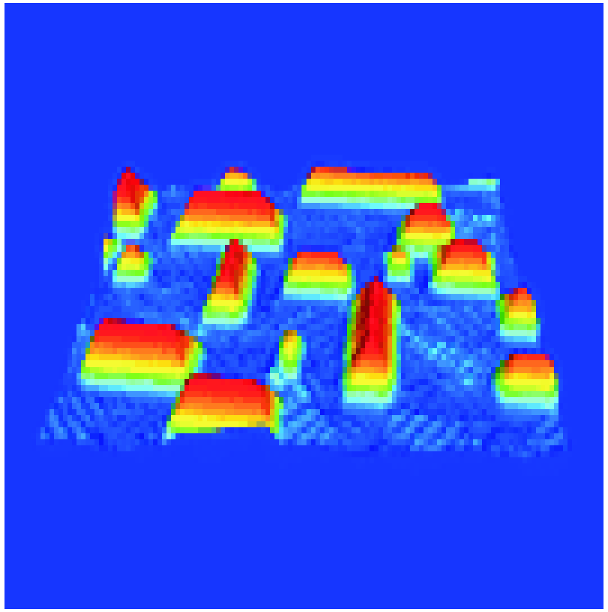
Applications: Nanoelectronic, Photonic, LEDs, ...



metal connects,
(F.H. Baumann, Bell Labs),



trench-MOS structure,
(O. Hellmund, RWTH Aachen),



Quantum-dots
(B. Voigtländer, FZ Jülich)

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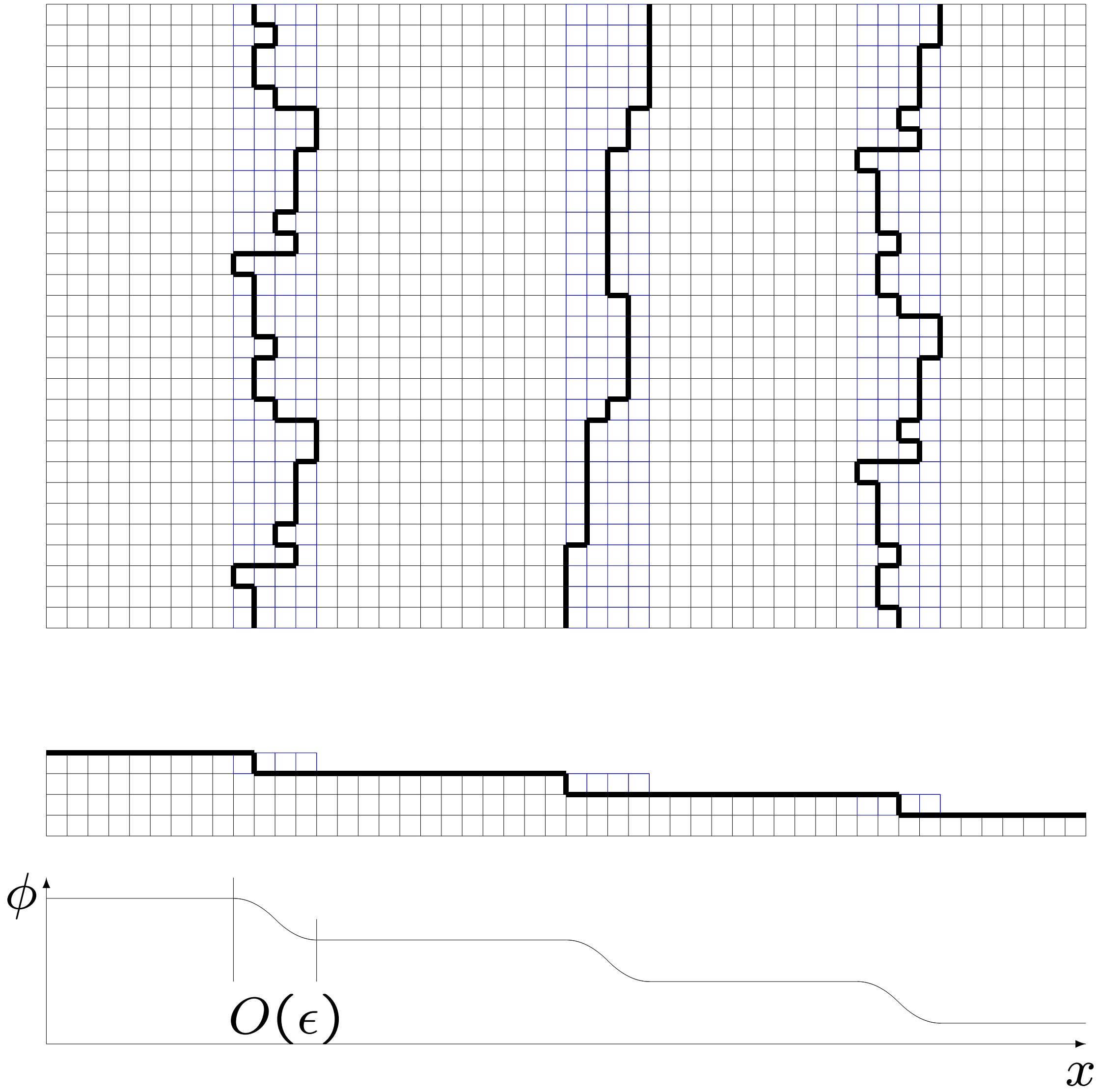
Towards a continuum description



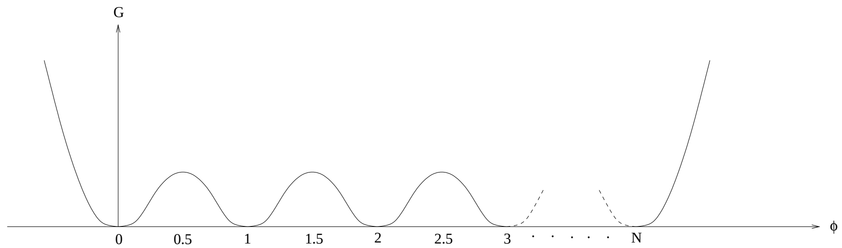
Diffuse interface

approximate rough steps

Multiwell potential

minimum at terraces $i = 0, \ldots, N$

$$G(\phi) = (\phi - i)^2(i + 1 - \phi)^2$$



Ginzburg-Landau free energy

ρ adatom density, ϕ height function

$$E = \int_\Omega \frac{\epsilon^2}{2}|\nabla\phi|^2 + G(\phi) - f(\rho, \phi)$$

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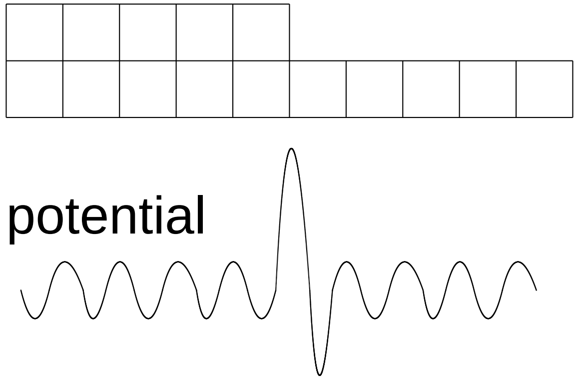
Phase-field model

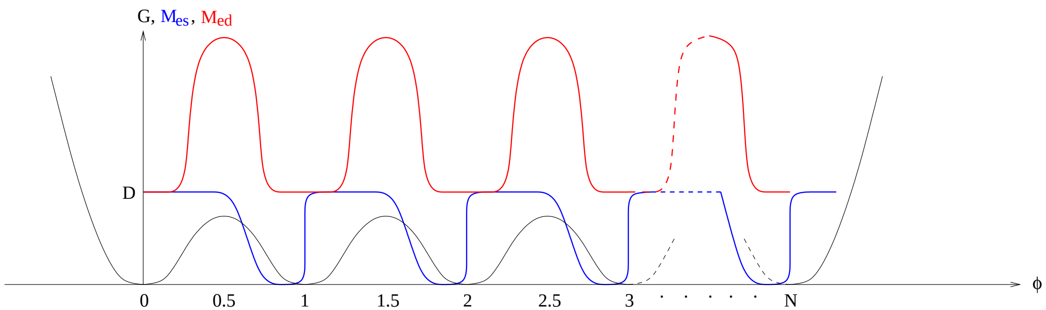
evolution equation $\partial_t \phi = -\frac{\delta E}{\delta \phi}$

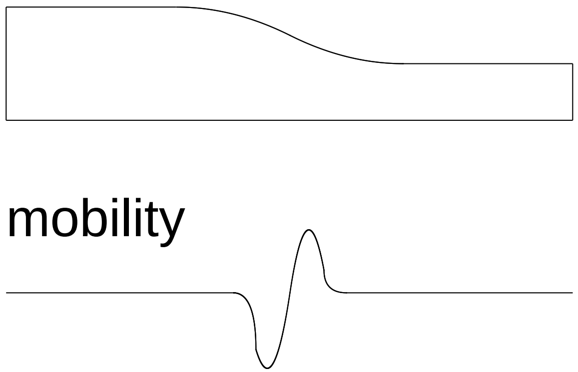
$$\alpha \epsilon^2 \partial_t \phi = \epsilon^2 \Delta \phi - G'(\phi) + \frac{\epsilon}{\rho^* \mu}(\rho - \rho^*)$$
$$\partial_t \rho = \nabla \cdot (D \nabla \rho) + F - \tau^{-1} \rho - \partial_t \phi$$

ρ^* equilibrium density, μ step stiffness



define mobility function D to account for effects at steps





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Asymptotic limit $\epsilon \to 0$, Burton-Cabrera-Frank model

$$\begin{aligned} \alpha\epsilon^2 \partial_t \phi &= \epsilon^2 \Delta\phi - G'(\phi) + \frac{\epsilon}{\rho^* \mu}(\rho - \rho^*) \\ \partial_t \rho &= \nabla \cdot (D \nabla \rho) + F - \tau^{-1}\rho - \partial_t \phi \end{aligned}$$

- diffusion limited, $\epsilon \to 0$, $\alpha \to 0$, $D = D$,

$$\begin{aligned} \partial_t \rho_i - \nabla \cdot (D \nabla \rho_i) &= F - \tau^{-1} \rho_i \\ \rho_i = \rho_{i-1} &= \rho^*(1 - \mu\kappa_i) \\ v_i &= [D \nabla \rho_i \cdot n_i] \end{aligned}$$

[Rätz,Voigt 2004]

- diffusion limited growth with edge-diffusion, $\epsilon \to 0$, $\alpha \to 0$, $D = M_{ed}$,

$$\begin{aligned} \partial_t \rho_i - \nabla \cdot (D \nabla \rho_i) &= F - \tau^{-1} \rho_i \\ \rho_i = \rho_{i-1} &= \rho^*(1 - \mu\kappa_i) \\ v_i &= [D \nabla \rho_i \cdot n_i] + \nu \partial_{ss} \kappa_i \end{aligned}$$

[Rätz,Voigt 2004]

Asymptotic limit $\epsilon \to 0$, Burton-Cabrera-Frank model

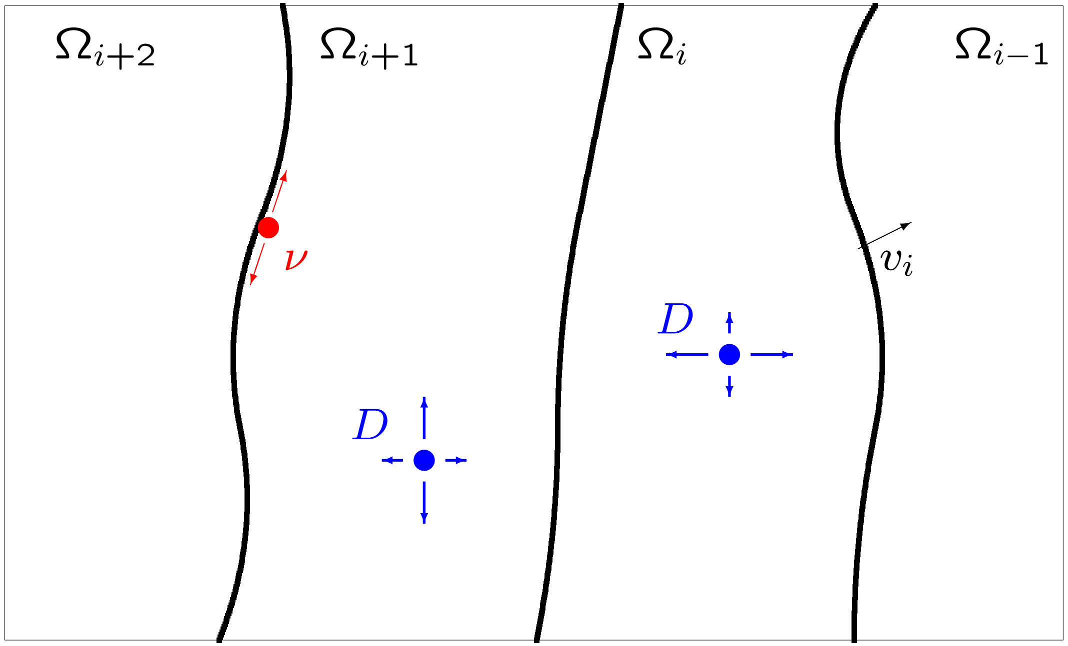
$$\begin{aligned} \alpha\epsilon^2 \partial_t \phi &= \epsilon^2 \Delta\phi - G'(\phi) + \frac{\epsilon}{\rho^* \mu}(\rho - \rho^*) \\ \partial_t \rho &= \nabla \cdot (D\nabla\rho) + F - \tau^{-1}\rho - \partial_t \phi \end{aligned}$$

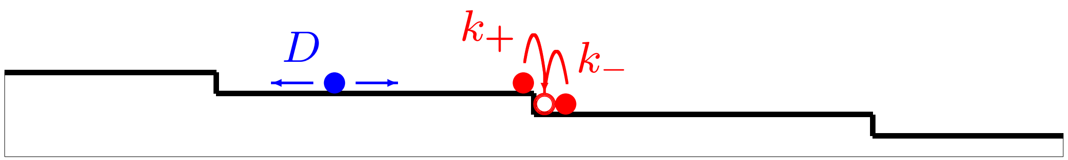
- attachment limited, $\epsilon \to 0$, $D = M_{es}$

$$\begin{aligned} \partial_t \rho_i - \nabla \cdot (D\nabla\rho_i) &= F - \tau^{-1}\rho_i \\ -D\nabla\rho_i \cdot n_i - v_i\rho_i &= k_+(\rho_i - \rho^*(1 - \mu\kappa_i)) \\ D\nabla\rho_{i-1} \cdot n_i - v_i\rho_{i-1} &= k_-(\rho_{i-1} - \rho^*(1 - \mu\kappa_i)) \\ v_i &= [D\nabla\rho_i \cdot n_i] + [\rho_i]v_i \end{aligned}$$

[Otto,Penzler,Rätz,Rump,Voigt 2004; Rätz,Voigt 2004]

Sharp interface step flow model





Free boundary problem

$$\partial_t \rho_i = \nabla \cdot (D \nabla \rho_i) + F - \tau^{-1} \rho_i$$

diffusion limited

$$\rho_i = \rho_{i-1} = \rho^*(1 + \mu\kappa_i)$$

attachment limited

$$\begin{aligned} q_i^+ &:= -D\nabla\rho_i \cdot n_i - v_i\rho_i \\ &= k_+(\rho_i - \rho^*(1+\mu\kappa_i)) \\ q_i^- &:= D\nabla\rho_{i-1} \cdot n_i + v_i\rho_{i-1} \\ &= k_-(\rho_{i-1} - \rho^*(1+\mu\kappa_i)) \end{aligned}$$

$$v_i = q_i^+ + q_i^- + \partial_s(\nu\partial_s(\mu\kappa_i))$$

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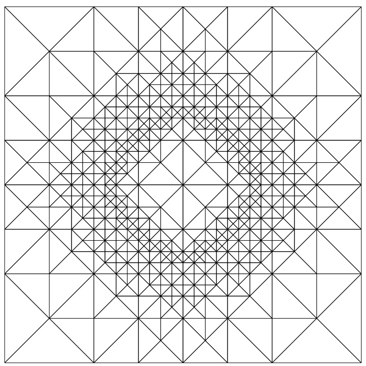
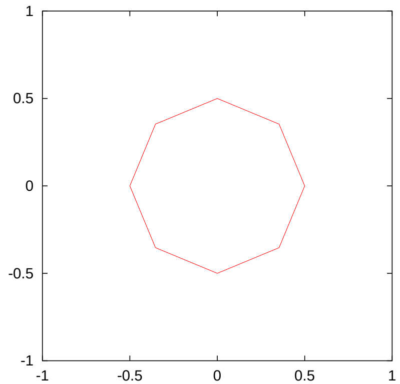
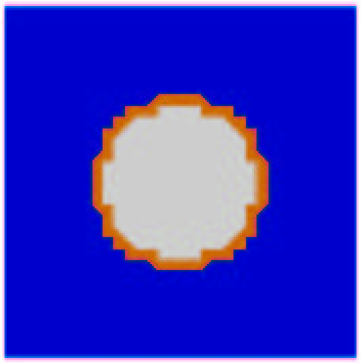
Numerical Algorithm, Operator Splitting

Discrete time partition: $t_0 < t_1 < \cdots < t_m < \cdots$
free Boundaries $\Gamma_i^m := \Gamma_i(t_m)$, adatom densities $\rho_i^m := \rho_i(t_m)$,
decouple adatom diffusion and boundary evolution, use independent grids

- Substep 1: Compute boundaries Γ_i^{m+1} using (Γ_i^m, ρ_i^m)
- Substep 2: Compute adatom densities ρ_i^{m+1} using $(\Gamma_i^{m+1}, \rho_i^m)$







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Adatom diffusion on terraces, diffusion limited

- One *continuous* adatom density ρ defined on whole domain Ω
  Weak formulation of diffusion equation ($[\nabla\rho\cdot\vec{n}_i]_i := \nabla\rho_i\cdot\vec{n}_i - \nabla\rho_{i-1}\cdot\vec{n}_i$)

$$\int_\Omega \partial_t\rho\phi + \int_\Omega D\nabla\rho\cdot\nabla\phi + \sum_{i=1}^N \int_{\Gamma_i} D[\nabla\rho\cdot\vec{n}_i]_i\phi = \int_\Omega F\phi - \int_\Omega \tau^{-1}\rho\phi.$$

- Boundary conditions at steps incorporated by penalty method ($\epsilon \ll 1$)

$$\int_\Omega \partial_t\rho\phi + \int_\Omega D\nabla\rho\cdot\nabla\phi + \sum_{i=1}^N \int_{\Gamma_i} \frac{1}{\epsilon}(\rho - \rho^*(1+\mu\kappa_i))\phi = \int_\Omega F\phi - \int_\Omega \tau^{-1}\rho\phi$$

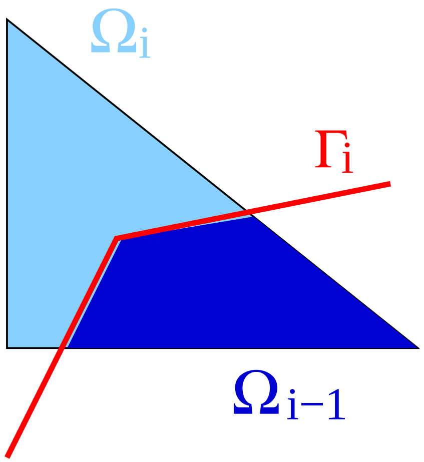
Thus (in a weak sense) $D[\nabla\rho\cdot\vec{n}_i]_i = \frac{1}{\epsilon}(\rho - \rho^*(1+\mu\kappa_i))$

Adatom diffusion on terraces, attachment limited

- Adatom densities $\rho_i \neq \rho_{i-1}$ at Γ_i, i.e. **no** global continuous density
- need two degrees of freedom at steps

Strategy: Composite Finite Elements, Extend each ρ_i trivially to the whole domain:

$$\left(\rho_i(x), D_i(x), F_i(x), \tau_i^{-1}(x)\right) = \begin{cases} (\rho_i(x), D, F, \tau^{-1}) & : x \in \bar{\Omega}_i \\ (0,0,0,0) & : x \in \Omega \setminus \Omega_i \end{cases}$$



- N diffusion equations on whole domain.
- at each boundary Γ_i we have a value for ρ_i and ρ_{i-1}

Weak formulation, attachment limited

$$\int_{\Omega_i} \partial_t \rho_i \phi + \int_{\Omega_i} D\nabla\rho_i \cdot \nabla\phi - \int_{\Gamma_i} D\nabla\rho_i \cdot \vec{n}_i \phi + \int_{\Gamma_{i+1}} D\nabla\rho_i \cdot \vec{n}_{i+1} \phi + \int_{\Omega_i} \tau^{-1} \rho_i \phi = \int_{\Omega_i} F\phi$$

Using

$$\frac{d}{dt}\int_{\Omega_i(t)} \rho_i = \int_{\Omega_i(t)} \partial_t \rho_i + \int_{\Gamma_i(t)} \rho_i v_i - \int_{\Gamma_{i+1}(t)} \rho_i v_i$$

and kinetic boundary conditions

$$-D\nabla\rho_i \cdot \vec{n}_i - \rho_i v_i = k_+(\rho_i - \rho^*(1+\mu\kappa_i)) \quad \text{on } \Gamma_i$$

$$D\nabla\rho_i \cdot \vec{n}_{i+1} + \rho_i v_{i+1} = k_-(\rho_i - \rho^*(1+\mu\kappa_{i+1})) \quad \text{on } \Gamma_{i+1}$$

yields

$$\frac{d}{dt}\int_{\Omega_i(t)} \rho_i \phi + \int_{\Omega_i(t)} D\nabla\rho_i \cdot \nabla\phi + \int_{\Omega_i(t)} \tau^{-1}\rho_i\phi + \int_{\Gamma_{i+1}} k_-\rho_i\phi + \int_{\Gamma_i(t)} k_+\rho_i\phi$$
$$= \int_{\Omega_i(t)} F\phi + \int_{\Gamma_{i+1}} k_-\rho^*(1+\mu\kappa_{i+1})) - \int_{\Gamma_i(t)} k_+\rho^*(1+\mu\kappa_i))$$

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Discretization, kinetic b.c.

Time discretization: $\frac{d}{dt}\int_{\Omega_i(t)} \rho_i \phi \longrightarrow \frac{1}{t_{m+1}-t_m}\left[\int_{\Omega_i^{m+1}} \rho_i^{m+1}\phi - \int_{\Omega_i^m} \rho_i^m \phi\right]$

Using extended variables

$$\left(\rho_i(x), D_i(x), F_i(x), \tau_i^{-1}(x)\right) = \begin{cases} (\rho_i(x), D, F, \tau^{-1}) & : x \in \Omega_i \\ (0,0,0,0) & : x \in \Omega \setminus \Omega_i \end{cases}$$

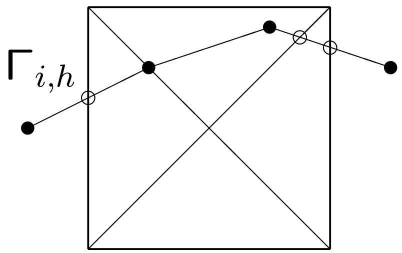
First order implicit in time, finite element method in space

$$\int_\Omega \frac{\rho_{i,h}^{m+1} - \rho_{i,h}^m}{t_{m+1} - t_m}\phi + \int_\Omega D_i \nabla \rho_{i,h}^{m+1} \cdot \nabla \phi + \int_\Omega \tau_i^{-1} \rho_{i,h}^{m+1} \phi + \int_{\Gamma_{i+1}} k_- \rho_{i,h}^{m+1} \phi$$
$$+ \int_{\Gamma_i} k_+ \rho_{i,h}^{m+1} \phi = \int_\Omega F_i \phi + \int_{\Gamma_{i+1}} k_- \rho^* (1 + \mu \kappa_{i+1}) - \int_{\Gamma_i} k_+ \rho^* (1 + \mu \kappa_i)$$

All integrals over whole domain Ω !

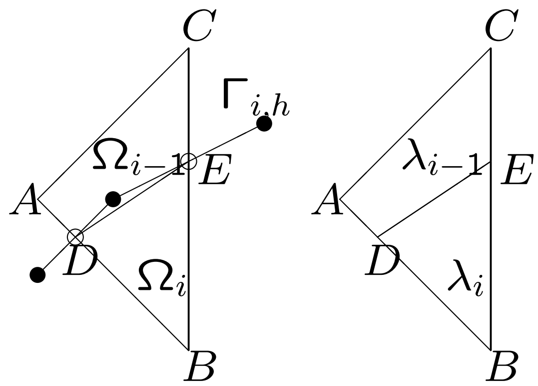
Integration routines

line integration



discontinuous coefficients $\int \phi \lambda$

$$\lambda = \begin{cases} \lambda_{i-1} & \text{in } T \cap \Omega_{i-1} \\ \lambda_i & \text{in } T \cap \Omega_i \end{cases}$$



$$\begin{aligned} \int_T \lambda \phi &\approx \int_{\triangle(DBE)} \lambda_i \phi + \int_{\square(ADEC)} \lambda_{i-1} \phi \\ &= \int_{\triangle(DBE)} \lambda_i \phi + \int_T \lambda_{i-1} \phi - \int_{\triangle(DBE)} \lambda_{i-1} \phi. \end{aligned}$$

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Free boundary evolution

nonlinear 4th order geometric evolution law

$$v_i = \underbrace{-D\nabla\rho_i \cdot \vec{n}_i - \rho_i v_i + D\nabla\rho_{i-1} \cdot \vec{n}_i + \rho_{i-1} v_i}_{\text{mass conservation}} + \underbrace{\partial_s(\nu\partial_s(\mu\kappa_i))}_{\text{edge diffusion}},$$

- diffusion limited: use $D[\nabla\rho \cdot \vec{n}_i]_i = \frac{1}{\epsilon}(\rho - \rho^*(1 + \mu\kappa_i))$ (from penalty method)

$$v_i = \frac{1}{\epsilon}(\rho - \rho^*) - \frac{1}{\epsilon}\rho^*\mu\kappa_i + \partial_s(\nu\partial_s(\mu\kappa_i)).$$

- attachment limited: use $-D\nabla\rho_i \cdot \vec{n}_i - v_i\rho_i = k_+(\rho_i - \rho^*(1 - \mu\kappa_i))$
  $D\nabla\rho_{i-1} \cdot \vec{n}_i + v_i\rho_{i-1} = k_-(\rho_{i-1} - \rho^*(1 - \mu\kappa_i))$

$$v_i = k_+(\rho_i - \rho^*) + k_-(\rho_{i-1} - \rho^*) - (k_+ + k_-)\rho^*\mu\kappa_i + \partial_s(\nu\partial_s(\mu\kappa_i)).$$

Free boundary evolution

nonlinear 4th order geometric evolution law

$$v_i = f_i - \beta\mu\kappa_i + \partial_s(\nu\partial_s(\mu\kappa_i))$$

parametric finite elements, for MCF [Dziuk 1991] for SD [Bänsch,Morin,Nochetto 2002]

write 4^{th} order PDE as 2^{nd} order system: position vector $\vec{x}_i$, curvature vector $\vec{\kappa}_i = \kappa\vec{n}_i$, velocity vector $\vec{v}_i = v_i\vec{n}_i$, geometric identity $\vec{\kappa}_i = -\partial_{ss}\vec{x}_i$

$$\begin{aligned}
\vec{\kappa}_i &= -\partial_{ss}\vec{x}_i \\
\mu\kappa_i &= \mu\vec{\kappa}_i \cdot \vec{n}_i \\
v_i &= f_i - \beta\mu\kappa_i + \partial_s(\nu\partial_s(\mu\kappa_i)) \\
\vec{v}_i &= v_i\vec{n}_i
\end{aligned}$$

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Time discretization

free boundary Γ_i^{m+1}: $\vec{x}_i^{m+1} = \vec{x}_i^m + \Delta t_m \vec{v}_i^{m+1}$

$$
\begin{aligned}
\vec{\kappa}_i &= -\partial_{ss}(\vec{x}_i + \Delta t_m \vec{v}_i) \\
\mu\kappa_i &= \mu\vec{\kappa}_i \cdot \vec{n}_i \\
v_i &= f_i - \beta\mu\kappa_i + \partial_s(\nu\partial_s(\mu\kappa_i)) \\
\vec{v}_i &= v_i \vec{n}_i
\end{aligned}
$$

geometric quantities $\vec{n}_i$, ∂_s explicit, unknowns $\vec{\kappa}_i$, $\mu\kappa_i$, v_i, $\vec{v}_i$ implicit

Variational formulation $\int \partial_{ss} uv = -\int \partial_s u \partial_s v$

$$
\langle \vec{\kappa}_i, \vec{\psi} \rangle - \Delta t_m \langle \partial_s \vec{v}_i, \partial_s \vec{\psi} \rangle = \langle \partial_s \vec{x}_i, \partial_s \vec{\psi} \rangle
$$

$$
\langle \mu\kappa_i, \psi \rangle - \langle \mu\vec{\kappa}_i \cdot \vec{n}_i, \psi \rangle = 0
$$

$$
\langle v_i, \psi \rangle + \langle \nu\partial_s(\mu\kappa_i), \partial_s\psi \rangle + \langle \beta\mu\kappa_i, \psi \rangle = \langle f_i, \psi \rangle
$$

$$
\langle \vec{v}_i, \vec{\psi} \rangle - \langle v_i \vec{n}_i, \vec{\psi} \rangle = 0
$$

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Finite element formulation and linear system

nodal bases (ψ_k) and $(\vec{\psi}_k^q)$

$$\begin{pmatrix} \vec{\boldsymbol{M}} & \boldsymbol{0} & \boldsymbol{0} & -\vec{\boldsymbol{N}} \\ \boldsymbol{0} & \boldsymbol{M} & -\vec{\boldsymbol{N}}_\mu{}^t & \boldsymbol{0} \\ -\Delta t_m \vec{\boldsymbol{A}} & \boldsymbol{0} & \vec{\boldsymbol{M}} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{A}_\nu + \boldsymbol{M}_\beta & \boldsymbol{0} & \boldsymbol{M} \end{pmatrix} \begin{pmatrix} \vec{V}_i \\ \mu K_i \\ \vec{K}_i \\ V_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vec{\boldsymbol{A}} \vec{X}_i \\ F \end{pmatrix}$$

Schur complement equation for $\vec{K}_i, V_i$ reads

$$\boldsymbol{S} \begin{pmatrix} \vec{K}_i \\ V_i \end{pmatrix} = \begin{pmatrix} \vec{\boldsymbol{A}} \vec{X}_i \\ F \end{pmatrix},$$

$$\boldsymbol{S} = \begin{pmatrix} \vec{\boldsymbol{M}} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{M} \end{pmatrix} - \begin{pmatrix} -\Delta t_m \vec{\boldsymbol{A}} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{A}_\nu + \boldsymbol{M}_\beta \end{pmatrix} \begin{pmatrix} \vec{\boldsymbol{M}} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{M} \end{pmatrix}^{-1} \begin{pmatrix} \boldsymbol{0} & -\vec{\boldsymbol{N}} \\ -\vec{\boldsymbol{N}}_\mu{}^t & \boldsymbol{0} \end{pmatrix}$$

$$= \begin{pmatrix} \vec{\boldsymbol{M}} & -\Delta t_m \vec{\boldsymbol{A}} \vec{\boldsymbol{M}}^{-1} \vec{\boldsymbol{N}} \\ (\boldsymbol{A}_\nu + \boldsymbol{M}_\beta) \boldsymbol{M}^{-1} \vec{\boldsymbol{N}}_\mu{}^t & \boldsymbol{M} \end{pmatrix}.$$

Schur complement equations

- solve for V_i

$$\left(\Delta t_m(\boldsymbol{A}_\nu + \boldsymbol{M}_\beta)\boldsymbol{M}^{-1}\vec{\boldsymbol{N}}_\mu{}^t\vec{\boldsymbol{M}}^{-1}\vec{\boldsymbol{A}}\vec{\boldsymbol{M}}^{-1}\vec{\boldsymbol{N}} + \boldsymbol{M}\right) V_i$$
$$= F - (\boldsymbol{A}_\nu + \boldsymbol{M}_\beta)\boldsymbol{M}^{-1}\vec{\boldsymbol{N}}_\mu{}^t\vec{\boldsymbol{M}}^{-1}\vec{\boldsymbol{A}}\vec{X}_i.$$

- solve for $\vec{V}_i$

$$\vec{\boldsymbol{M}}\vec{V}_i = \vec{\boldsymbol{N}}V_i,$$

- update position X_i, assemble again over new interface

- solve for μK_i

$$\mu K_i = -\boldsymbol{M}^{-1}\vec{\boldsymbol{N}}_\mu\vec{\boldsymbol{M}}^{-1}\vec{\boldsymbol{A}}\vec{X}_i.$$

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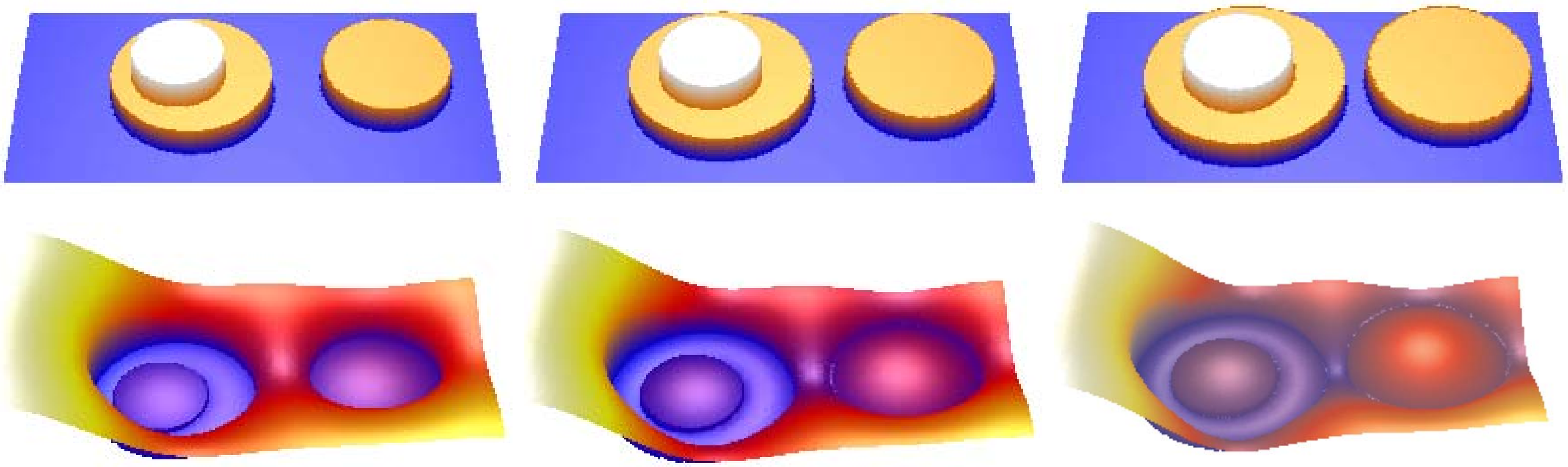
Numerical tests for isotropic situations

- area conservation for geometric evolution
- comparison with analytic solution for circular domain
- mass conservation

[Bänsch,Haußer,Lakkis,Li,Voigt 2004]



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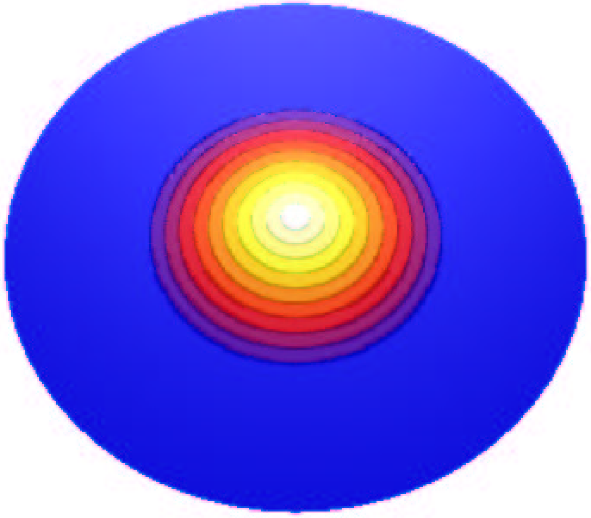
Thermal decay

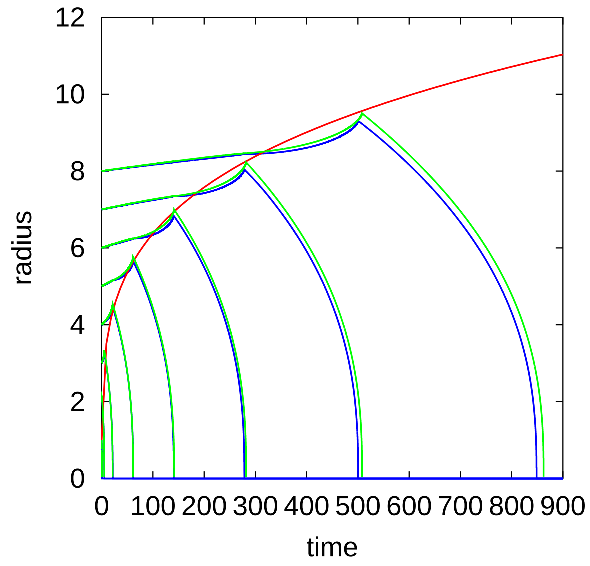


$$\rho_i''(r) + \frac{1}{r}\rho_i'(r) = 0 \qquad R_{i+1}(t) < r < R_i(t)$$

$$D\rho_i'(R_{i+1}) = k_-\left(\rho_i(R_{i+1}) - \rho^*\left(1 + \frac{\mu}{R_{i+1}}\right)\right)$$

$$-D\rho_{i+1}'(R_{i+1}) = k_+\left(\rho_{i+1}(R_{i+1}) - \rho^*\left(1 + \frac{\mu}{R_{i+1}}\right)\right)$$

scaling law $R \approx t^{1/4}$



— PDE, — ODE

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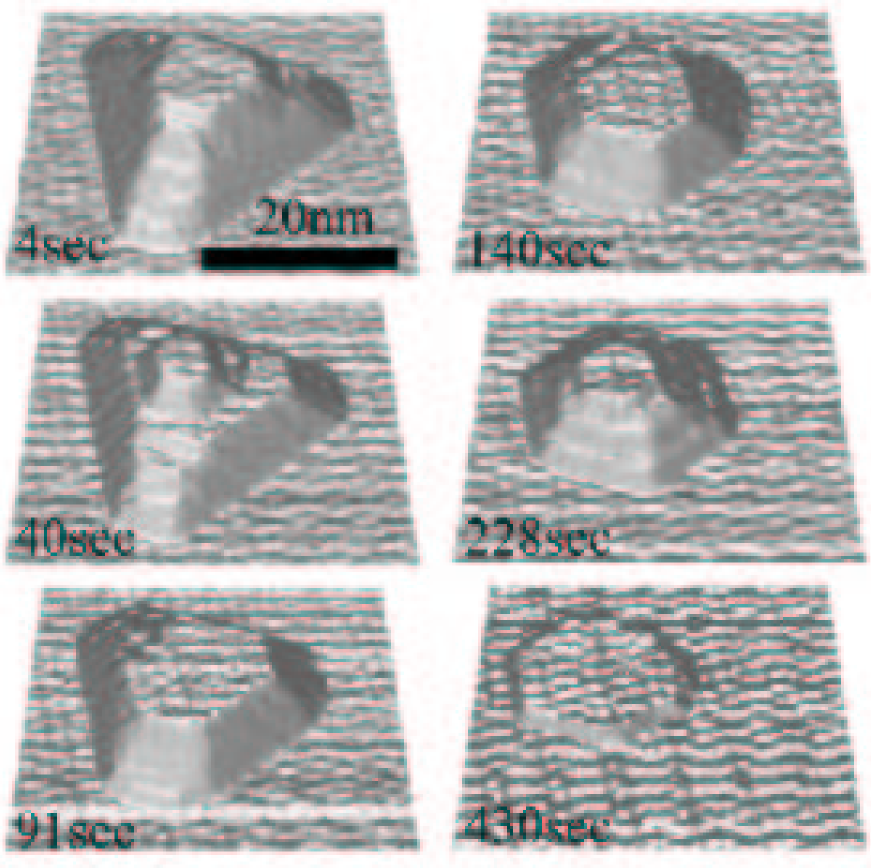
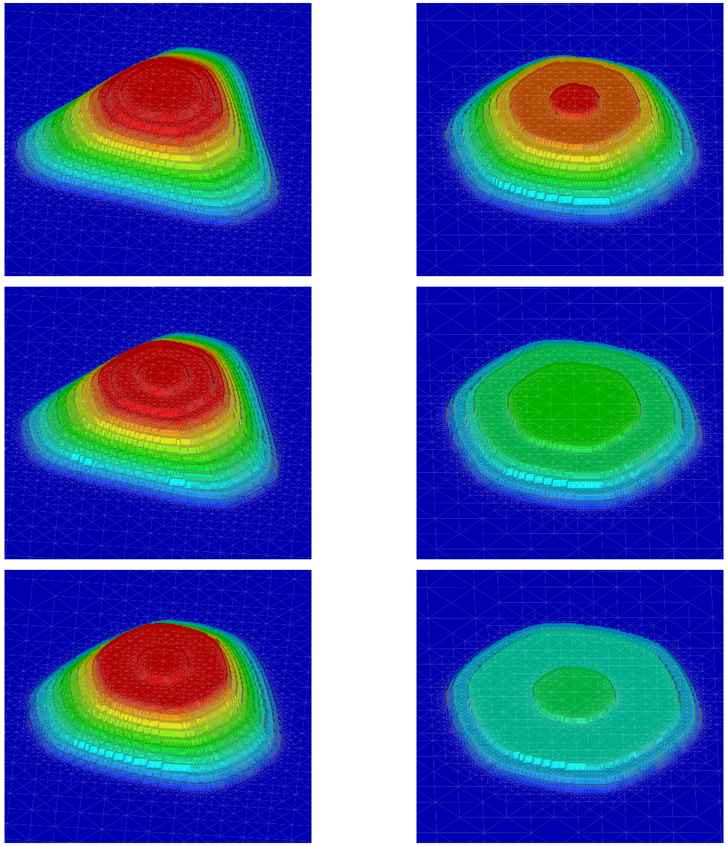
Anisotropic decay of a nanomound

Thermal relaxation of a 12-layer mound on a substrate: $200a \times 200a$, $a = 0.25nm$.



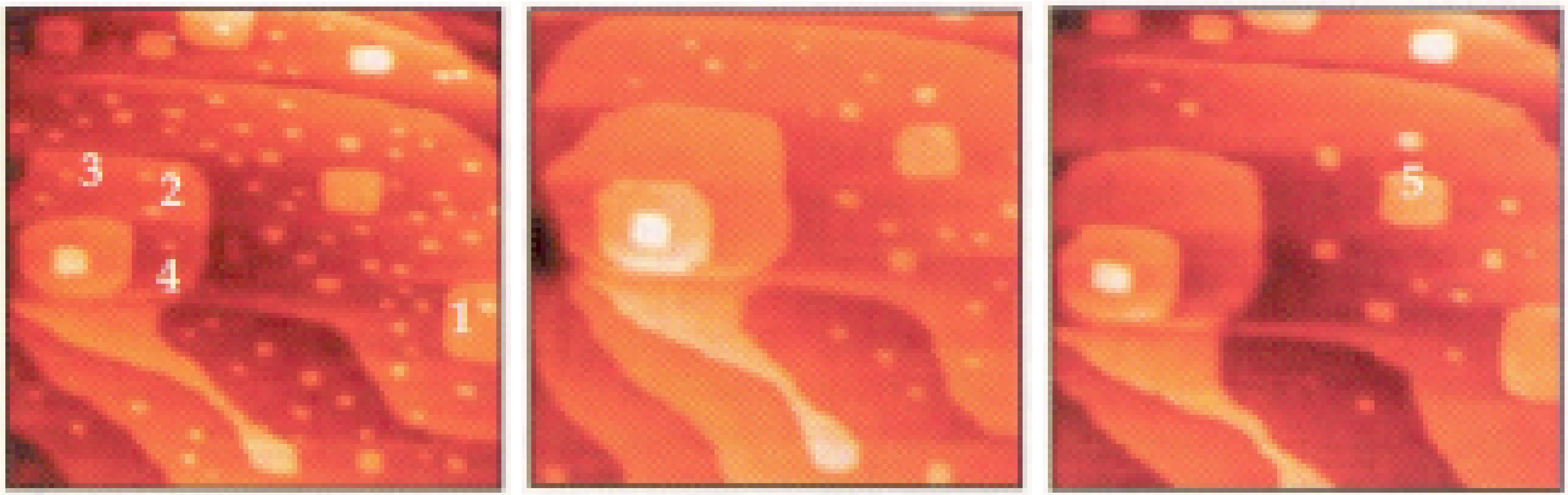
STM snapshots, Si(111) nanomound
[Ichimiya et al. 2001]



12, 27, 65, 157, 476, 1330sec
[Haußer,Voigt 2004]

Coarsening and Ostwald ripening, experiments

coarsening of islands; small islands shrink, large islands grow

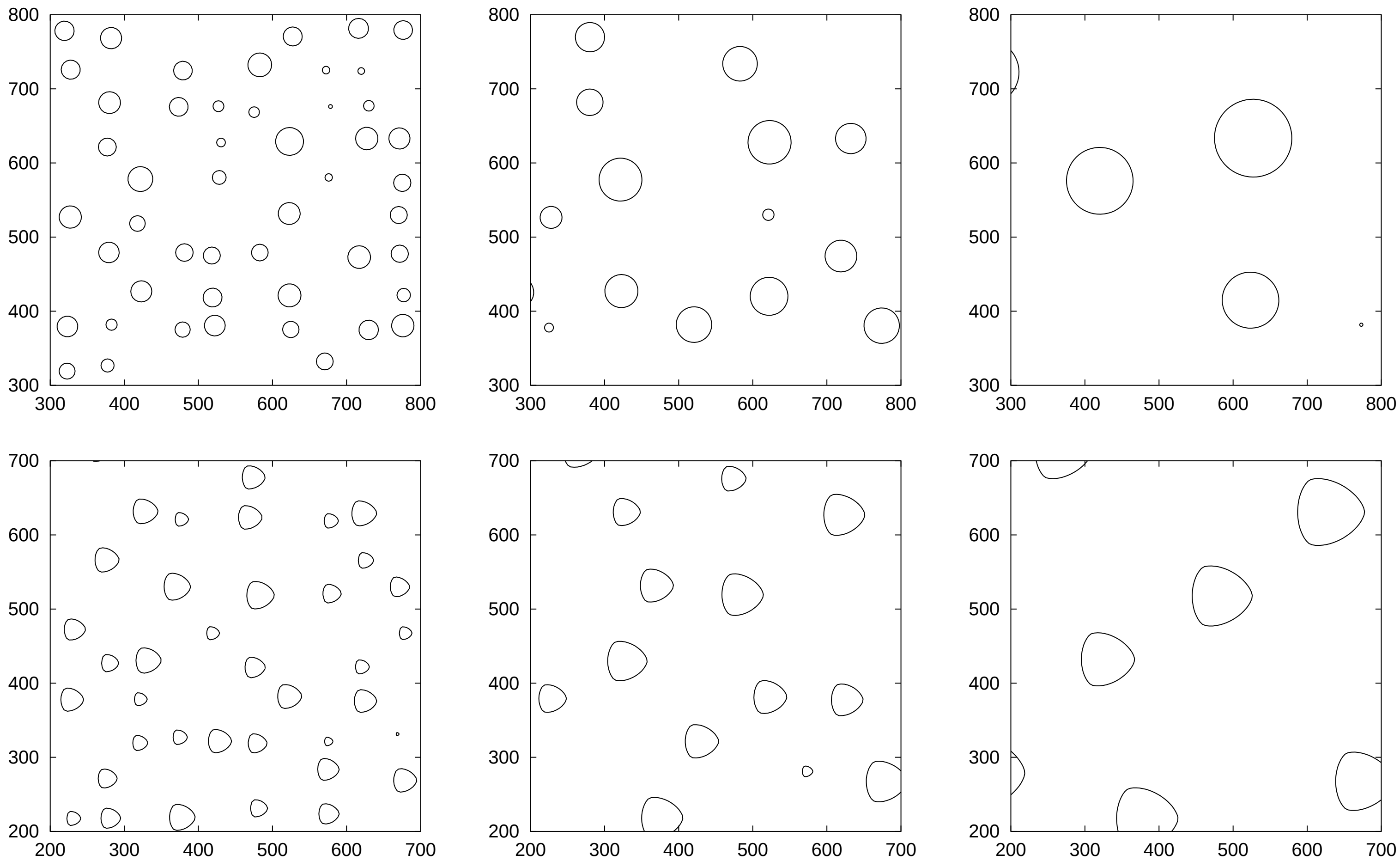


TiN(001) during annealing [I. G. Petrov et al. 2001]

Crystal Growth Group
c a es a r

Coarsening and Ostwald ripening, simulation

coverage $\phi = 0.085$, $k = 10^4$, $t = 600s, 3000s, 15000s$, 1000×1000



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Ostwald ripening - Mean field theory

Lifshitz, Slyozov, Wagner (LSW) reduce Mullins-Sekerka system

$$\begin{aligned} \Delta u &= 0 && \text{in } \mathbb{R}^3 \backslash \partial G \\ v &= [\nabla u \cdot \vec{n}] && \text{on } \partial G \\ u &= \kappa && \text{on } \partial G \end{aligned}$$

to equation for radius of each particle R_i.

small volume fraction: $u \approx \overline{u}(t)$ away from particle, solve for isolated particle with $u(t,\infty) = \overline{u}(t)$.

$$\begin{aligned} \dot{R}_i &= \frac{1}{R_i^2}(R_i \overline{u}(t) - 1) \\ \overline{u}(t) &= \frac{\sum_{i;R_i>0} 1}{\sum_{i;R_i>0} R_i(t)} \end{aligned}$$

distribution of particle radii $\nu(t,r)$

$$\int_{r_1}^{r_2} \nu(t,r)\, dr = \text{number of particles with radius in } (r_1, r_2)$$

<u>two-dimensional situation</u>

divergence of logarithmic Green's function, introduce screening length

$$\begin{aligned} \dot{R}_i &\approx \frac{1}{\ln(\frac{1}{\phi^{1/2}})} \frac{1}{R_i^2}(R_i \overline{u}(t) - 1) \\ \overline{u}(t) &= \frac{\sum_{i;R_i>0} \frac{1}{R_i}}{\sum_{i;R_i>0} 1} \end{aligned}$$

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Homoepitaxial Ostwald ripening - Mean field theory

Burton-Cabrera-Frank model yields

$$\dot{R}_i \approx (\overline{\rho} - \rho^*) \frac{Dk}{D + kR_i \ln(\frac{1}{\phi^{1/2}})}$$

$$\overline{\rho}(t) = \frac{\sum_{i;R_i>0} \frac{R_i}{D+kR_i \ln(1/\phi^{1/2})} \rho^*}{\sum_{i:R_i>0} \frac{R_i}{D+kR_i \ln(1/\phi^{1/2})}}$$

Diffusion limited $k\overline{R} \gg D$

$$\dot{R}_i \approx \frac{D}{R_i \ln(\frac{1}{\phi^{1/2}})} (\overline{\rho} - \frac{\nu}{R_i})$$

$$\overline{\rho}(t) = \nu \frac{\sum_{i;R_i>0} \frac{1}{R_i}}{\sum_{i:R_i>0} 1} = \nu \overline{\left(\frac{1}{R}\right)}$$

Attachment limited $k\overline{R} \ll D$

$$\dot{R}_i \approx (\overline{\rho} - \frac{\nu}{R_i}) k$$

$$\overline{\rho}(t) = \nu \frac{\sum_{i;R_i>0} 1}{\sum_{i:R_i>0} R_i} = \nu \frac{1}{\overline{R}}$$

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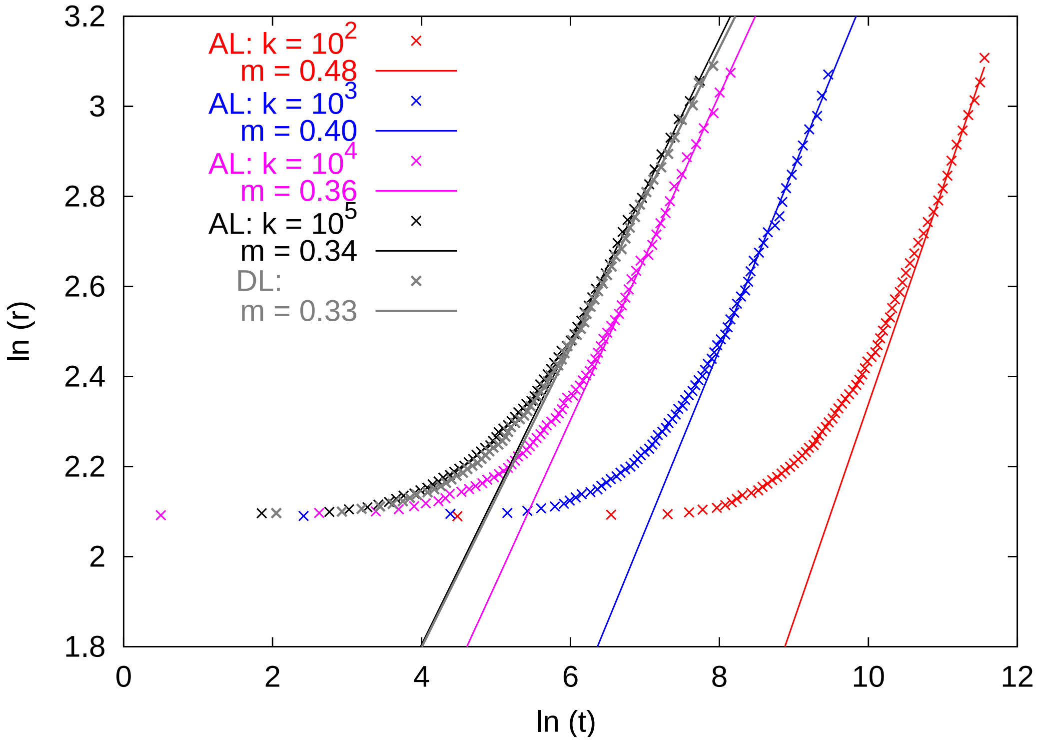
Homoepitaxial Ostwald ripening - Mean field theory and Simulation

Diffusion limited

$$\bar{R}(t) = (\bar{R}^3 + K(\phi)t)^{\frac{1}{3}}$$

Attachment limited

$$\bar{R}(t) = (\bar{R}^2 + K(\phi)t)^{\frac{1}{2}}$$



400 islands
substrate $1000 \times 1000a$
coverage 0.085
initial distribution radius and midpoints chosen randomly according to coverage
zero asymptotic distribution.

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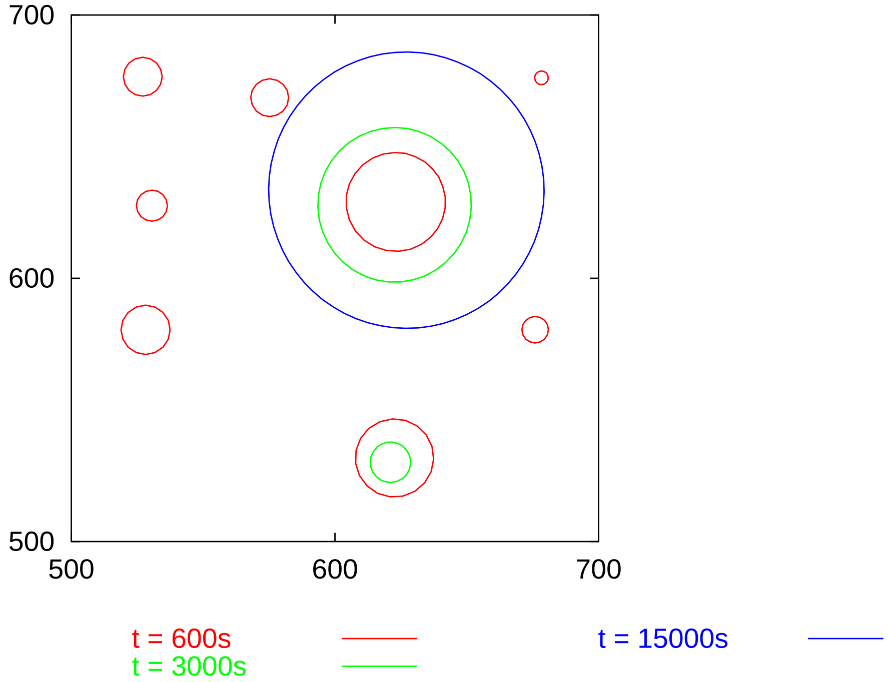
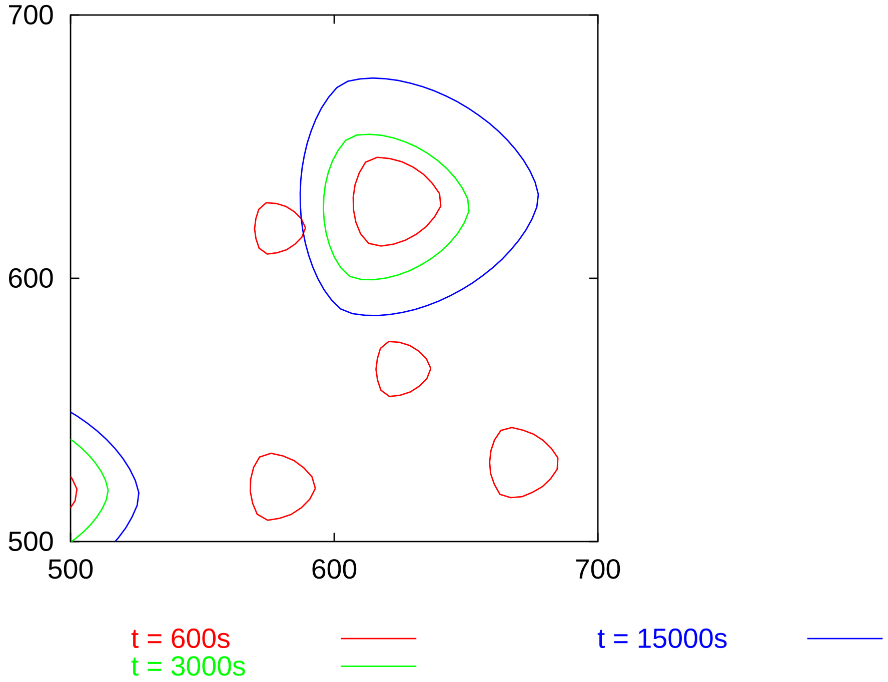
Homoepitaxial Ostwald ripening, island motion





assumption of mean field theories, that the center of the islands is fixed is not satisfied

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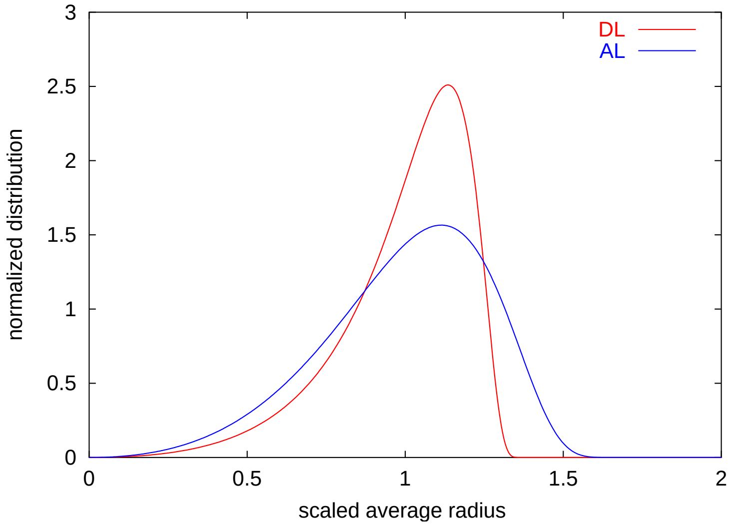
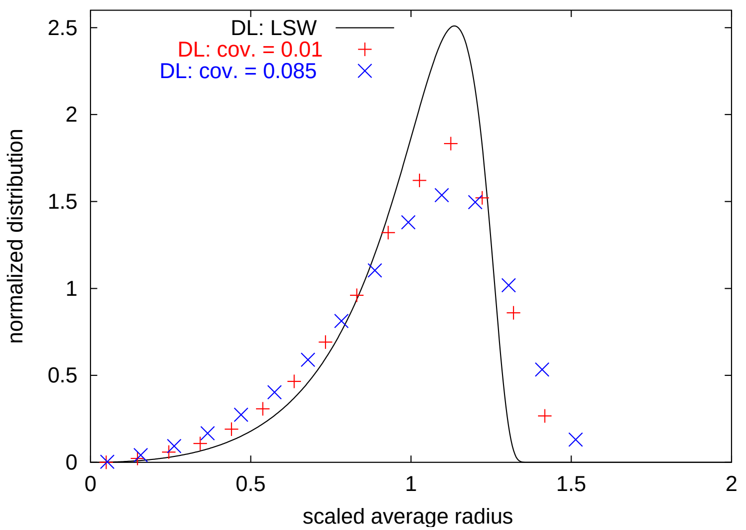
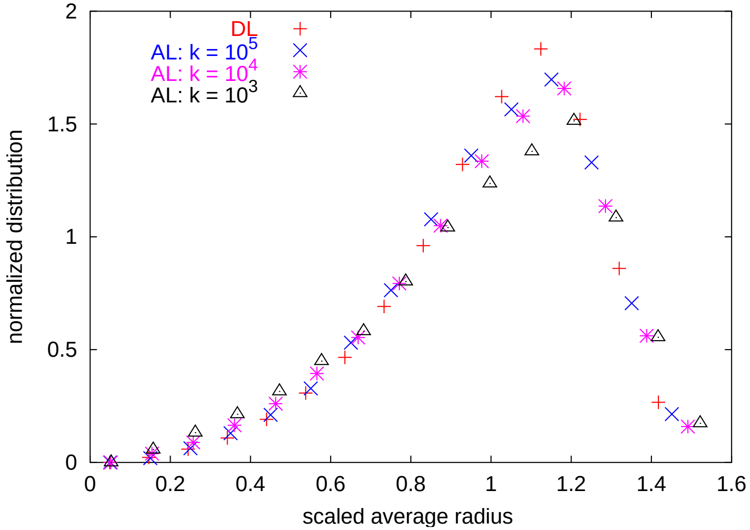
Ostwald ripening, island size distribution

LSW island size distribuition function

diffusion limited and attachment limited







More information

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