(Lecture II)

From discrete schemes to macroscopic evolution laws: Coarse graining and homogenization in epitaxial relaxation

Dionisios Margetis
Department of Mathematics, &
Institute for Physical Science and Technology, &
Ctr. for Scientific Computation and Math. Modeling
University of Maryland, College Park

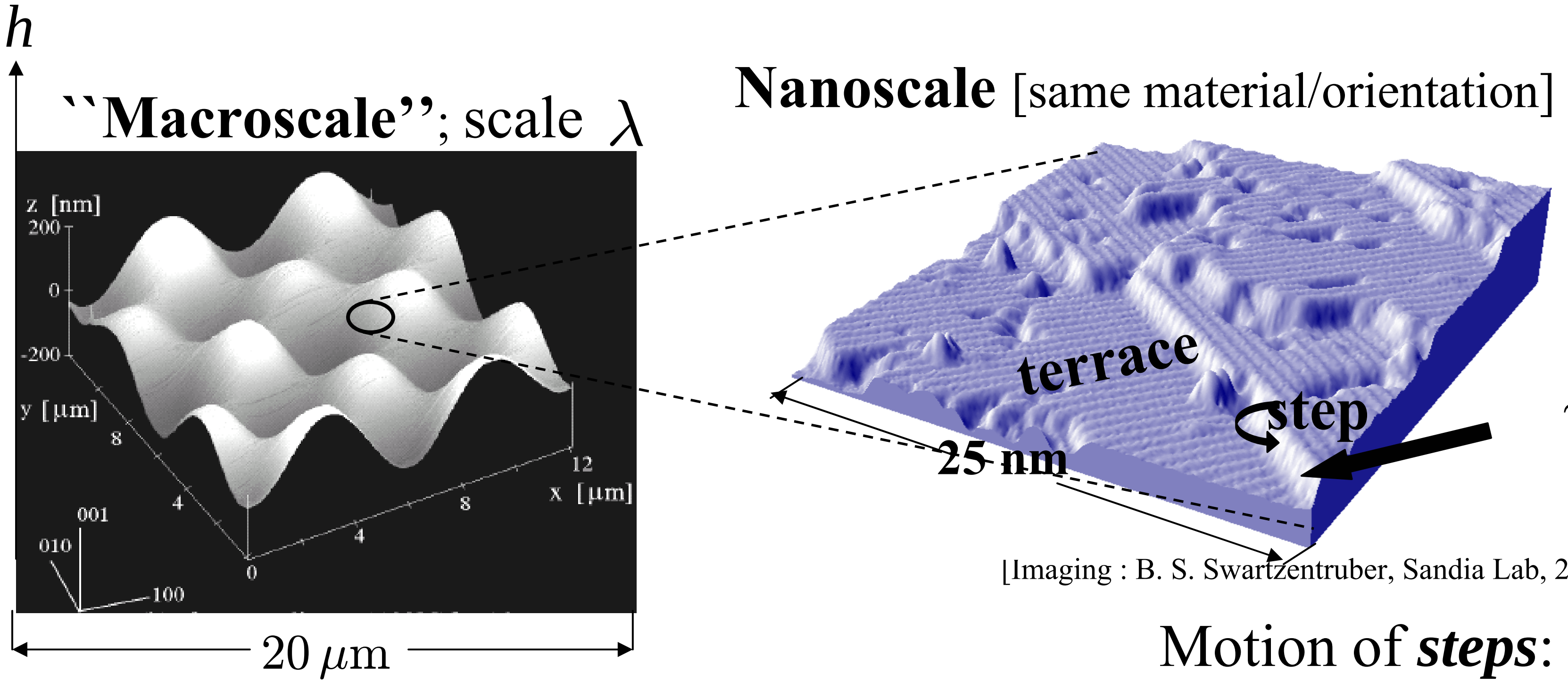
*Research supported by **NSF** DMS-0847587*

Interdisciplinary Conference "**Mathematical Aspects of Crystal Growth**"
Hokkaido University
Sapporo, Japan -- July 26-30, 2010

Recalling physical setting

``Macroscale''; scale λ

Nanoscale [same material/orientation]



[Imaging of Si(001): Blakely,Tanaka, 1999]

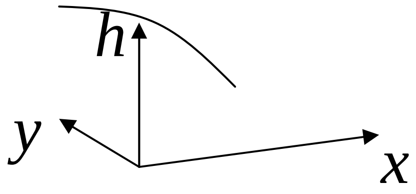
[Imaging : B. S. Swartzentruber, Sandia Lab, 2002]

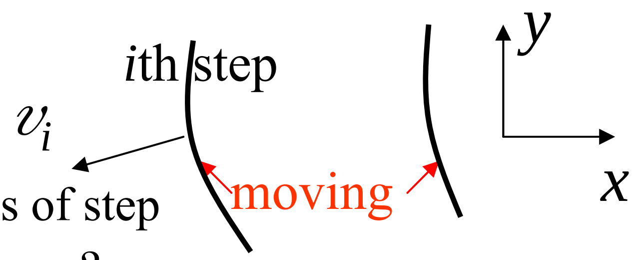
~1 atom; height a

Motion of ***steps***:

Discrete scheme

PDE for height h ?



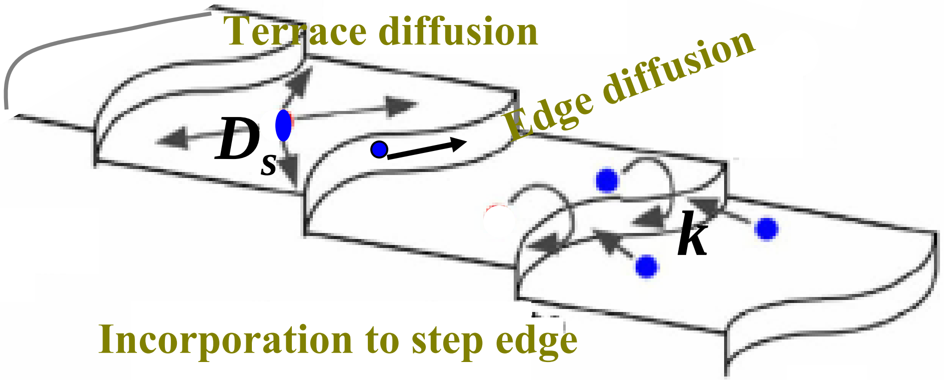


: In terms of step positions ?

[Nozières, 1987; Rettori, Villain, 1988; Lancon, Villain, 1990; Ozdemir, Zangwill, 1990; Israeli, Kandel, 1999; E, Yip, 2001; Xiang, 2002; DM, Aziz, Stone, 2005; DM, Kohn, 2006; DM, Fok, Aziz, Stone, 2006; DM, 2007; Quah, DM, 2008; Fok, Rosales, DM, 2008; DM, Tzavaras, 2009; Quah, DM, 2010]

Microscopic processes

[BCF, 1951]


Terrace diffusion

Edge diffusion

D_s

k

Incorporation to step edge

(Asymmetrically with
ES=Ehrlich-Schwoebel barrier;
rates k_- & k_+)

Macroscopic limit: Overview

For what macroscopic theory is step motion a consistent discrete scheme?

Main assumptions:

- Evolution/relaxation *near equilibrium* (BCF theory)
- Motion by *surface diffusion*
- *Monotone* step trains -- **away from facets**

Early theories of epitaxial relaxation for $T < T_R$ are fully continuum, analogous to theory for $T > T_R$:
mass conservation and **continuum thermodynamics**;
e.g., Spohn (1993), Hager and Spohn (1995)

Today we know that care should be exercised:
Continuum theories may *not* be consistent with steps (Lec. III)

Ingredients of continuum theory below roughening

height flux

(1) $h_t + \mathrm{div}\, J = 0$ mass conservation law (in relaxation)

mobility

(2) $J = -M(\nabla h) \cdot \nabla \mu$ Fick's law/flux

(3) $\mu = \left(\frac{\delta E}{\delta h} \right)_{L^2}$ surface free energy variational-thermdn. principle/chem. potential

Equations (1) and (3) stem from fully continuum principles [Spohn, 1993; Shenoy, Freund, 2002; Chan, Ramasubramaniam, Shenoy, Chason, 2004]

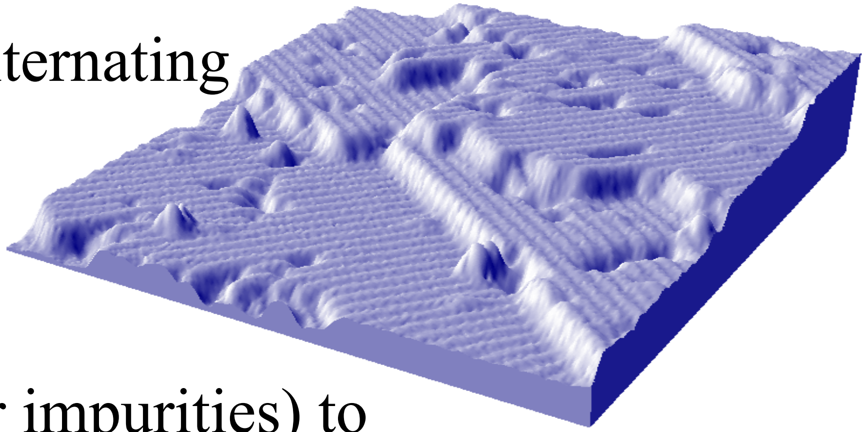
By contrast, *Fick's law* (2) must be derived from step kinetics.
In **1D** [Nozières, 1987; Rettori, Villain, 1988; Ozdemir, Zangwill, 1990]:

$$M(\nabla h) \propto \frac{D_s}{1 + Q|\nabla h|}, \qquad Q = \frac{2D_s}{ka}$$

Also used in **2D** [DM, Aziz, Stone, 2005; Shenoy *et al.*, 2004]
However: 2D case is richer: **tensor** M
1D case: Averaging in case of surface reconstructions

Surface-reconstruction-inspired model: homogenization in 1D

Surface reconstruction



Naturally: Si(001) has terraces with alternating properties (e.g., diffusivities)

[Monch, 1995; Lifshits, Salanin, Zotov, 1994; Swartzentruber, Kitamura, Lagally, Webb, 1993]

Artificially: Attachment of solutes (or impurities) to vicinal crystals can alter stability and shape dramatically

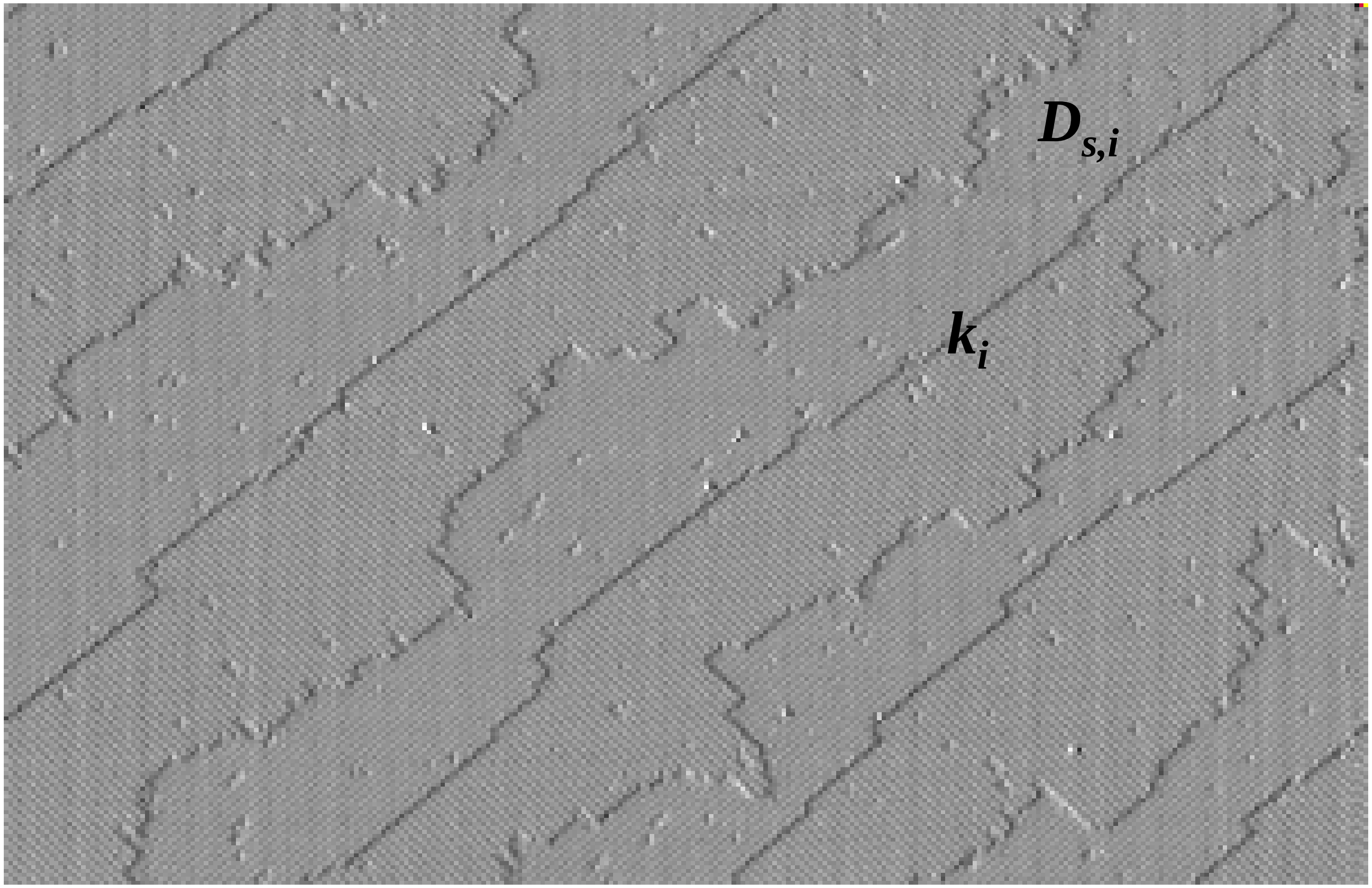
[Hansen *et al* 2002; Qiu *et al* 2004; Stasevich *et al* 2009]

Goal: Prediction of possibilities for surface ***"composites"***

The usual coarse graining by Taylor expansions is not adequate

[DM, 2009]

View of reconstructed Si(001) surface



[B. S. Swartzentruber, Sandia National Labs; www.sandia.gov/surface_science/stm/images/IMAGES.HTM]

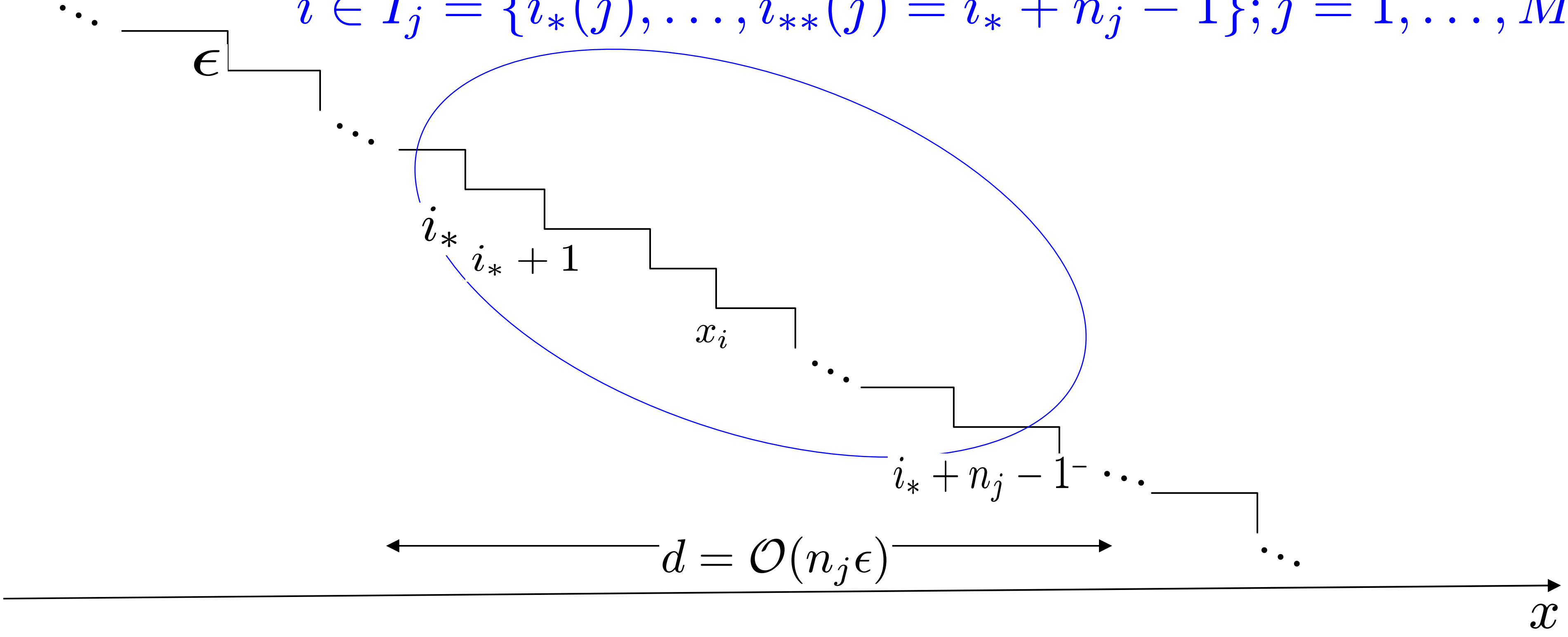
Large-scale evolution laws ?

1D Model: Notion of mesoscale

[Milton, 2002]

Consider M groups of consec. steps; n_j (:fixed) steps in jth group

$$i \in I_j = \{i_*(j), \ldots, i_{**}(j) = i_* + n_j - 1\}; j = 1, \ldots, M$$



Assumption: Microscale parameters vary appreciably within each I_j.
(Appropriate) *Averages* vary *slowly* across different I_j

$\epsilon \ll d \ll \lambda$ $\qquad$ $n_j \to \infty, \quad n_j \epsilon \downarrow 0, \quad M \to \infty$

Proposition (Effective Fick's law in 1D) [DM, 2009] *Suppose the step model has (positive, bounded) kinetic rates k_i and diffusivities $D_{s,i}$. By classical homogenization, the continuum-scale flux is*

$$\boxed{J = -M_e(x)\,\partial_x \mu} \qquad \text{where}$$

$$M_e = \frac{\rho_s}{\vartheta}\,\frac{D_{\mathrm{av}}}{1+Q_{\mathrm{av}}\,m}, \qquad \vartheta = k_B T$$

$$D_{\mathrm{av}}(x)^{-1} := \lim_{n_j\to\infty}\left[(x_{i_{**}} - x_{i_*})^{-1}\sum_{i\in I_j}\frac{x_{i+1}-x_i}{D_{s,i+1}(x)}\right], \quad Q_{\mathrm{av}} := \frac{2D_{\mathrm{av}}}{k_{\mathrm{av}}\,a},$$

$$k_{\mathrm{av}}^{-1} := \lim_{n_j\to\infty}\left(n_j^{-1}\sum_{i\in I_j}k_i^{-1}\right), \qquad \boxed{m(x) := \lim_{n_j\to\infty}\frac{n_j\,\varepsilon}{x_{i_{**}}-x_{i_*}} = |h_x|}$$

mesoscopic
slope

Sketch of proof Classical homogenization: Microscale:

Diffusion

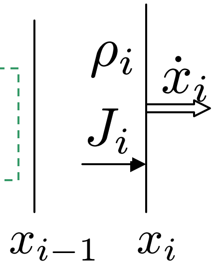
$$D_{s,i}\partial_x^2\rho_i = \partial_t\rho_i \qquad x_{i-1} < x < x_i;\ i = 1,\dots,N$$

Attach./Detach.
at *i*th step edge
(from left)

$$\boxed{\underbrace{-D_{s,i}(\partial_x\rho_i)}_{=:\,J_i} - \underset{\text{convection}}{\dot{x}_i\rho_i} = k_i(\rho_i - \rho_i^{\mathrm{eq}}) \qquad x = x_i}$$

Step velocity law

$$\dot{x}_i = \epsilon[J^- - J^+ - \dot{x}_i(\rho_i^- - \rho_i^+)]$$



- Scale separation. Multiscale expansion at mesoscale.

$$y := x/\epsilon, \qquad \tau := \epsilon^2 t = O(1)$$

$$\rho_i(x,t) = \varrho(x,t) =: \varrho^{(0)}(x,y,\tau) + \epsilon\varrho^{(1)}(x,y,\tau) + \epsilon^2\varrho^{(2)}(x,y,\tau) + \dots$$

$$J_i(x,t) = -D_{s,i}(x)[\partial_x + \epsilon^{-1}\partial_y]\varrho =: \epsilon^{-1}\mathcal{J}^{(-1)}(x,y,\tau) + \mathcal{J}^{(0)}(x,y,\tau) + \dots$$

[Bensoussan, Lions, Papanicolaou, 1978]

1. Conditions at $y_i = x_i/\epsilon$; $\mathcal{J}^{(0),(-1)}$ **cont.** by dom. balance in step vel.
2. Leading order: By dom. balance in diffusion eq., boundedn. of $\varrho^{(0)}$,

$$\boxed{\varrho^0(x,y,\tau) = B(x,\tau) \Rightarrow \mathcal{J}^{(-1)} \equiv 0}$$

3. Next higher-order, $O(\epsilon)$, terms:

$$D_{\mathrm{av}}\partial_x B = D_{i_*}(C_{i_*} + \partial_x B)(1 + q_{\mathrm{av}}m) \Rightarrow \mathcal{J}^{(0)} = -D_{i_*}(C_{i_*} + \partial_x B) = -D_{\mathrm{e}}\partial_x B$$

4. By dom. balance in boundary conds., $B(x)$ is identified with $\rho^{\mathrm{eq}}(x)$ $\square$

Relaxation laws for 1D model

[DM, *in prep.*]

Fick's law should be complemented by:

- Mass conservation [by step velocity law, kinetic bc's to $\mathcal{O}(\epsilon^2)$]:

$$\boxed{\overbrace{m(x,\tau)\bar{v}(x,\tau)}^{=\partial_\tau h}+\partial_x\mathcal{J}^{(0)}(x,\tau)=0;}\qquad \bar{v}(x,\tau)=\lim_{n_j\to\infty}\left(n_j^{-1}\sum_{i\in I_j}\dot{x}_i^0(\tau)\right)$$

- Thermodynamic force : chemical potential. **Start with**:

$$\sum_{i=0}^{N-1}\dot{x}_i\mu_i=\dot{E}_N;\quad E_N=\sum_{i=0}^{N-1}\tilde{g}_i\left(\frac{\epsilon}{x_{i+1}-x_i}\right)^2,\quad \tilde{g}_i=O(1)>0$$

Macroscale: $\epsilon\downarrow 0,\quad m_i:=\epsilon/(x_{i+1}-x_i)=O(1)$

$$\boxed{\mu=(\delta E[h]/\delta h)_{L^2},}\qquad E[h]=\frac{1}{3}\int g_{\rm av}(x)\,|h_x|^3\,dx$$

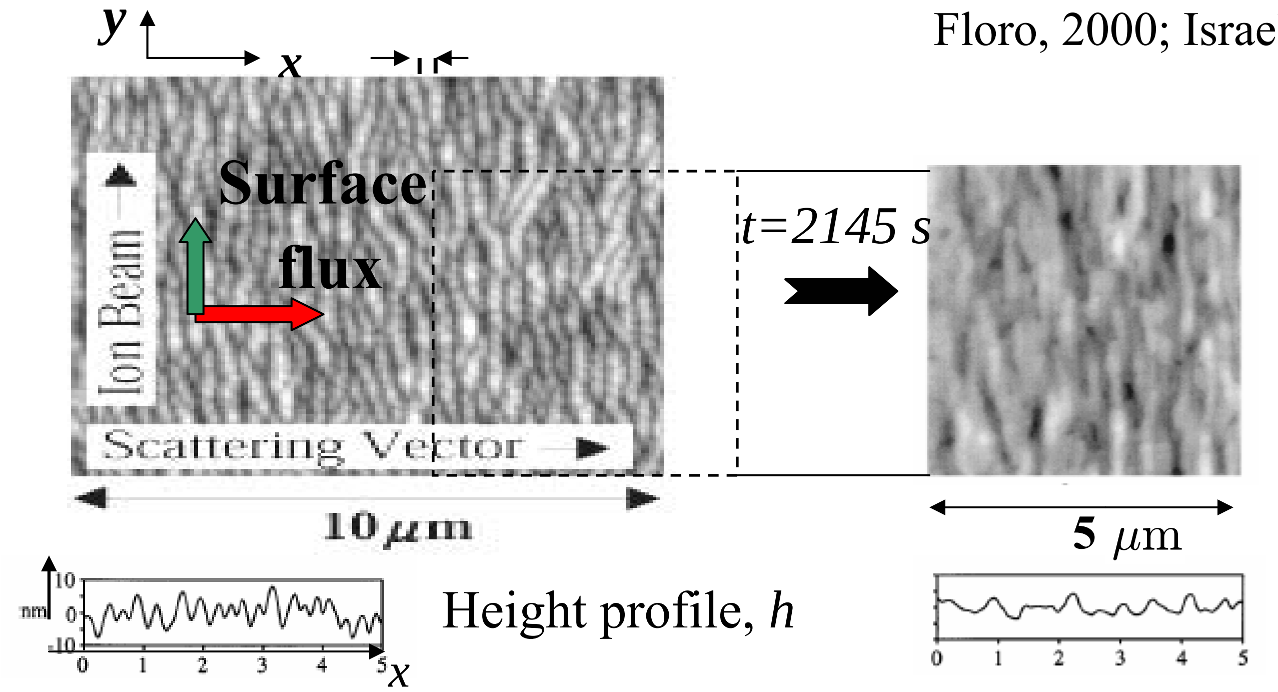
$$g_{\rm av}(x)m(x)^2:=\lim_{n_j\to\infty}\left[n_j^{-1}\sum_{i\in I_j}(3\tilde{g}_i)m_i^2\right]$$

Coarse-graining of step flow: evolution laws in **2D**

Motivation: Relaxation experiments

Si(001) T = 920 –1020 K [Erlebacher, Aziz, Chason, Sinclair, Floro, 2000; Israeli, Kandel, 2001]

Top view:



Height profile, *h*

$$\lambda_x/\lambda_y \sim 10^{-1}$$

$$\boxed{\text{Peak-to-valley height variation} \quad \delta_{\mathrm{pv}} h = O\left(\frac{1}{t}\right)}$$

inverse linear decay

Similar observation on Ag(110) [Pedemonte,Bracco,Boragno, de Mongeot,Valbusa, 2003]

By contrast, for lithography-made **1D** corrugations on Si(001) [Keefe, Umbach, Blakely, 1994]:

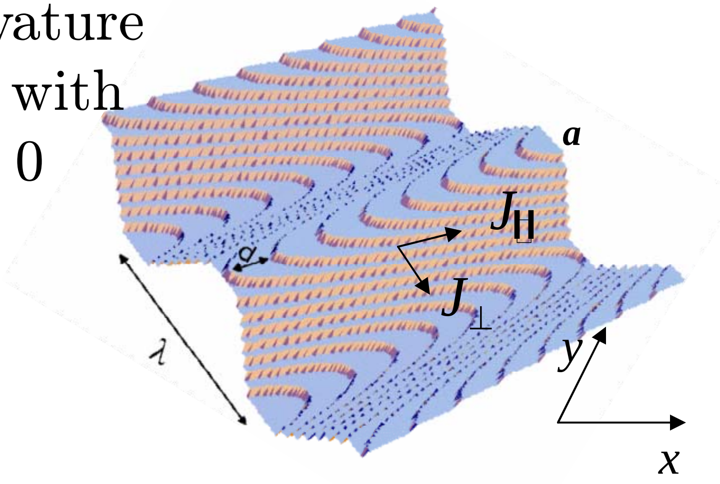
$$\boxed{\delta_{\mathrm{pv}} h = O(e^{-ct})}$$

exponential decay

$$\lambda_x/\lambda_y \sim 10^{-3}$$

Macroscopic surface flux in 2+1 dims

Proposition [DM, Kohn, 2006] If step curvature $\kappa_i = O(\lambda^{-1})$ and sufficiently slowly varying with arc length, step-step spacing$= O(a)$, $a/\lambda \to 0$ with **fixed step density**, THEN:

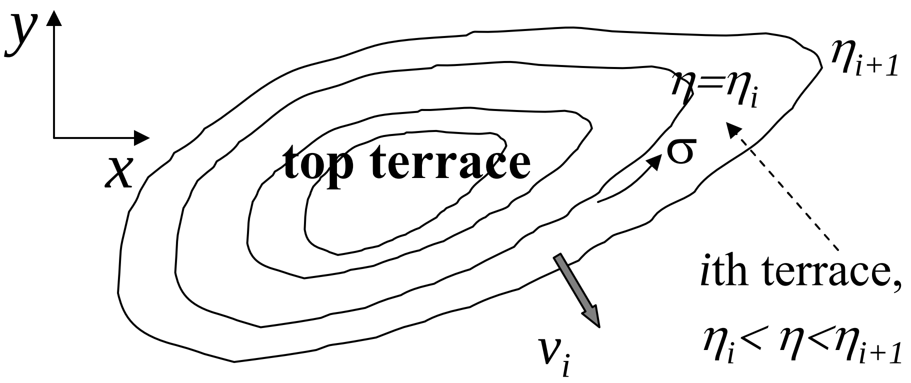


Continuum flux on (x,y) plane:

$$\boldsymbol{J} = \begin{pmatrix} J_{\perp} \\ J_{//} \end{pmatrix} = -\frac{D_s \rho_s}{k_{\mathrm{B}} T} \underset{\mathbf{M}}{\boxed{\begin{pmatrix} \dfrac{1}{1+Q|\nabla h|} & 0 \\ 0 & 1 \end{pmatrix}}} \begin{pmatrix} \partial_{\perp}\mu \\ \partial_{//}\mu \end{pmatrix} \; ; \qquad \overset{\text{Step kinetics}}{Q} = \frac{2D_s}{ka}$$

Sketch of proof (by discrete step flow in 2+1 dims)

Local coordinates (η,σ);
descending steps, height a;
ith step at $\eta = \eta_i$



- Step normal (scalar) **velocity** :

$$v_i = a^2 (J_{i-1,\perp} - J_{i,\perp})$$

- Adatom **flux** on ith terrace

$$\boldsymbol{J}_i(\mathbf{r},t) = -D_s \nabla \rho_i , \ \eta_i < \eta < \eta_{i+1}; \quad D_s \Delta \rho_i = \frac{\partial \rho_i}{\partial t} \approx 0$$

Boundary conditions for diffusion eq. on ith terrace:

$$-J_{i,\perp} = k\,[\rho_i - \rho_i^{\text{eq}}(\sigma,t)] \ @\, \eta = \eta_i; \quad J_{i,\perp} = k\ [\rho_i - \rho_{i+1}^{\text{eq}}(\sigma,t)] \ @\, \eta = \eta_{i+1}$$

$$\rho_i^{\text{eq}} = \rho_s \exp \frac{\mu_i}{k_{\text{B}} T} \approx \rho_s \left(1 + \frac{\mu_i}{k_{\text{B}} T} \right)$$

- $\mu_i(\sigma,t)$: **step chemical potential**

[**B**urton, **C**abrera, **F**rank, 1951]

Difficulty: Solving Laplace's eqn. for ρ_i on i th terrace.

Method: η is ``fast'' and $\sigma$ is ``slow'' : Use of asymptotics

$$\rho_{\mathrm{i}}(\eta,\sigma,t) \sim K_i(\sigma,t)\int_{\eta_i}^{\eta} d\eta' \, \frac{\xi_\eta}{\xi_\sigma} + N_i(\sigma,t), \quad \xi_\sigma = |\partial_\sigma \mathbf{r}|, \xi_\eta = |\partial_\eta \mathbf{r}|$$

Continuum limit: $\eta_{i+1} - \eta_i \rightarrow 0$

$$\boxed{J_{i,//} = J_{i,//}\,|_{\eta=\eta_i} = -\frac{D_s\rho_s}{k_B T}\,\partial_{//}\mu,}$$

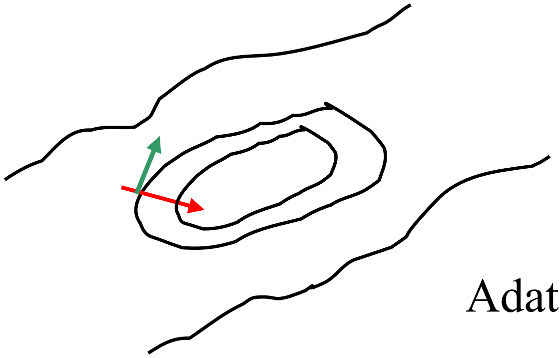
longitudinal current

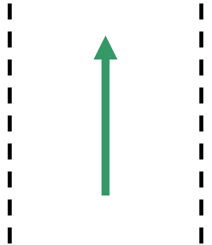
from $\rho_i \sim \rho_i^{eq}$, $\eta=\eta_i$

$$\boxed{J_{i,\perp} = \boldsymbol{J}_{i,\perp}\,|_{\eta=\eta_i} = -\frac{D_s\rho_s}{k_B T}\,\frac{1}{1+Q\,|\nabla h|}\,\partial_\perp \mu}$$

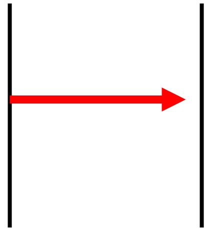
transverse current

$$Q = \frac{2D_s}{ka} \qquad \square$$





Adatoms hop `freely' on terrace



Restriction by attach.-detach. @ steps

Evolution laws in 2+1 dims

(Step density → surface slope= $m=|\nabla h|$)

- Surface **velocity**/mass conservation (from step velocity law):

$$\partial_t h + \overset{\text{atomic volume}}{\Omega}\,\mathrm{div}\,J = 0$$

- **Mass flux** (from boundary conditions at step edges):

$$\boldsymbol{J} = \begin{pmatrix} J_\perp \\ J_{//} \end{pmatrix} = -\frac{D_s \rho_s}{k_B T} \begin{pmatrix} \dfrac{1}{1+Q|\nabla h|} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \partial_\perp \mu \\ \partial_{//} \mu \end{pmatrix} ; \qquad Q = \frac{2D_s}{ka}$$

- **Chemical potential**:

$$\mu(\mathbf{r},t) = \Omega\left(\underbrace{-\,g_1 \nabla \bullet \frac{\nabla h}{|\nabla h|}}_{\text{Step curvature}} \underbrace{-\,g_3 \nabla \bullet \left[\partial_m (m\mathsf{V}) \frac{\nabla h}{|\nabla h|} \right]}_{\text{Step interactions}} \right)$$

$$\mathsf{V} = \mathsf{V}(m)$$

Elastic-dipole & entropic, repuls. interactions:

$V=m^2, \quad g_3>0$

→ **PDE for height *h***

outside facets

Outline of microsc. derivation of μ

[Change in energy of step by adding or removing a point defect]

[DM, Kohn, 2006]

*i*th step moves: $\eta_i \rightarrow \eta_i + (\delta\eta)$

$$\mu_i \propto \frac{\delta_\eta [U\ \delta s]}{(\delta s)(\delta R)}$$

energy per unit step length

step arc length

distance vertical to step

$$\Rightarrow \mu_i = a^2 \left(\kappa_i U + \frac{1}{\xi_\eta} \partial_\eta U \right), \ \xi_\eta = |\partial_\eta \mathbf{r}|$$

step curvature $\rightarrow -\nabla \bullet \dfrac{\nabla h}{|\nabla h|}$

$$U = \gamma + U^{\text{int}}$$

step line tension $= \boldsymbol{g_1 a}$

step interactions

Nearest-neighbor interactions; strength $\boldsymbol{g_3 a}$

$$U^{\text{int}} = \frac{\boldsymbol{g_3 a}}{3} \left[\mathsf{V}\left(m_i, \frac{R_i}{\lambda}, \frac{R_{i+1}}{\lambda} \right) + \mathsf{V}\left(m_{i-1}, \frac{R_i}{\lambda}, \frac{R_{i-1}}{\lambda} \right) \right]$$

step density

Formula for μ by $\eta_{i+1} - \eta_i \rightarrow 0$

□

Relaxation PDE outside facets (minimal model)

$$h_t = -\mathrm{div}\left\{\mathbf{M}\cdot\nabla\left[g_1\,\mathrm{div}\left(\frac{\nabla h}{|\nabla h|}\right) + g_3\,\mathrm{div}\left(|\nabla h|\nabla h\right)\right]\right\}; \qquad h = h(x,y,t)$$

Cartesian coordinates :

$$\mathbf{M}_{(x,y)}(\nabla h) \propto \frac{h_x^2}{|\nabla h|^2}\begin{pmatrix} \frac{1}{1+Q|\nabla h|} + \frac{h_y^2}{h_x^2} & -\frac{Q|\nabla h|}{1+Q|\nabla h|}\frac{h_y}{h_x} \\ -\frac{Q|\nabla h|}{1+Q|\nabla h|}\frac{h_y}{h_x} & \frac{h_y^2/h_x^2}{1+Q|\nabla h|} + 1 \end{pmatrix}$$

In previous theories for 2D, M is a scalar:

$$\mathrm{M} \propto \frac{1}{1+\mathrm{Q}|\nabla h|} \qquad \left(\mathrm{Q} = \frac{2D_s}{ka}\right)$$

[Shenoy et al., 2005; DM et al., 2006]

Extension : Effect of electric field

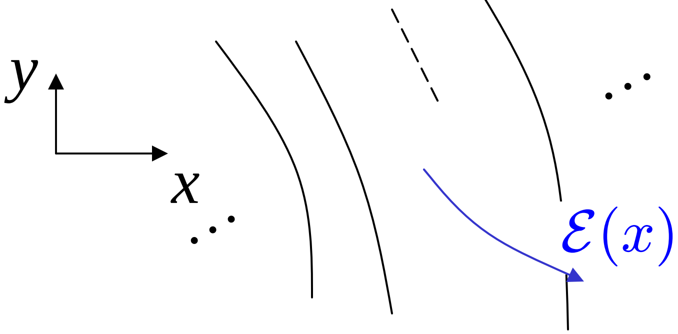
[Quah, DM, 2010]

- Microscale: On ith terrace,

$$\underbrace{D_s\Delta\rho_i - \mathbf{v}\cdot\nabla\rho_i = \partial_t\rho_i} \approx 0, \qquad \mathbf{v}(x) = \frac{D_s(Z^*e)\mathcal{E}(x)}{T}$$

Drift velocity

[Fu *et al*,1996]



- Macroscale: Evolution (relaxation) laws:

$$\begin{cases} h_t = -\mathrm{div}\mathbf{J} \\[2ex] \mathbf{J} = -\dfrac{D_s\rho_s}{T}\mathbf{M}(\nabla h)\cdot\left[\nabla\mu - \mathbf{v}(x)\dfrac{T}{D_s}\left(1+\dfrac{\mu}{T}\right)\right]; \\[2ex] \mu = -\mathrm{div}\left(g_1\dfrac{\nabla h}{|\nabla h|} + g_3|\nabla h|\nabla h\right); \; x \in \mathbf{R}^2 \end{cases}$$

Numerics by Finite Element Method

[Bonito, Nochetto, Quah, DM, 2009]

$$\mu^n = \mu(\cdot, n\tau_n),\ h^n = h(\cdot, n\tau_n)$$

Semi-Implicit Euler scheme

$$\text{PDE splitting}\left\{\begin{array}{l} \iint \mu^{n+1}\phi - \left(\dfrac{g_1}{|\nabla h^n| + \tilde{\varepsilon}} + g_3 |\nabla h^n|\right)\nabla h^{n+1}\cdot\nabla\phi = 0 \\[2ex] \iint \dfrac{h^{n+1} - h^n}{\tau_n}\phi + \mathbf{M}(\nabla h^n; \tilde{\varepsilon})\nabla\mu^{n+1}\cdot\nabla\phi = 0 \end{array}\right.$$

Regularization

To suppress facets : $g_1 = 0$

Set $Q >> 1$ (**ADL** regime)

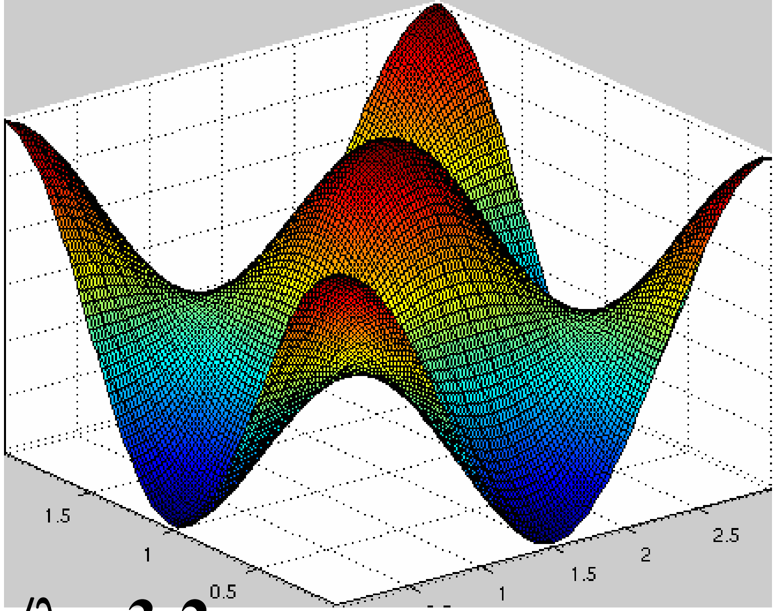
Alternate numerical method: Fourier series for height profile

[Shenoy, Ramasubramaniam, Ramanarayan, Tambe, Chan, Chason, 2004;
Chan, Ramasubramaniam, Shenoy, Chason, 2004]

Numerical Simulations: Bi-periodic profiles

[Bonito, Nochetto, Quah, DM, 2009]

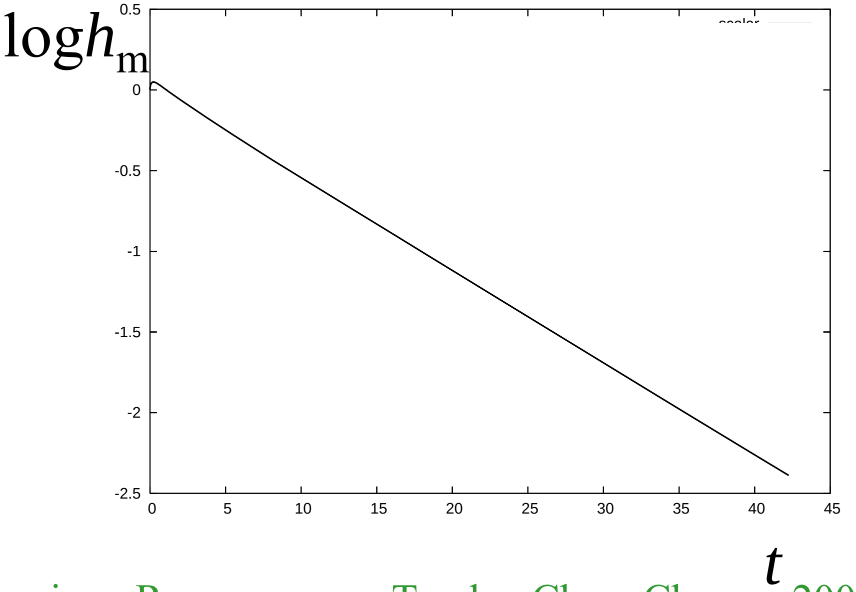
h



Scalar

M

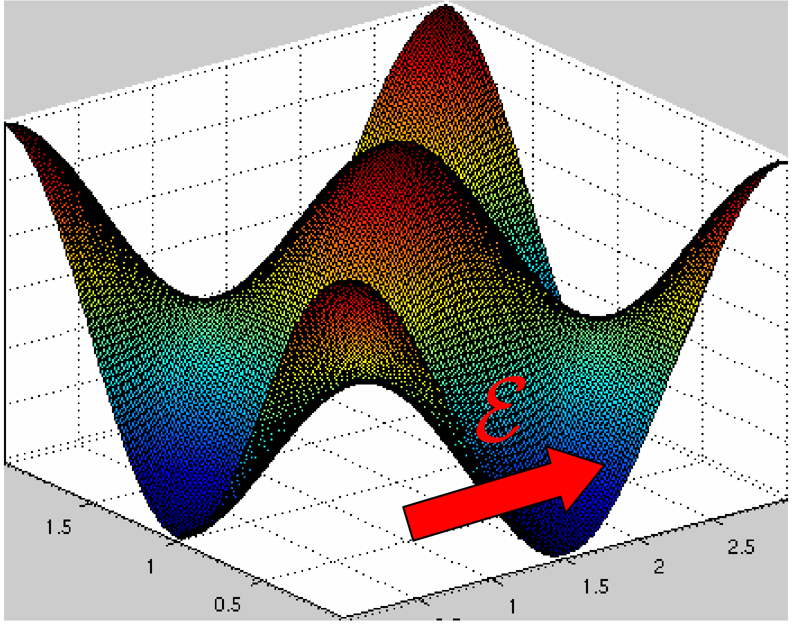
$\lambda_y / \lambda_x = 3:2$

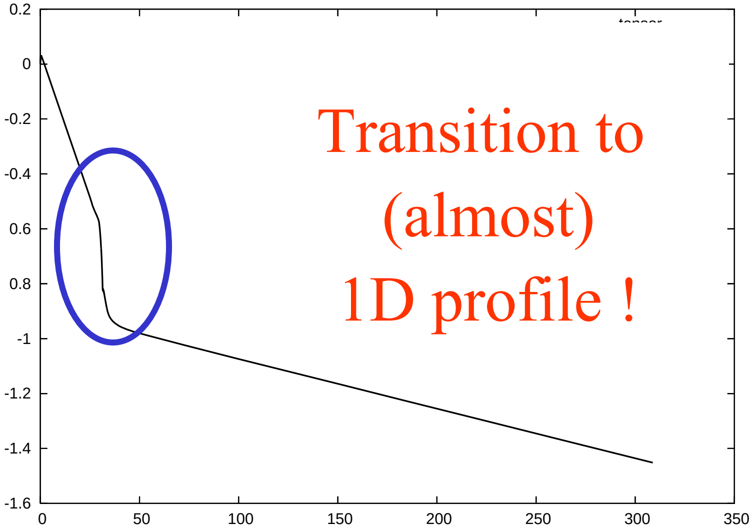


[Shenoy, Ramasubramaniam, Ramanarayan, Tambe, Chan, Chason, 2004]

Tensor

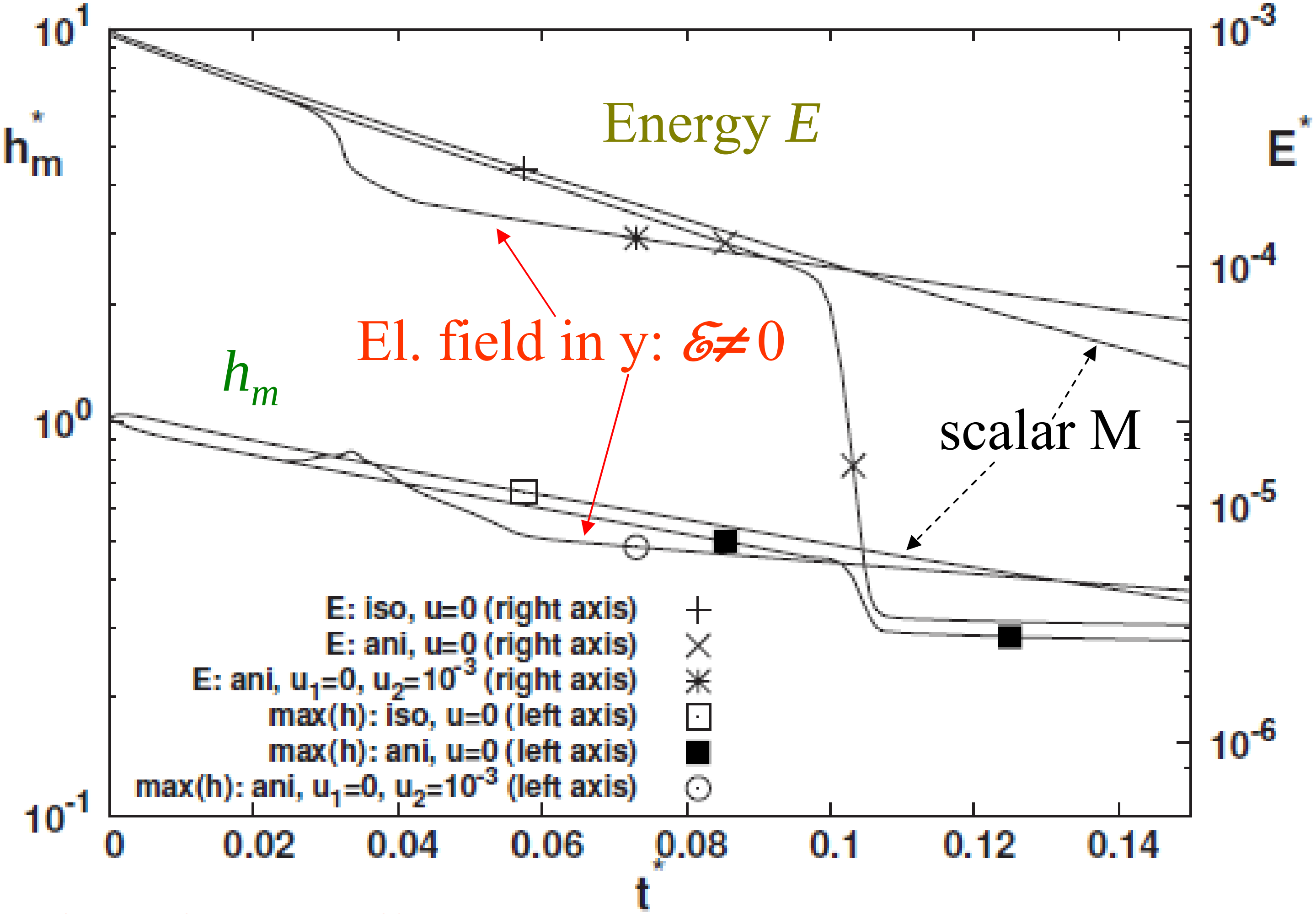
M





Transition to
(almost)
1D profile !

Interplay of anisotropy and **electric field**: Height peak and energy



Energy E

El. field in y: $\mathcal{E} \neq 0$

h_m

scalar M

Analytical understanding ?

On decay laws in surface relaxation

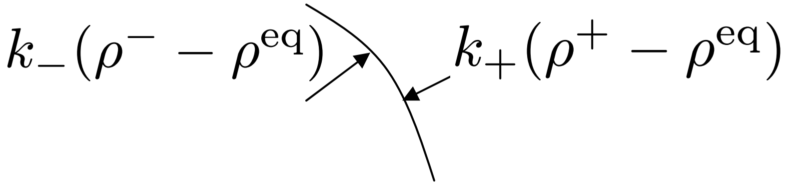
- Numerical results for *nonzero but very small line tension* (g_1) are similar for various (incl. non-sinusoidal) initial data
  [Bonito, Nochetto, Quah, DM, 2009]
- The variational formulation inherent to FEM is not consistent with steps near facets, when $g_1 \neq 0$ (**Lecture III**)
- For appreciable line tension, numerical studies via Fourier series for **scalar *M*** *w/* ADL kins. report decay depending on init. data, g_1/g_3.
  For Cu(001), $g_1/g_3 \approx 1$, initial sinusoidal profile [Shenoy *et al*., 2004] :
  $$h_{peak}(t) \sim c\sqrt{t^* - t}$$
  For initial non-sinusoidal profile [Shenoy et al., 2004] : "propensity" for *inverse linear* time decay; no theoretical argument todate.
- Self-similar solutions have been observed numerically (**Lec. III**):eg,
  1D periodic profiles [Israeli, Kandel, 2000; Odisharia, 2006] ;
  radial setting [Israeli, Kandel, 1999; DM, Fok, Aziz, Stone, 2006]

Extensions of macroscopic theory (via limit of step flow)

Asymmetric barriers of attachment/detachment

Microscale

[**Ehrlich**, Hudda, 1966; **Schwoebel**, Shipsey, 1966]



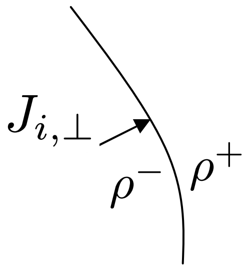
Macroscale

Fick’s law has

$$k = 2\left(\frac{1}{k_+} + \frac{1}{k_-}\right)^{-1}$$

Step transparency

Microscale [Ozdemir, Zangwill, 1992; Chalmers, Tsao, Gossard, 1992; Tanaka, Bartelt, Umbach, Tromp, Blakeley, 1997; Métois, Stoyanov, 1999; Pierre-Louis, Métois, 2004; Sato, Uwaha, Saito, 2000; Sato, 2007]



Attachment-detachment law at ith step with permeability:

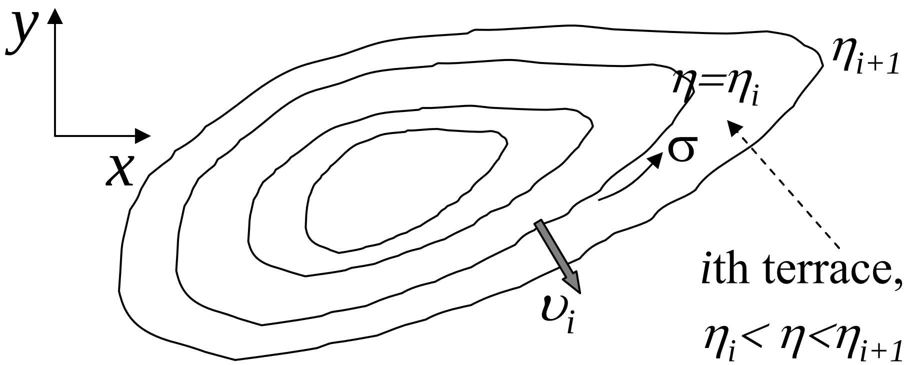
$$J_{i,\perp} = k(\rho^- - \rho_i^{\mathrm{eq}}) + p\,(\rho^- - \rho^+) \qquad (p > 0)$$

Macroscale [**1D**: E, Yip, 2001; Israeli, Kandel, 1999; **2D**: Quah, Young, DM, 2008]

Fick’s law: $k \Rightarrow k + 2p$

Step edge & anisotropic terrace diffusion

Microscale



- Step **velocity**:

$$\upsilon_i = (up\ \text{flux})_\perp - (down\ \text{flux})_\perp + \boxed{\partial_s\left[D_e\,\partial_s\left(\frac{\mu_i(\sigma)}{k_B T}\right)\right]}$$

Edge diffusion

- Adatom **flux** on *i*th terrace

$$\boldsymbol{J}_i^t(\boldsymbol{r},t) = -\boldsymbol{D}_T\cdot\nabla\rho_i,\quad \text{div}(\boldsymbol{D}_T\cdot\nabla\rho_i) = \frac{\partial\rho_i}{\partial t} \approx 0;\quad \eta_i < \eta < \eta_{i+1}$$

Tensor

Step edge & anisotropic terrace diffusion (cont)

Macroscale [Quah, DM, 2008]

Fick’s law:

$$\mathbf{J} = \mathbf{J}^T + \mathbf{J}^e \propto - \overset{\mathbf{M}}{\boxed{\begin{pmatrix} \dfrac{D_{\eta\eta}/k_B T}{1+Q\,|\nabla h|} & \dfrac{D_{\eta\sigma}/k_B T}{1+Q\,|\nabla h|} \\[2ex] \dfrac{D_{\sigma\eta}/k_B T}{1+Q\,|\nabla h|} & \dfrac{1}{k_B T}\,\dfrac{D_{\sigma\sigma}+\widetilde{D}\,|\nabla h|}{1+Q\,|\nabla h|} + \dfrac{D_e}{\rho_s}\,|\nabla h| \end{pmatrix}}} \cdot \begin{pmatrix} \partial_\perp \mu \\ \partial_{/\!/} \mu \end{pmatrix};$$

$$Q := \frac{2D_{\eta\eta}}{ka}, \qquad \widetilde{D} := \frac{2\det(\mathbf{D}_T)}{ka}, \quad \mathbf{D}_T =: \begin{pmatrix} D_{\eta\eta} & D_{\eta\sigma} \\ D_{\sigma\eta} & D_{\sigma\sigma} \end{pmatrix}$$

Take-home messages/Challenges

- Continuum elements: *mass conservation, Fick's law, chem. potential.*

  PDE consistent with step flow away from facets

- Homogenization of **1D** models inspired by *reconstructed surfaces*

  Effective material parameters; analogy with *composites*

2D ?

$$J = \begin{pmatrix} J_\perp \\ J_{//} \end{pmatrix} = -\frac{\mathcal{D}_{\mathrm{av}}\rho_{\mathrm{s}}}{k_B T}\begin{pmatrix}(1+Qm)^{-1} & 0 \\ 0 & 1\end{pmatrix}\begin{pmatrix}\partial_\perp \mu \\ \partial_{//}\mu\end{pmatrix}; \qquad Q = \frac{2\mathcal{D}_{\mathrm{av}}}{k_{\mathrm{av}}\varepsilon},\ m = |\nabla h|$$

- **2D** anisotropy in surface mobility under conventional step kinetics

  FEM numerics: **topographic transition**; understanding ?

- Relation of PDE solutions to experimental data (relaxing profiles) ?

Lec. III: Continuum theory near facets