The Dynamics of Epitaxy

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Outline

- Burton-Frank-Cabrera Model for solid-vapor surfaces

- The Dynamics of steps:
  - Step-step interactions and step bunching
  - meandering and stability

- Role of deposition in surface roughness

References

- A. Pimpinelli and J. Villian, *Physics of Crystal Growth*, Cambridge 1998.

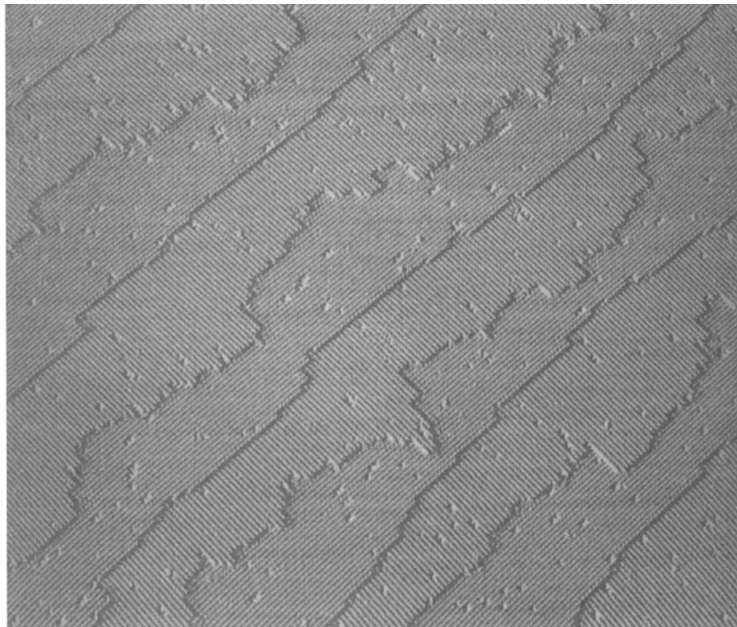- P. Noziéres, *Shape and Growth of Crystals*, in Solids Far from Equilibrium, Ed. C. Goodrèche, Cambridge 1992.
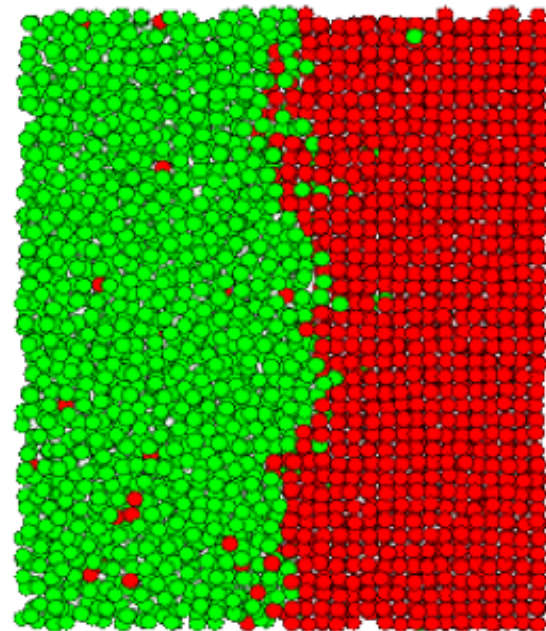
Solid-Vapor Surfaces at T<T$_R$

Step

Kink

Vacancy
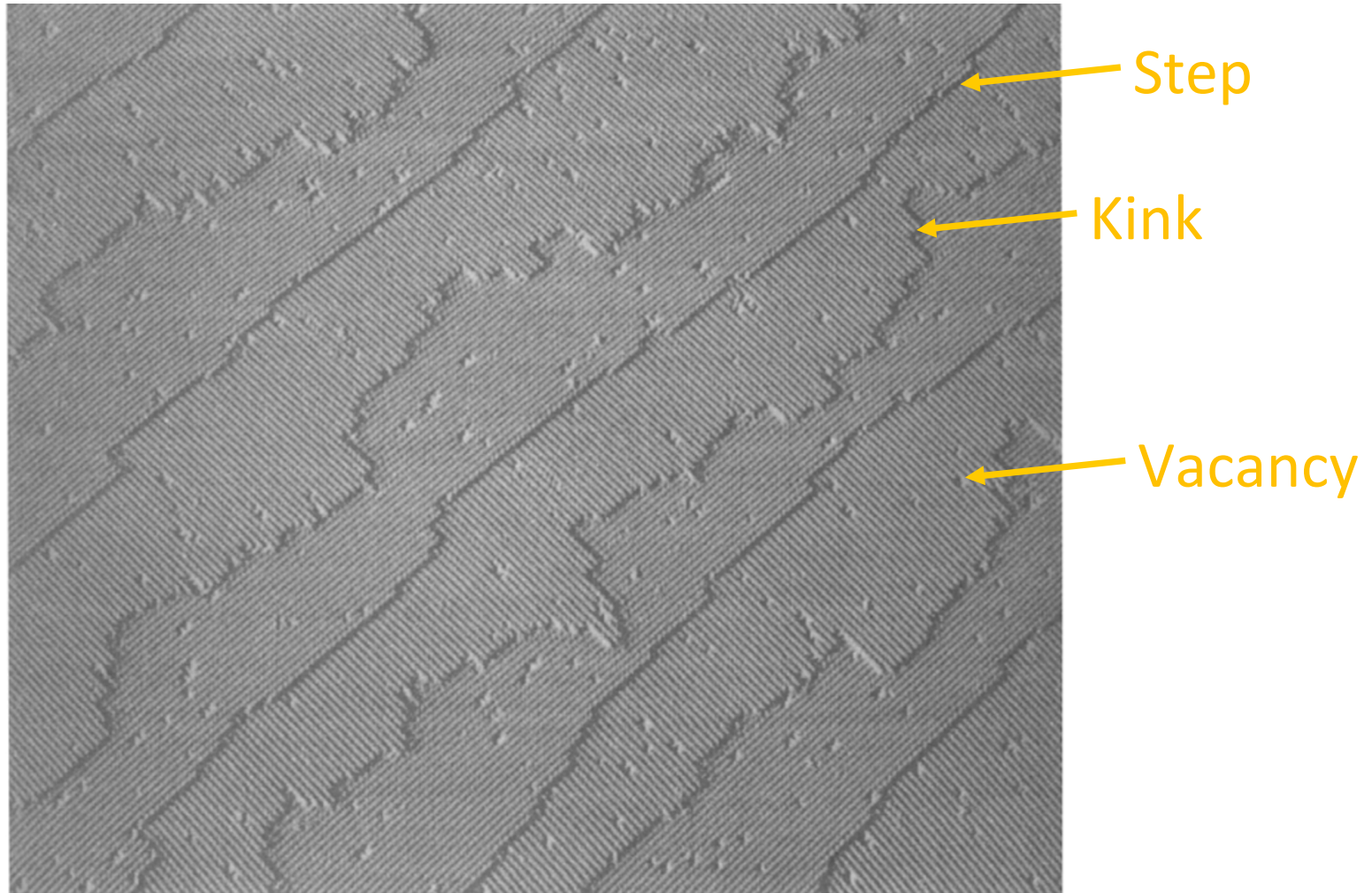
(Swartzendruber, B.S., et al. (1990) Phys. Rev. Lett. 65, 1913.)

Step Energy

- The step energy, β is positive
- It is very approximately, $\beta \sim \gamma a$
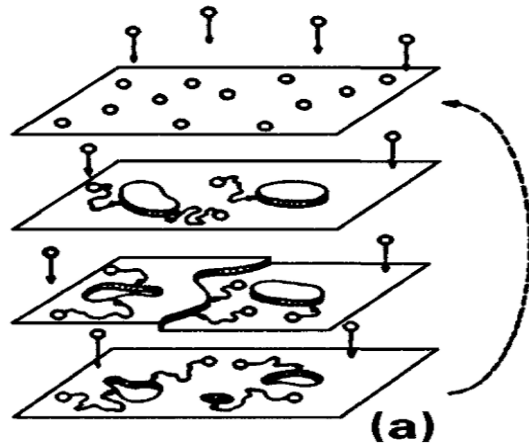- It goes to zero at the roughening transition

Below T_R

Above T_R

(M. Asta)

Growth Modes During MBE

Surface diffusion possible

Step flow

Island nucleation
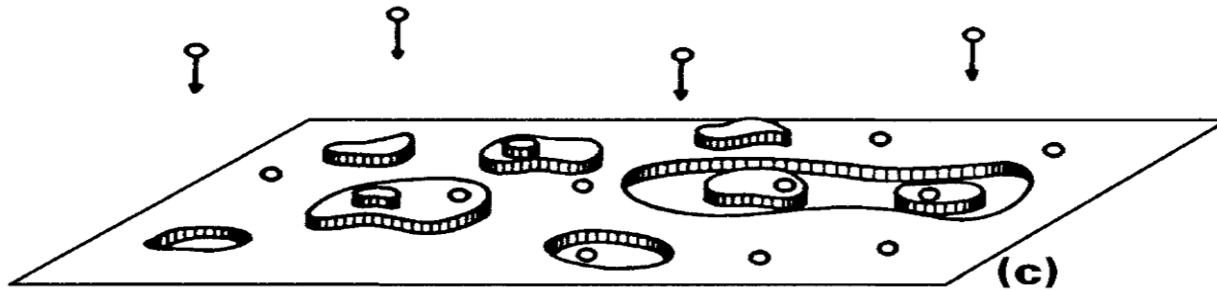
Surface diffusion not possible

(A. Pimpinelli and J. Villian)
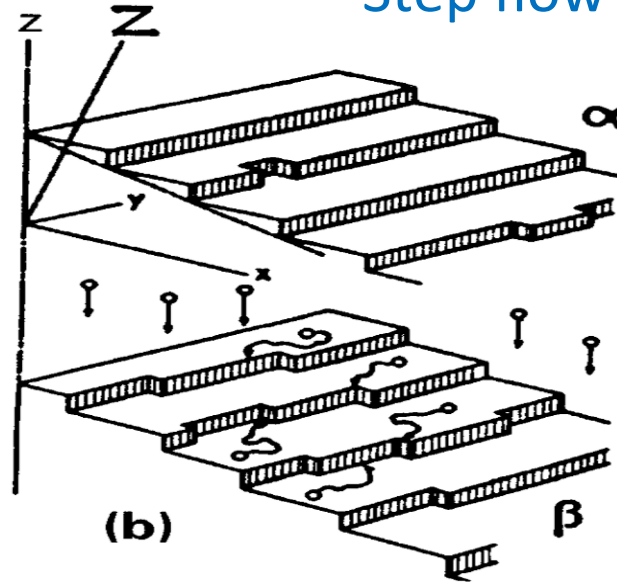
Defects Can Act as Sources of Steps
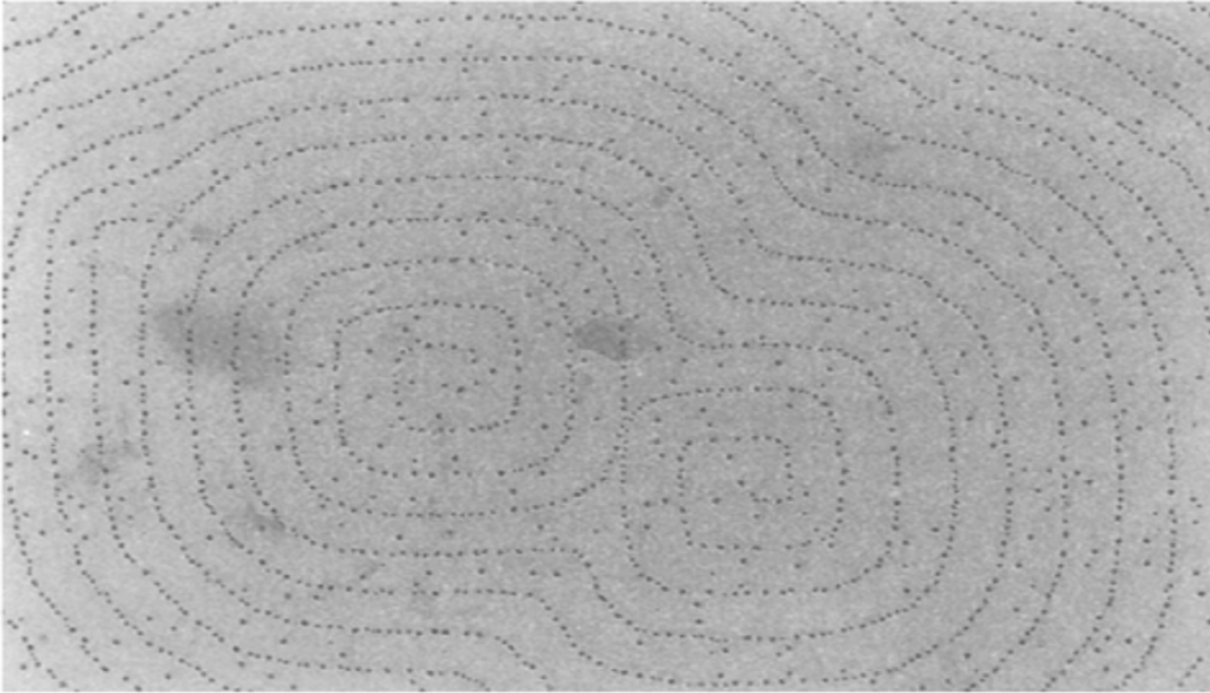
Growth from screw dislocations that intersect the surface

(Heyraud & Metois, CRMC2, Marseille)

Other defects are common in semiconductor systems: stacking faults and twins

(Gamalski, et al. 2013)

Step motion: BFC model

- Infinite vicinal surface
- Parallel straight steps

Deposition

(a)

F

Incorporation at step

Evaporation (b)

$1/\tau_v$

$$\frac{\partial \rho}{\partial t} = D_s \frac{\partial^2 \rho}{\partial x^2} - \frac{1}{\tau_v}\rho + F$$

Surface diffusion
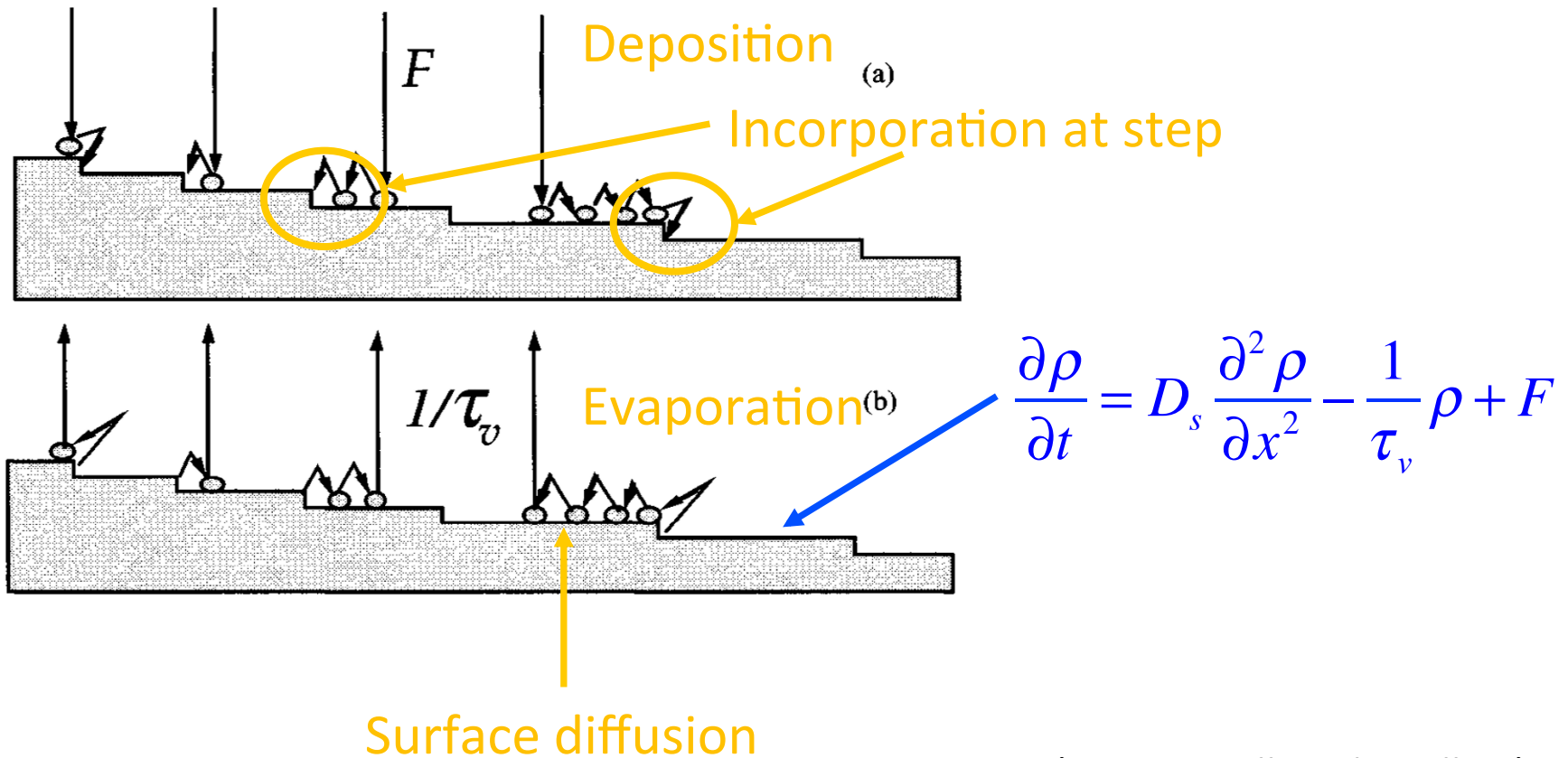
(A. Pimpinelli and J. Villian)

Step motion: BFC model

First approximation:
- Emission and adsorption of adatoms is fast
- Thus, local equilibrium is present at a step edge

$$\rho_e(L(t))$$

$$\frac{\partial \rho}{\partial t} = D_s \frac{\partial^2 \rho}{\partial x^2} - \frac{1}{\tau_v}\rho + F$$

Quasistationary Approximation

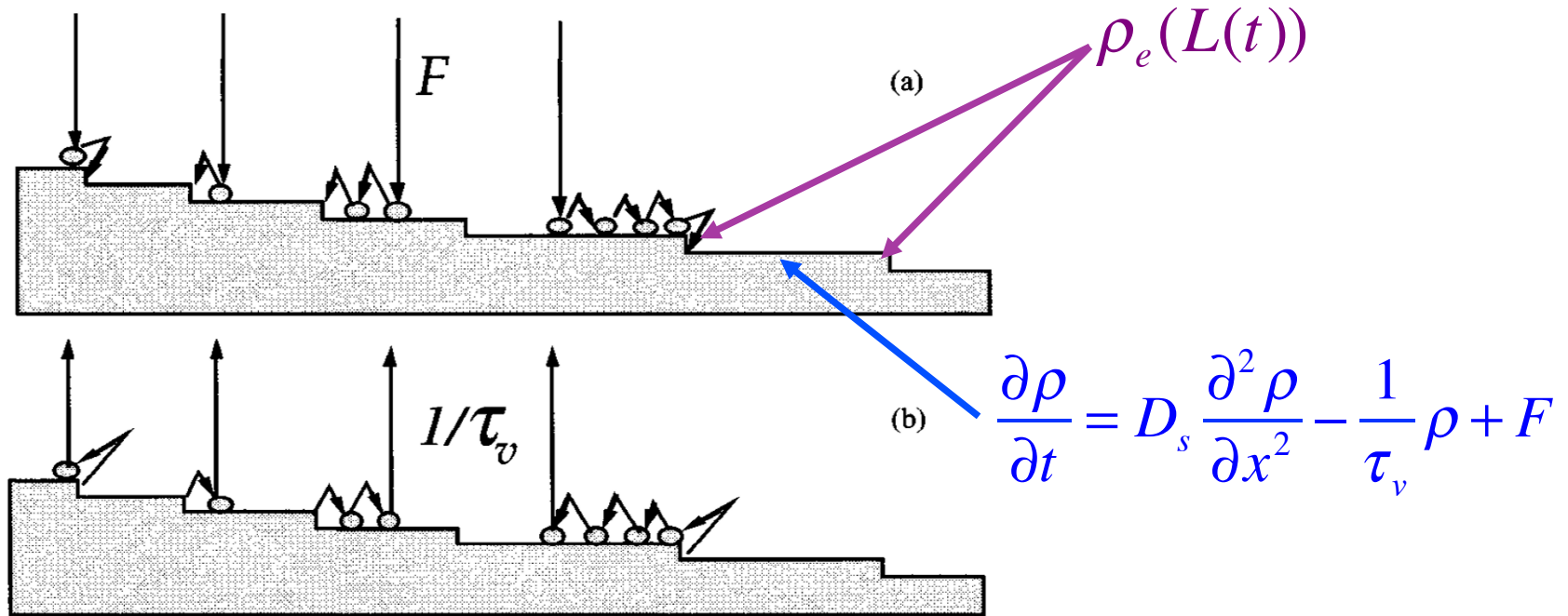- Assume that the diffusion field relaxes to its steady state value very quickly:

$$\frac{1}{D_s}\frac{\partial \rho}{\partial t} = 0 = \frac{\partial^2 \rho}{\partial x^2} - \frac{1}{D_s \tau_v}\rho + \frac{F}{D_s}$$

- With the solution:

$$\rho(x) = F\tau_v + \frac{\cosh(\kappa x)}{\cosh(\kappa l / 2)}(\rho_e - F\tau_v) \quad \text{where} \quad \kappa = (D_s \tau_v)^{-1/2}$$

where the origin has been located at the center of a terrace

Deposition
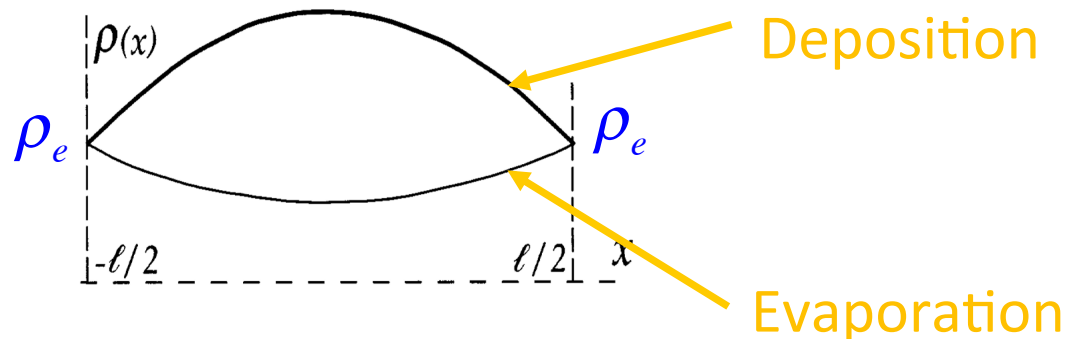
Evaporation

The Limit of No Evaporation

- This is case in certain MBE growth situations (Ge or Si)
- Residence time on the surface is long $\tau_v \to \infty$
- This implies that the screening distance is very small $\kappa\ell \ll 1$

$$\rho(x) = \rho_e + F\tau_v\kappa^2\left(\frac{\ell^2}{8} - \frac{x^2}{2}\right)$$

Deposition

Evaporation
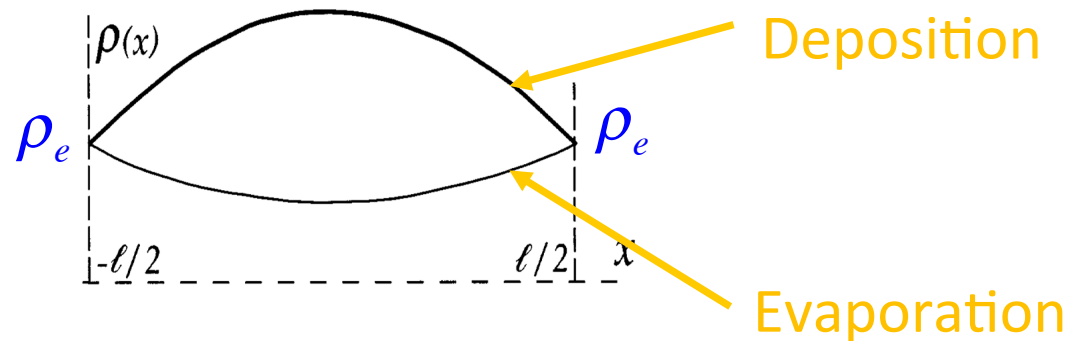
Step Velocity

- Mass balance at a step edge:
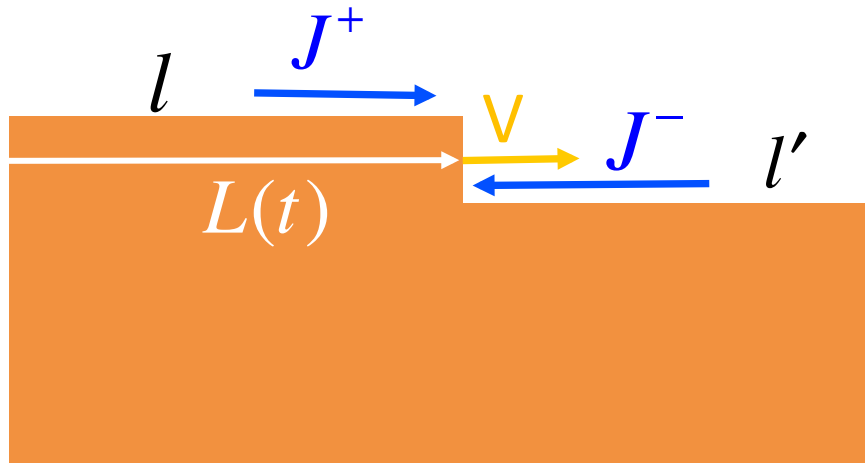
$$\frac{dL}{dt} = V = \Omega \left(D_s \frac{\partial \rho}{\partial x}\bigg|_{L^+} - D_s \frac{\partial \rho}{\partial x}\bigg|_{L^-} \right)$$

Thus:

$$V = D_s \left(F\tau_v - \rho_e \right) \kappa \left[\tanh(\kappa l / 2) + \tanh(\kappa l' / 2) \right]$$

Stable Step Flow Growth (Nucleation)
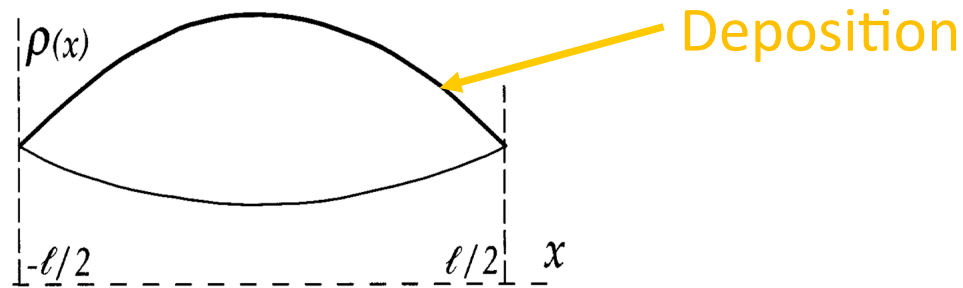
- If the adatom supersaturation is sufficiently large and there atoms do not have time to attach to a step, nucleation of an island can occur on a terrace

- The diffusion length depends on the atom flux,

$$l_s = \sqrt{D_s \tau_a} \sim (D_s / F)^{1/6}$$

- Then if $l_s \gg l$ then nucleation does not occur and step flow takes place

Ehrlich-Schwoebel Barrier

- Previously we assumed that the attachment and emission of atoms at a step edge is fast, thus

$$\mu(L) = \mu_e(\rho) \Rightarrow \rho(L) = \rho_e$$

- However, there can be to barriers to atom motion at the step edges:
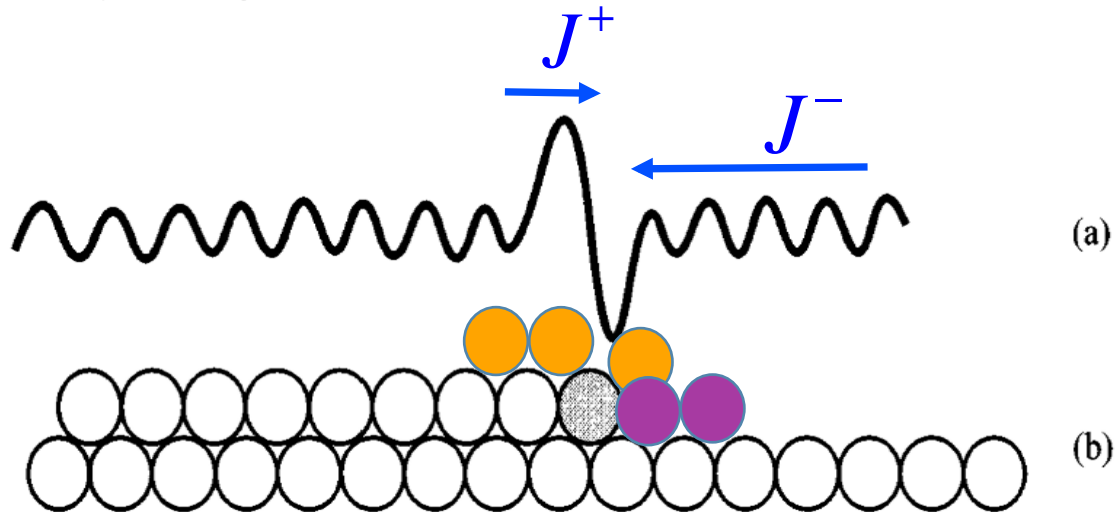
Ehrlich-Schwoebel Barrier

$$J^{+\rightarrow-} = \alpha^+ \exp(-\mu_a / kT)$$

$$J^{-\rightarrow+} = \alpha^+ \exp[(\mu^+ - \mu_e + \mu_a)/kT]$$

$$J_T^{+\rightarrow-} = J^{+\rightarrow-} - J^{-\rightarrow+-}$$

$J^{-\rightarrow+}$

$J^{+\rightarrow-}$

μ_a

$\mu^+ - \mu_e$

μ_e

Upper Terrace

Lower Terrace

Energy

Reaction Coordinate (Not Distance)

Total Flux From Upper to Lower Terrace

$$J^{+\to-} = \alpha^+ \exp(-\mu_a/kT) \qquad J^{-\to+} = \alpha^+ \exp[-(\mu^+ - \mu_e + \mu_a)/kT]$$

Since the total flux going from the upper to lower terrace is:
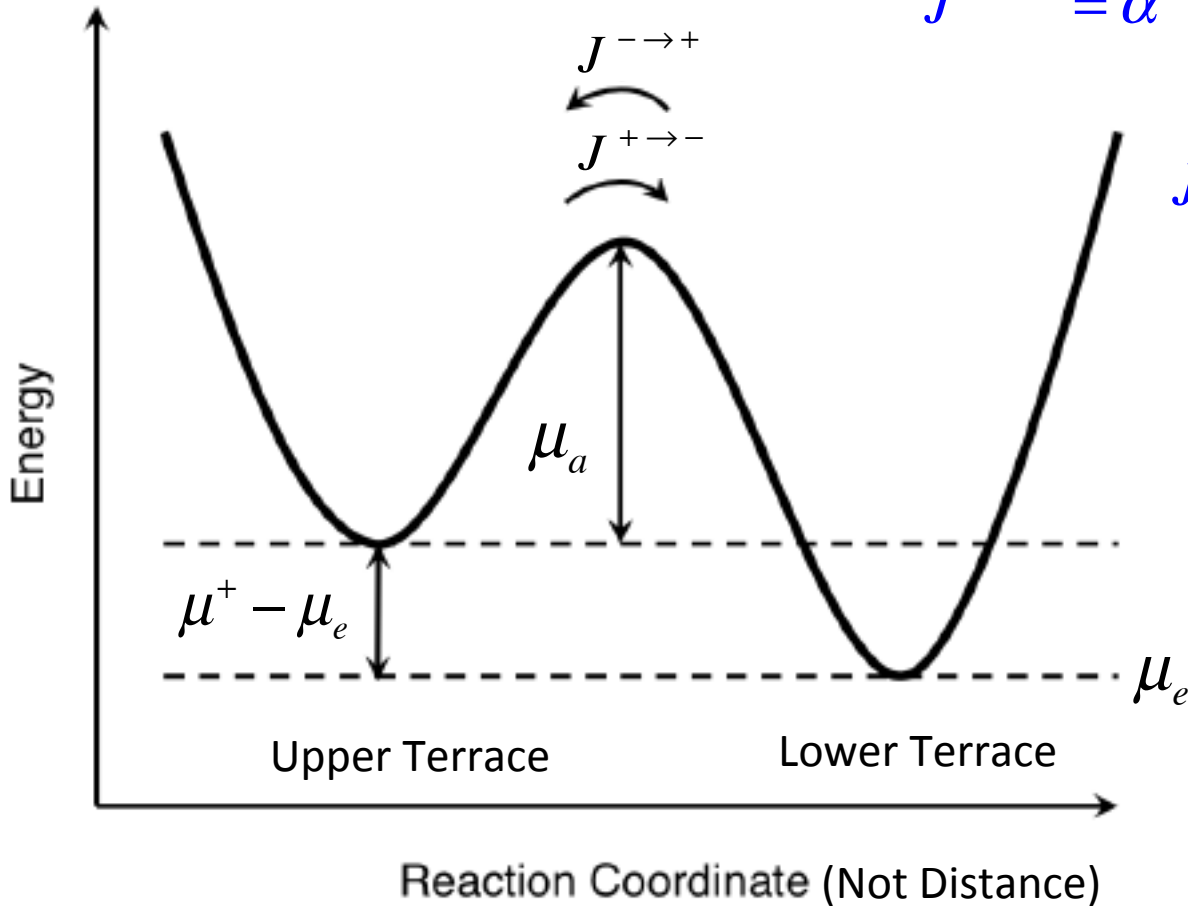
$$J_T^{+\to-} = J^{+\to-} - J^{-\to+}$$

Thus,

$$J_T^{+\to-} = \alpha^+ \exp(-\mu_a/kT)\left(1 - \exp[-(\mu^+ - \mu_e)/kT]\right)$$

If we assume a small driving force,

$$J_T^{+\to-} = \tilde{k}^+(\mu^+ - \mu_e)$$

Conclusions:
- The chemical potential at the step edge of the upper terrace is not equal to its equilibrium value
- The magnitude of the difference depends on the kinetic coefficient
- In unusual cases the kinetic coefficient can be infinity

Total Flux From Upper to Lower Terrace

Since the chemical potential is a function of the adatom density and assuming small changes from equilibrium

$$\mu^{+}(\rho) = \mu_e(\rho_e) + \frac{\partial \mu}{\partial \rho}(\rho - \rho_e)$$

Since,

$$J_T^{+ \rightarrow -} = \tilde{k}^{+}(\mu^{+} - \mu_e)$$

The flux can be expressed in terms of the adatom concentration:

$$J_T^{+ \rightarrow -} = k^{+}(\rho^{+} - \rho_e)$$

The flux of adatoms that is going over the step is supplied by diffusion from the upper step,

$$-D\frac{d\rho^{+}}{dx} = k^{+}(\rho^{+} - \rho_e)$$

Step motion: Erhlich-Schwoebel barrier

Note with an ES barrier k^+ is less than k^-

$$D\frac{d\rho^-}{dx} = k^-(\rho^- - \rho_e)$$

$$-D\frac{d\rho^+}{dx} = k^+(\rho^+ - \rho_e)$$

F

$1/\tau_v$

(b)

$$\frac{\partial \rho}{\partial t} = D_s \frac{\partial^2 \rho}{\partial x^2} - \frac{1}{\tau_v}\rho + F$$
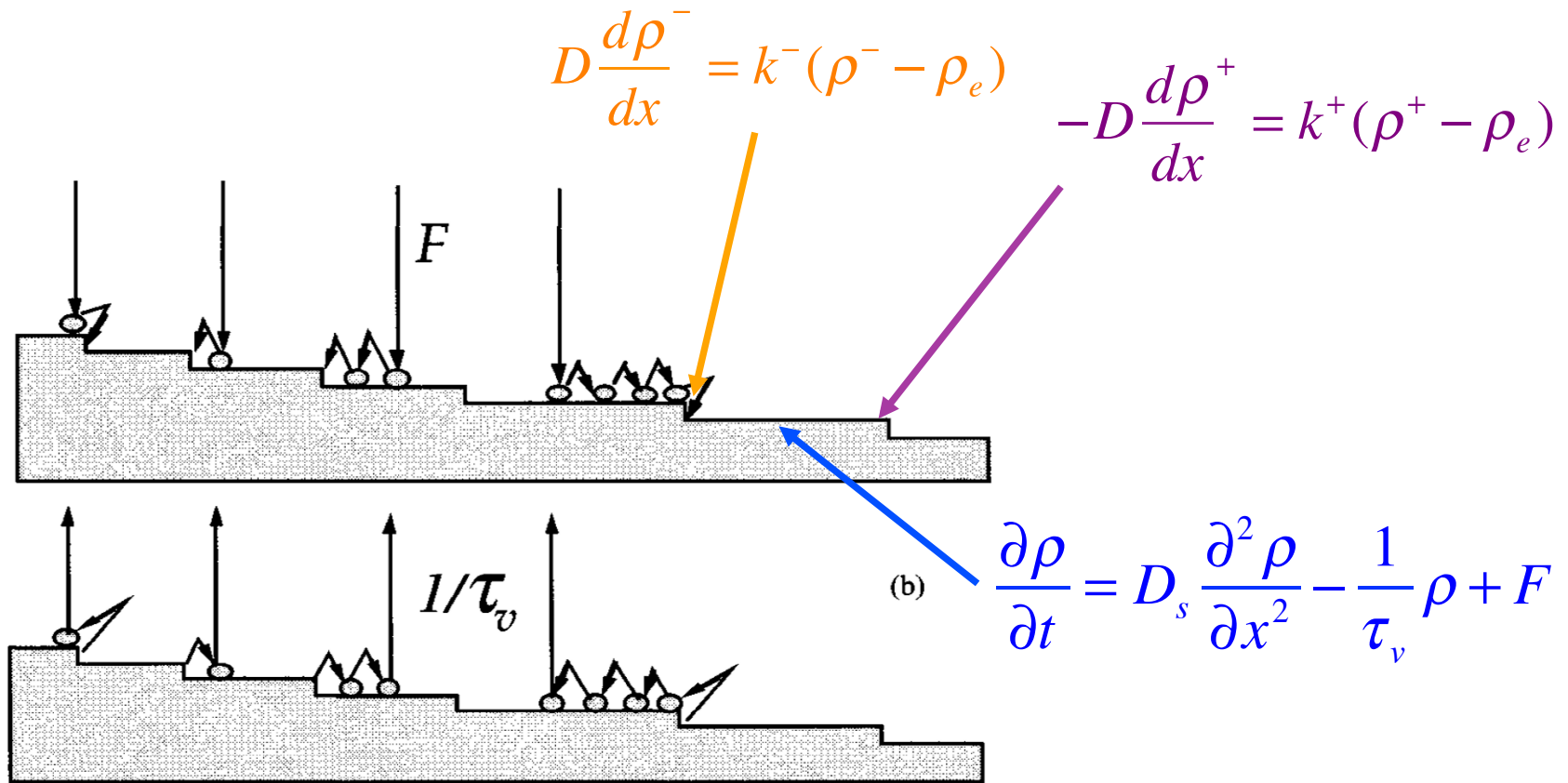
Step motion: Erhlich-Schwoebel barrier
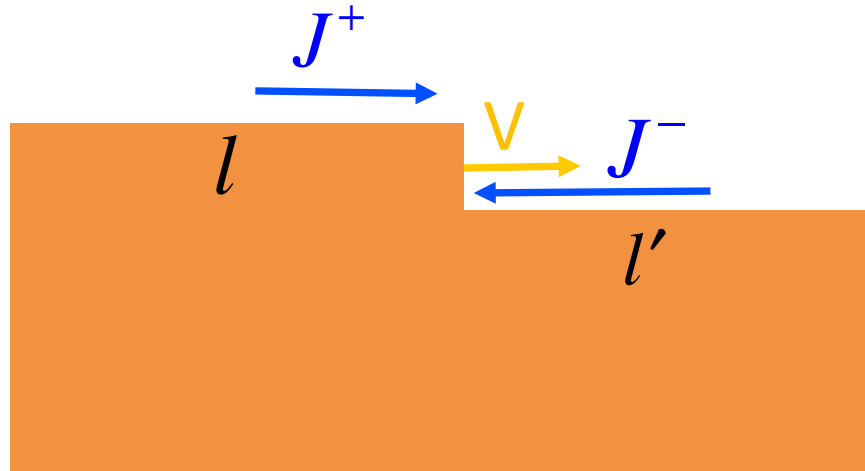
$$V = \Omega \left(D_s \left. \frac{\partial \rho}{\partial x} \right|_{L^+} - D_s \left. \frac{\partial \rho}{\partial x} \right|_{L^-} \right) = k^+ \rho^+ - k^- \rho^- - 2\rho_e$$

This equation can be used to couple the gradients and concentrations

Solutions to the Diffusion Problem

- Surface diffusion along a terrace: Pimpinelli and Villan (appendix)

- Nanowire with a catalyst containing a single cylindrical step, Golovin et al, JAP (2008) (bulk and surface diffusion)

- Growth from a liquid: Chernov JCG, 2004
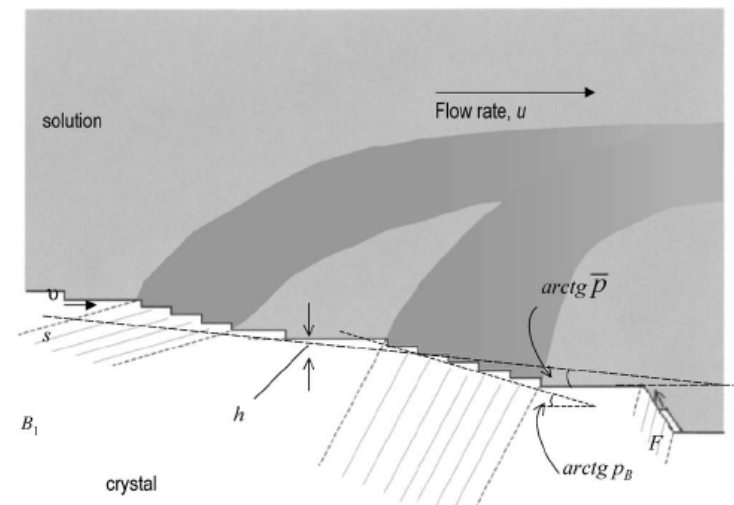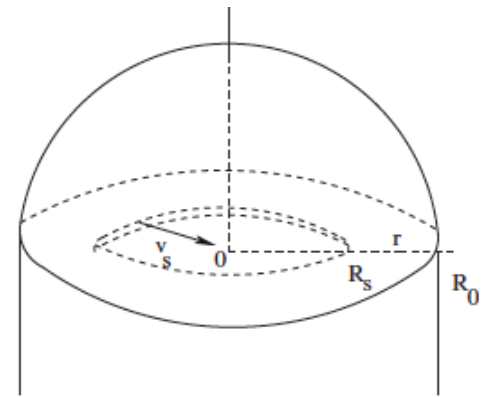
What Happens with More than Two Steps?

Is a train of straight steps stable to bunching?

Initial state

Step bunch

Final state
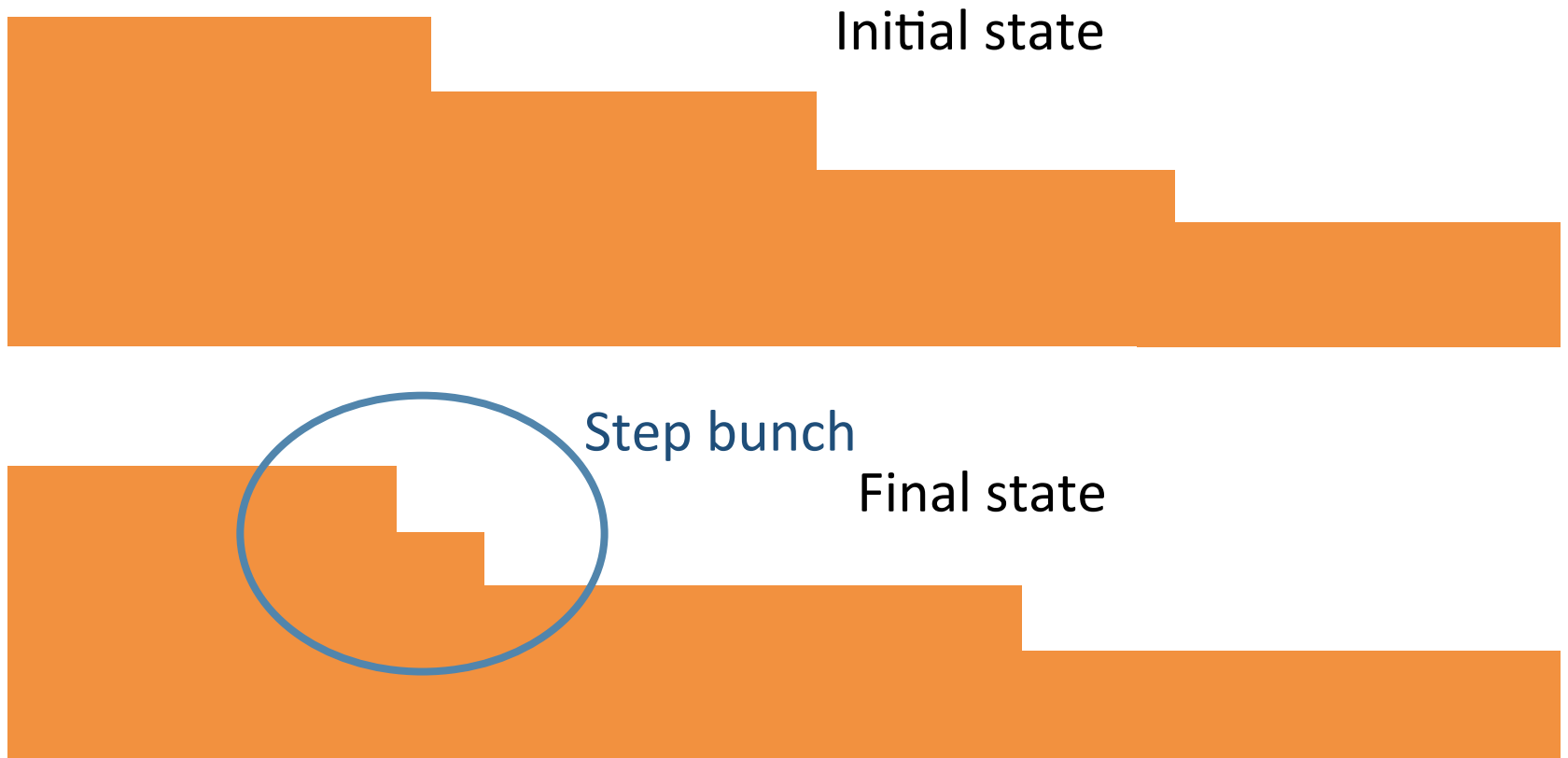
Examples: Erhlich-Schwoebel Barrier

Deposition : Terrace A is larger than the surrounding facets

final

Initial
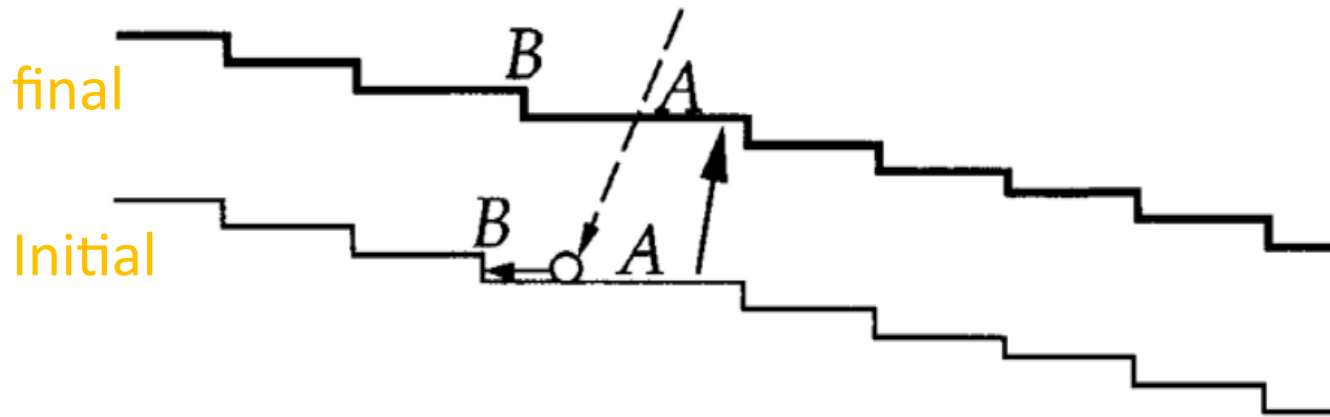
(A. Pimpinelli and J. Villian)

- Terrace A collects more atoms than other terrace and then feeds them to the step edge
- Due to the ES barrier most of the atoms feeding the step edge come from terrace A
- Thus the step at B moves faster and the size of terrace A decreases: ES barrier is stabilizing

Examples: Erhlich-Schwoebel barrier

Evaporation: Terrace A is larger than the surrounding facets
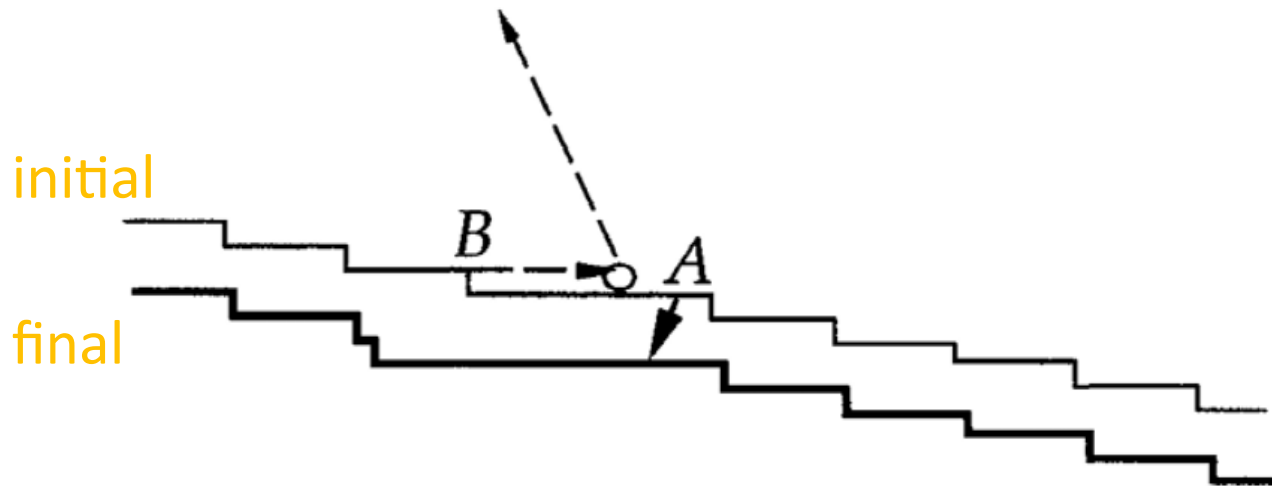
(A. Pimpinelli and J. Villian)

- Terrace A loses more atoms than other terraces
- So step a B recedes faster and due to the ES barrier most of the atoms feeding the evaporation from terrace A come from the motion of step B
- Thus the step a B recedes faster than other steps and the size of terrace A increases: ES barrier is destabilizing on evaporation

Example: Effects of Initial Size of Terraces

- Very long, singular facet during deposition
- No Erhlich-Schwoebel barrier

initial

(a)
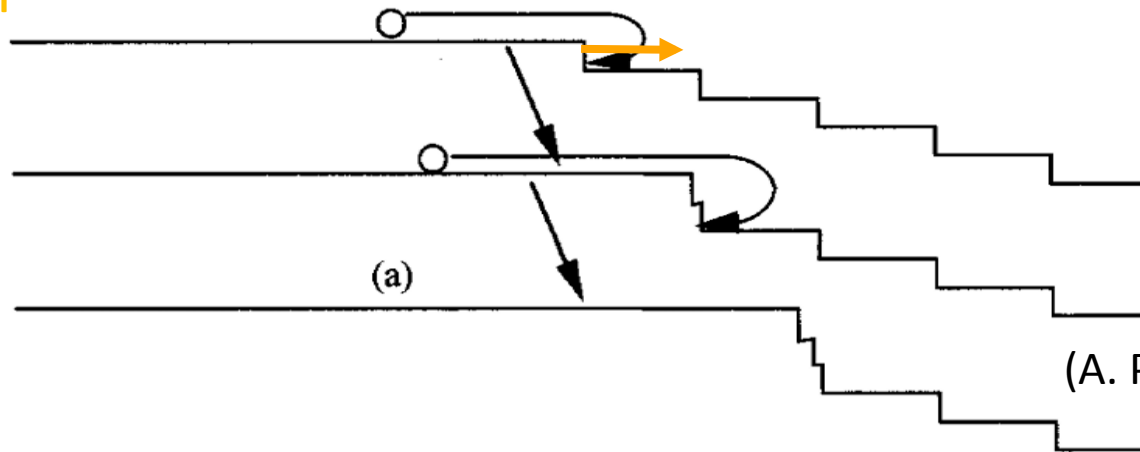
(A. Pimpinelli and J. Villian)

- Large facet collects more atoms than others
- These atoms are fed to the the steps closest to this facet
- Thus these steps move faster
- Result: Step bunching due to the initial large terrace

Example: Thermodynamically Unstable Surface Orientation, Herring Faceting

$$\left(T > T_R\right)$$

$$\gamma = \gamma_o\left(1 + \gamma_4\cos(4\theta)\right) \quad \gamma_4 = 0.3$$

$$\mu = \mu_o + V_m\left(\gamma + \frac{\partial^2\gamma}{\partial\theta^2}\right)\kappa$$

n θ

Metastable

Metastable

$$\left(\gamma + \frac{\partial^2\gamma}{\partial\theta^2}\right) = 0$$

$$\left(\gamma + \frac{\partial^2\gamma}{\partial\theta^2}\right) = 0$$
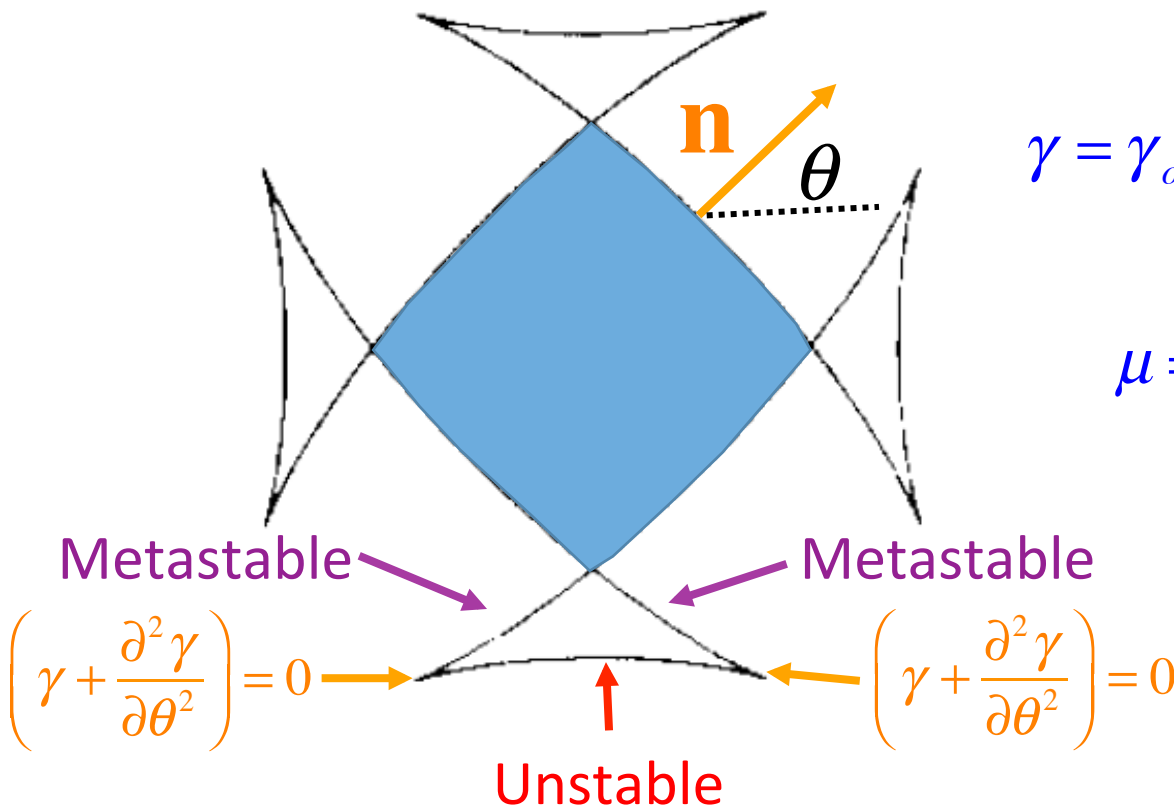
Unstable

(PWV, Coriell and McFadden, J. Cryst. Growth, 1984)

- Shape which gives constant chemical potential
- Convex region is the Wulff shape

Example: Thermodynamically Unstable Surface Orientation, Herring Faceting
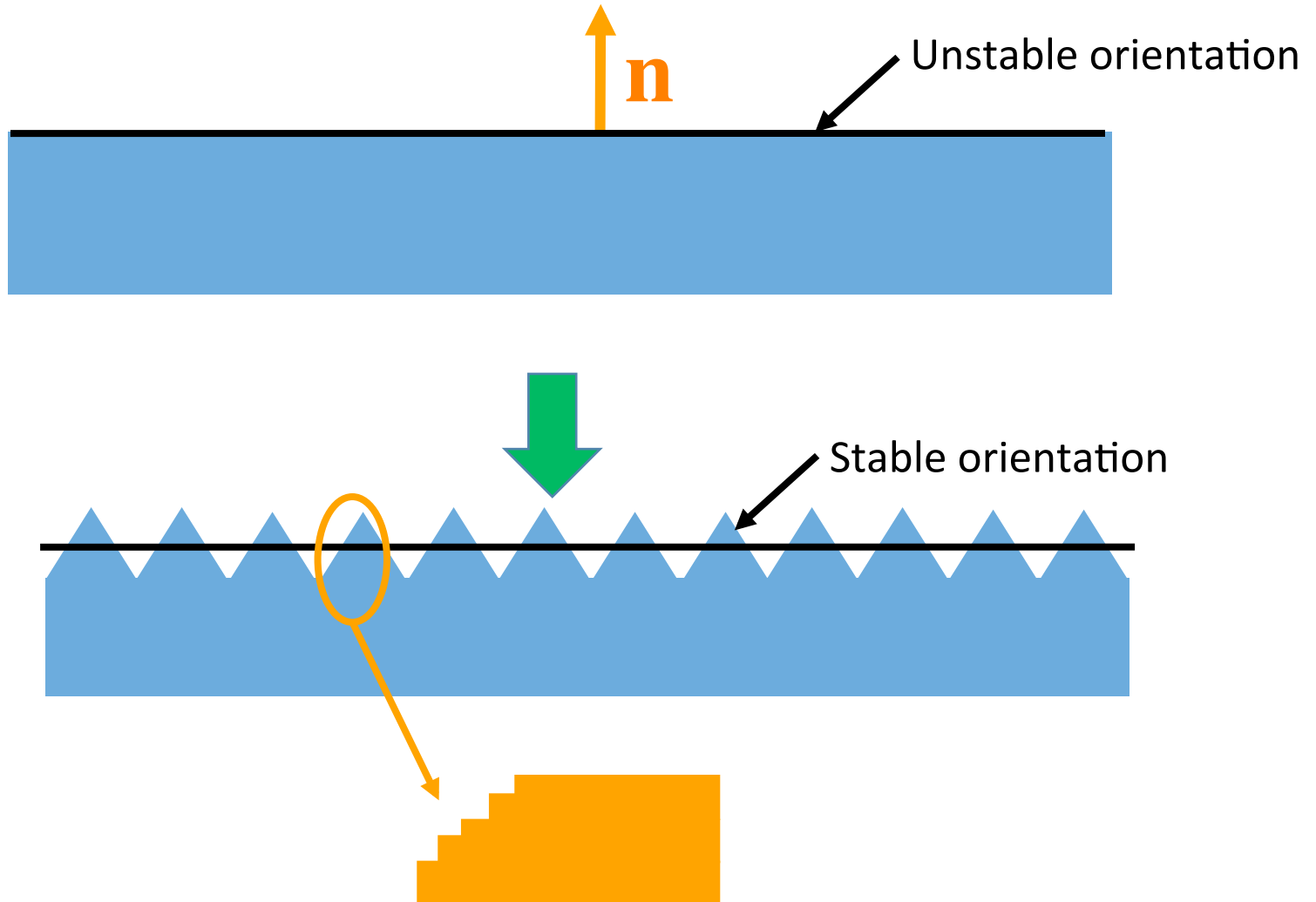
n

Unstable orientation

Stable orientation

What Sets the Smallest Spacing Between Steps?

- Only discuss two:
  - Surface stress
  - Entropic repulsion
- Other possibilities
  - Surface reconstructions (e.g. Si surface)
  - Composition

Surface Stress and Surface Energy

- The presence of a crystalline lattice allows us to differentiate between energy variations that involve deformation and those that involve growth

Deformation: surface stress f

Growth: surface energy γ
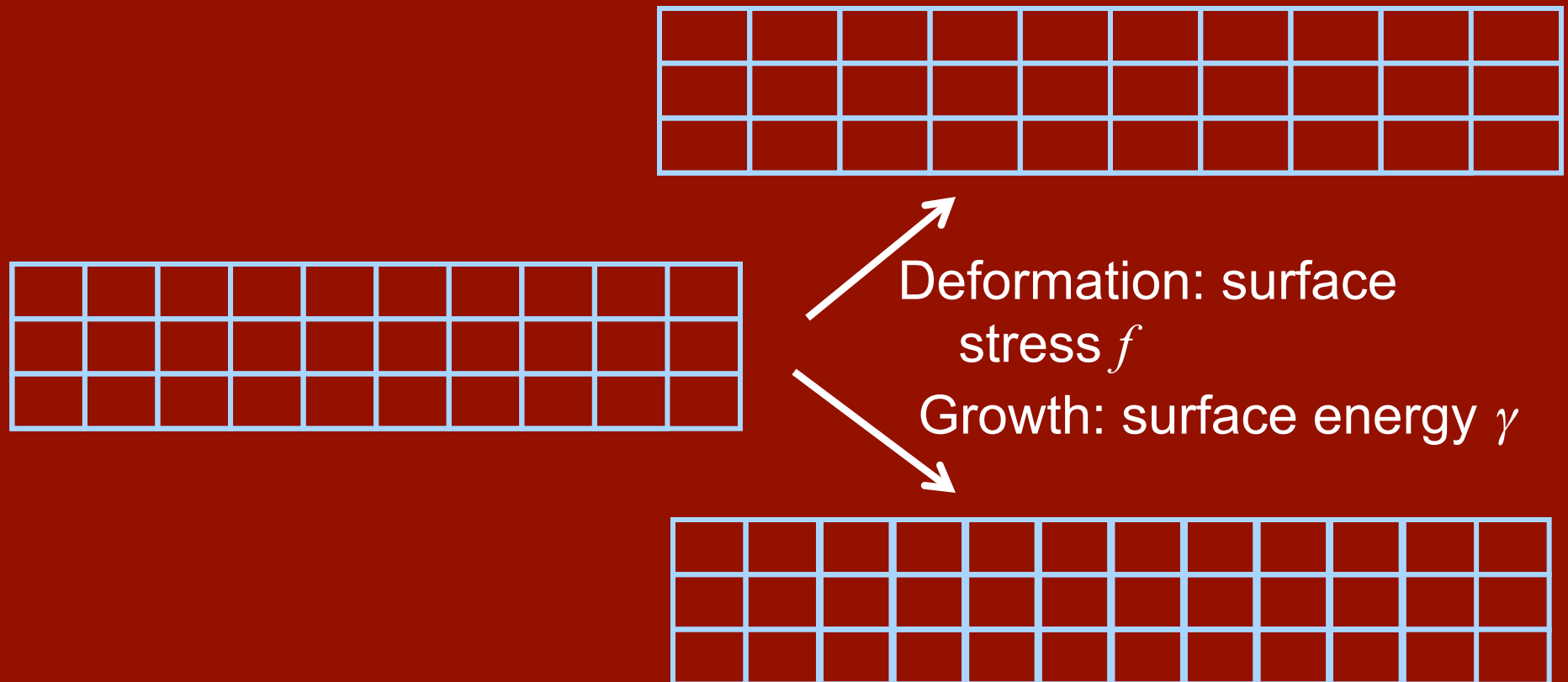
Surface Stress and Surface Energy

- For a fluid as soon as the block is deformed, atoms move from the bulk to the surface, thus $f = \gamma$

- Surface stress can be either positive or negative!

- Surface energy must be positive for stability. This prevents surfaces from spontaneously creating interfacial area

- Is there a relationship between surface stress and surface energy?

Surface Stress and Surface Energy

A_R
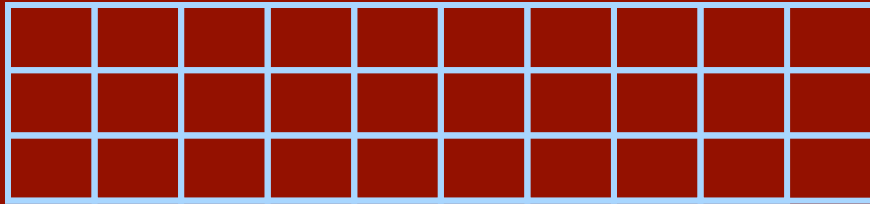
Surface energy per area in the reference state:

$$\gamma_R = \gamma_R(T, \mu_i, e_{ii})$$

z

x
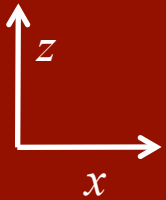
A
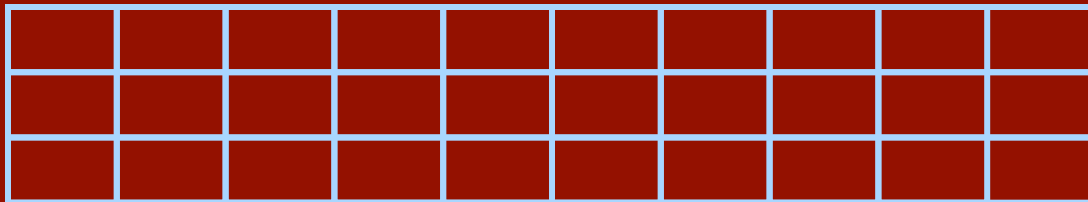
Surface energy per area in the physical state:

$$\gamma = \gamma(T, \mu_i, e_{ii})$$

$$A = A_R(1 + e_{ii}) \qquad e_{ii} = e_{xx} + e_{yy}$$

Surface Stress and Surface Energy

$$f_{ij} = \frac{\partial \gamma_R}{\partial e_{ij}}$$

Energy must be independent of reference state:

$$\gamma A = \gamma_R A_R$$

Using the expression for the area change:

$$A = A_R \left(1 + e_{ii}\right)$$

$$\gamma \left(1 + e_{ii}\right) = \gamma_R$$

Using this in the above:

$$f_{ij} = \frac{\partial \gamma}{\partial e_{ij}} + \gamma \delta_{ij} + O(e_{ij}^2)$$

Surface Stress Enters the Force Balance

- Surface stress is a force per unit length along the surface
- Consider a cylindrical surface, a portion of which is:

$$P\widehat{r} \qquad T_{\theta\theta}^{\alpha} = f$$

$$T_{rr}^{\alpha}$$

$$f \qquad\qquad f$$

$$R$$

$$r$$

$$\theta$$

$$\hat{x}$$
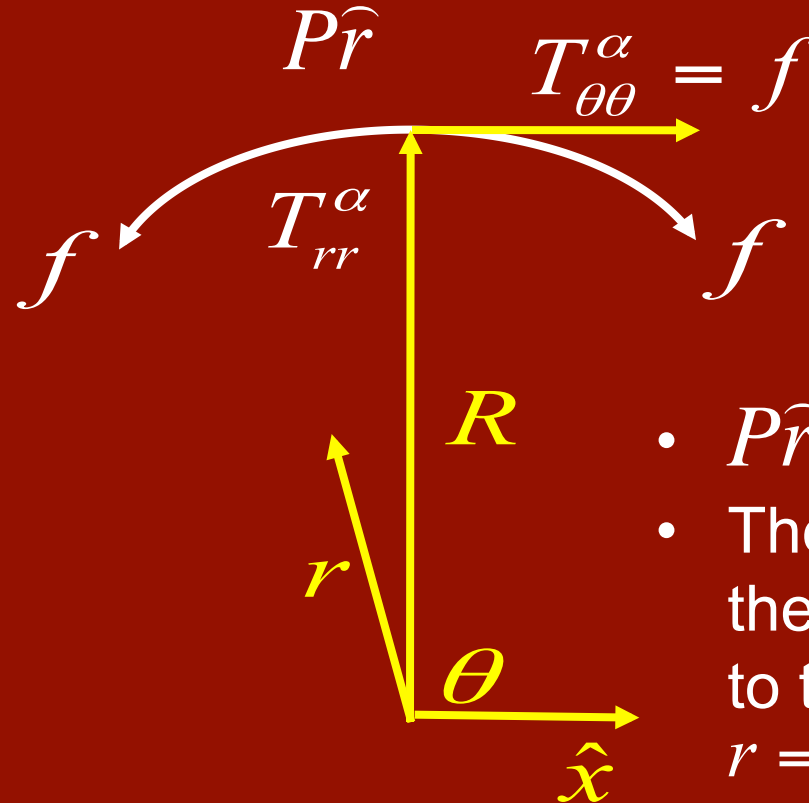
- $P\widehat{r} \neq T_{rr}^{\alpha}$
- There is a jump in the force tangential to the interface at $r = R$

Surface Stress Enters the Force Balance

For a smooth surface, the force balance is:

$$\mathbf{T}\mathbf{n} - P\mathbf{n} = \nabla_s \bullet \mathbf{f}$$

Surface stress has no effect at a planar surface, with constant **f**

For curved surfaces, e.g. spherical surface, and **f** dilatational

$$\mathbf{T}\mathbf{n} - P\mathbf{n} = 2f / R$$

Surface Stress

- In most cases, the magnitude of the surface stress is on the order of the surface energy

- Using the equations for the jump in the stress, the stress generated by a typical surface stress with a 100 nm diameter wire equal to putting the entire weight of a garbage truck on your fingernail

- Using a Lagrangian representation of the area,

$$f_{ij} = \frac{\partial \gamma}{\partial \hat{e}_{ij}} \qquad (\hat{e}_{ij} \text{ is the surface strain})$$

- Letting $f_{ij} = f \delta_{ij}$ (true for any surface with inversion symmetry) and integrating (to first order in strain)

$$\gamma = \gamma_o + f \delta_{ij} \hat{e}_{ij}$$

Surface Stress

- Thus the surface energy depends on the surface stress as

$$\gamma = \gamma_o + f\hat{e}_{ii}$$

- So as the surface strain changes the surface energy changes. It can increase or decrease depending on the sign of f

- This can be important in many semiconductor surfaces, e.g. Ge (001)

Consider a Surface With a Step

Surface is no longer smooth, so the previous result for the effects of stress at the surface does not hold

$$\mathbf{F} = \mathbf{g}\delta'(x)$$
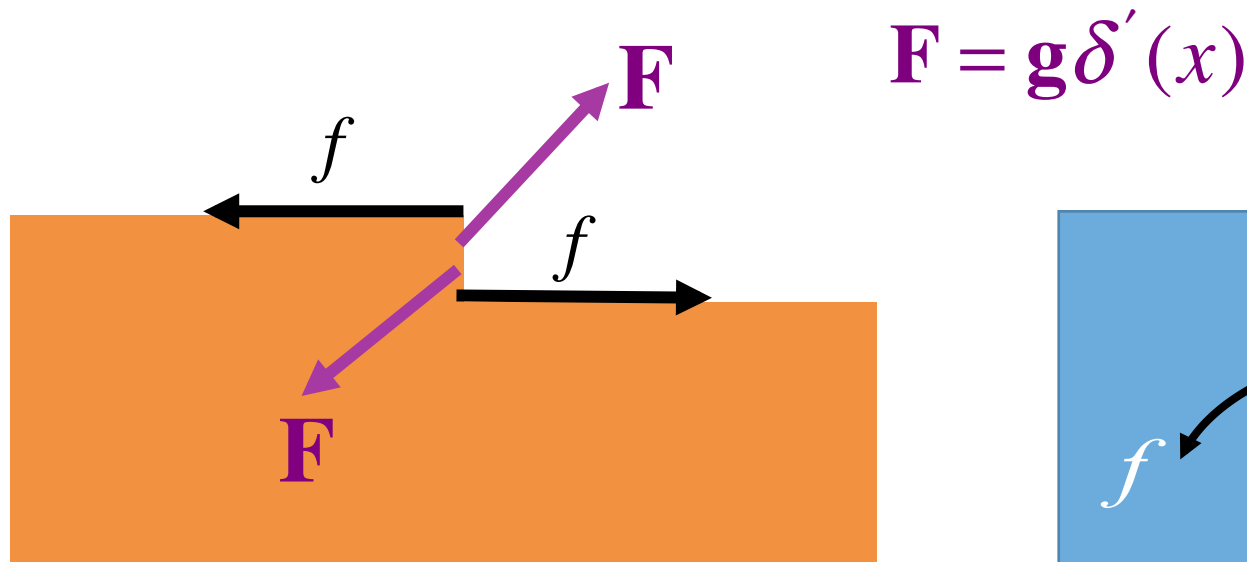
A step produces a long-ranged strain field given by a force dipole located at the step edge
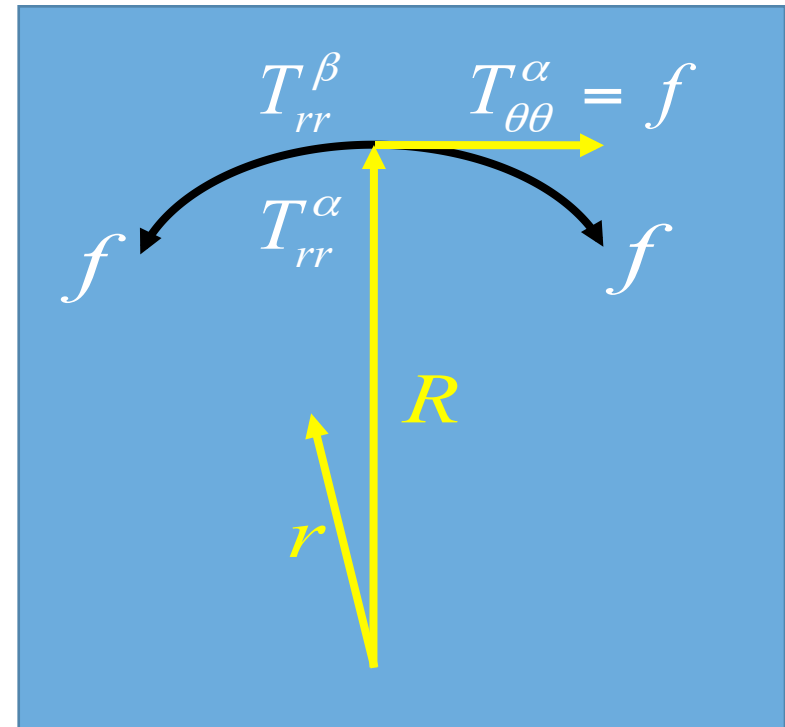
Stress Field due to a Step

- Sufficiently close to the step the field is not dipolar
- The component of the force along the surface induces an expansion
- The component of the force normal to the surface induces a torque
- The force dipole induces a long-range strain field ~ $1/d^2$
- Consider two steps,

$$u_{i,j} = u_{i,j}^{(1)} + u_{i,j}^{(2)} \quad T_{ij} = T_{ij}^{(1)} + T_{ij}^{(2)}$$

- Using the expression for the elastic energy.

$$W = \frac{1}{2}\int T_{ij}E_{ij}\,dV$$

and elastic equilibrium conditions,

$$W = -\frac{1}{2}\int T_{ij}n_i u_j\,dx = -\frac{1}{2}\int F_j u_j\,dx$$

Interaction Energy Between Steps

- The interaction energy,

$$\Delta W_{12} = g_i^{(2)} u_{i,x}^{(1)}(x^{(2)}) = g_i^{(1)} u_{i,x}^{(2)}(x^{(1)})$$

- For an elastically isotropic solid along the surface:

$$u_i(x) = -\frac{2(1-v^2)}{\pi E}\frac{g_i}{x}$$

- Thus,

$$\Delta W_{12} = \frac{2(1-v^2)}{\pi E}\frac{g_i^{(1)} g_i^{(2)}}{d^2}$$

- The sign depends on the dot product of the dipole moments, hence the signs of the two steps

Interaction Energy Between Steps

- For two steps of the same direction:

  the force is repulsive
- For two steps of opposite direction:

  the force can be either attractive or repulsive
- The force goes as $1/d^2$

What Happens with More than Two Steps?
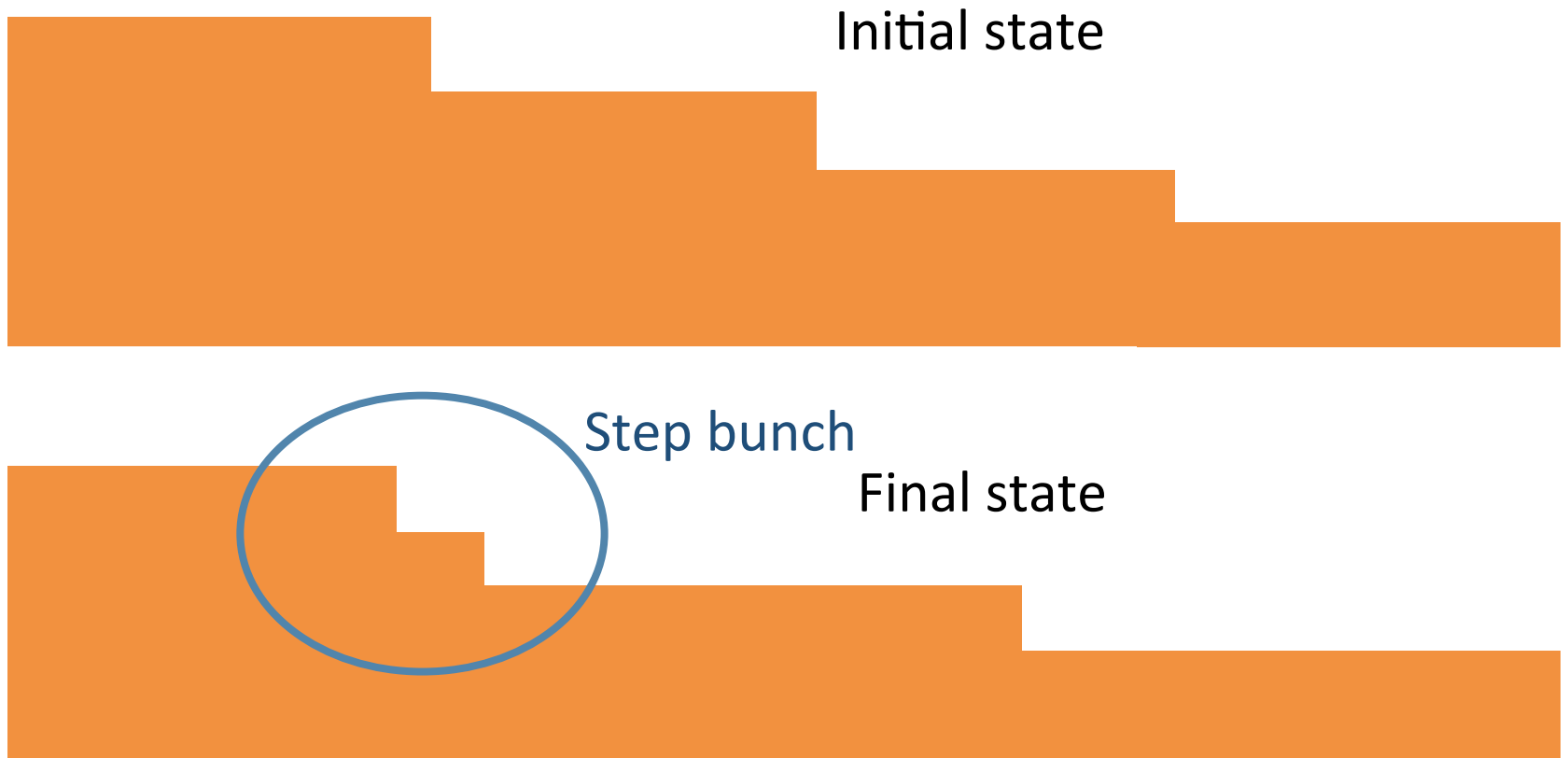
Is a train of straight steps stable to bunching?

Initial state

Step bunch

Final state

What Sets the Smallest Spacing Between Steps?

- Only discuss two:
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- Other possibilities
    - Surface reconstructions (e.g. Si surface)
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Step-Step Interactions: Entropy

- Steps have kinks

- Thus, it is possible to consider the fluctuations of a step edge like a vibrating string

- Calculate the energy change associated with an increase in length of the step and ascribe this to thermal fluctuations

- The step is confined to live between two neighboring steps

- Gruber and Mullins ca. 1960
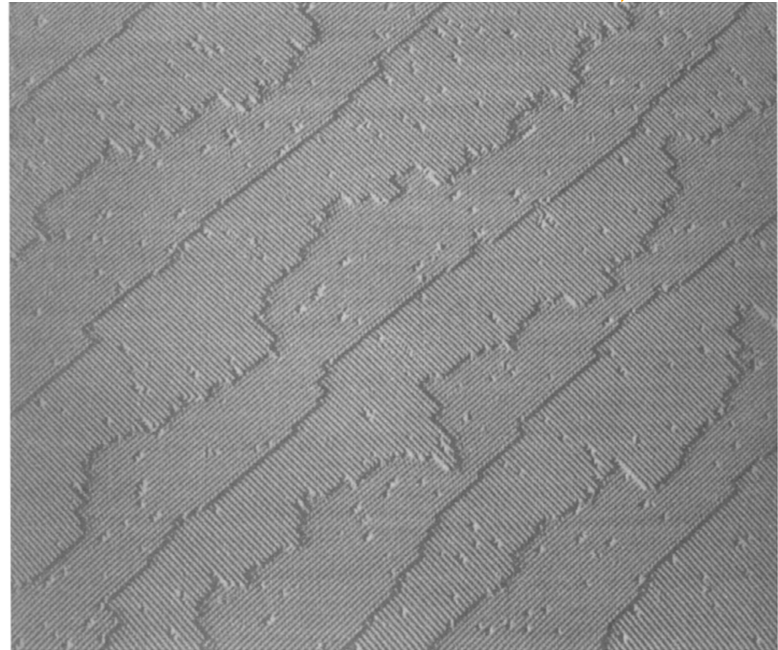
Complicated calculation, consider a simple qualitative argument

Entropy of a Fluctuating Step
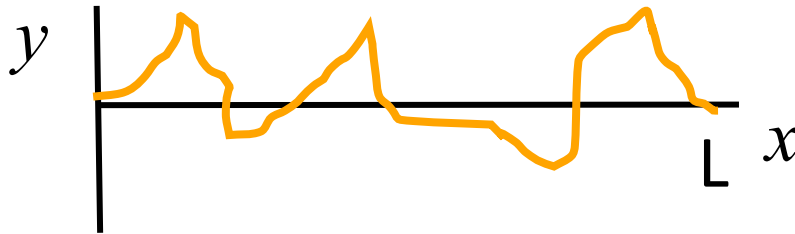
- Expand in Fourier series:

$$y(x) = \sum_k a_k \exp(ikx)$$

- The energy of the string increases, since it is not straight,

$$E = \sum_k L\beta k^2 a_k^2 / 2 \qquad \left(ds = (1 + (y_x)^2)^{1/2} \approx \frac{1}{2}(y_x)^2 \right)$$

- Each mode carries an energy $k_B T/2$,

$$\left\langle a_k^2 \right\rangle = \frac{k_B T}{L\beta k^2}$$

Entropy of a Fluctuating Step

- The mean square displacement is,

$$\left\langle x^2 \right\rangle = \sum_k \left\langle a_k^2 \right\rangle = \frac{1}{2\pi} \int_0^\infty \frac{k_b T}{\beta k^2} dk$$

- Diverges for small k, or large wavelength
- *The mean square displacement must be less than d*
- Long wavelength modes are cut off up to k_c

$$\left\langle x^2 \right\rangle \sim d^2 = \frac{1}{\pi} \int_{k_c}^\infty \frac{k_b T}{\beta k^2} dk$$

Entropy of a Fluctuating Step

- Thus,

$$k_c \sim \frac{k_b T}{\beta d^2}$$

- For each suppressed mode we lose free energy $\sim -k_B T \log T$

- Neglecting the log, the free energy thus increases by an amount

$$\Delta E \sim k_c L k_b T$$

- Thus,

$$\Delta E_L \sim \frac{(k_b T)^2}{\beta d^2}$$

- So the entropic interaction energy between goes as $1/d^2$

Entropy of a Fluctuating Step

$$\Delta E_L \sim \frac{(k_b T)^2}{\beta d^2}$$
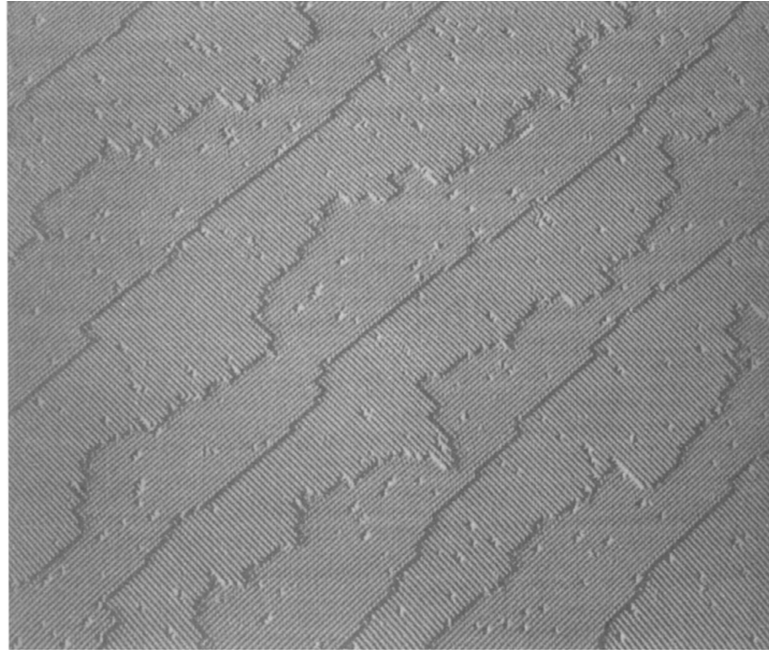
Summary: Both elastic and entropic interactions go as $1/d^2$

What Happens with More than Two Steps?

Is a train of straight steps stable to bunching?

Initial state

Final state

Do Steps Remain Straight During Growth?

- Bales-Zangwill or Mullins-Sekerka instability
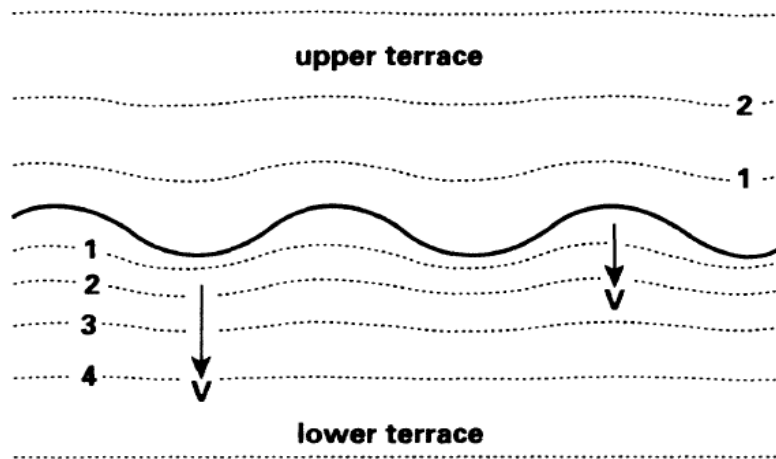
(Bales and Zangwill, PRB 1990)

- Diffusion-driven instability
- To see this let the ES barrier be large
- The adatom concentration gradient is larger at the peaks than the troughs. "Lightning rod effect"
- Since $V \sim d\rho / dx$ the peaks move faster than troughs
- Thus, the curvature at the tip increases, this increases the gradient. Thus κ and V go to infinity in finite time

Missing Physics: Capillarity

- From before:

$$J_T^{+\rightarrow-} = \tilde{k}^+(\mu^+ - \mu_e)$$

- The equilibrium chemical potential is a function of the curvature of the step edge, due to a nonzero step energy

$$\mu_e = \mu_o + \beta\kappa$$

Chemical potential at a flat interface

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Chemical potential at a flat interface

- If the step is positively curved the chemical potential is increased above its value at a flat interface

- If the step is negatively curved it is depressed

Missing Physics: Capillarity

$\mu_e < \mu_o$

$\mu_e > \mu_o$
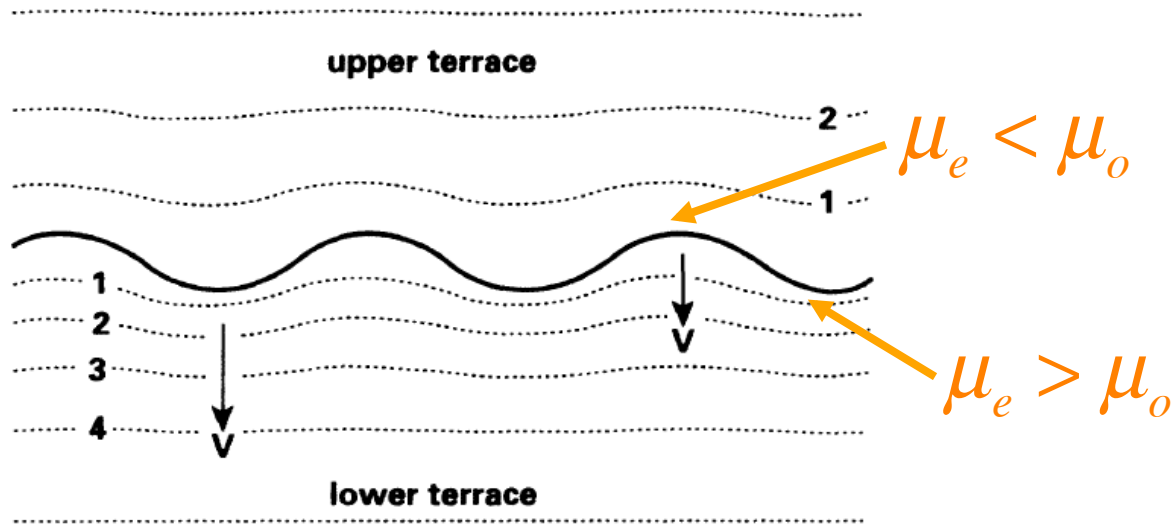
Capillarity tends to flatten the interface, and prevents cusp formation due to diffusion

$$-D\frac{d\rho^+}{dx} = k^+(\rho^+ - \rho_o - \beta\kappa)$$

One Last Piece of Physics

- Diffusional interaction between steps:
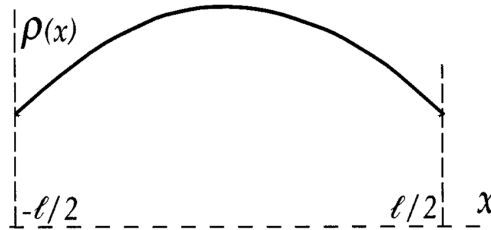
- So, can a non-planar upper step affect the shape of the lower step?
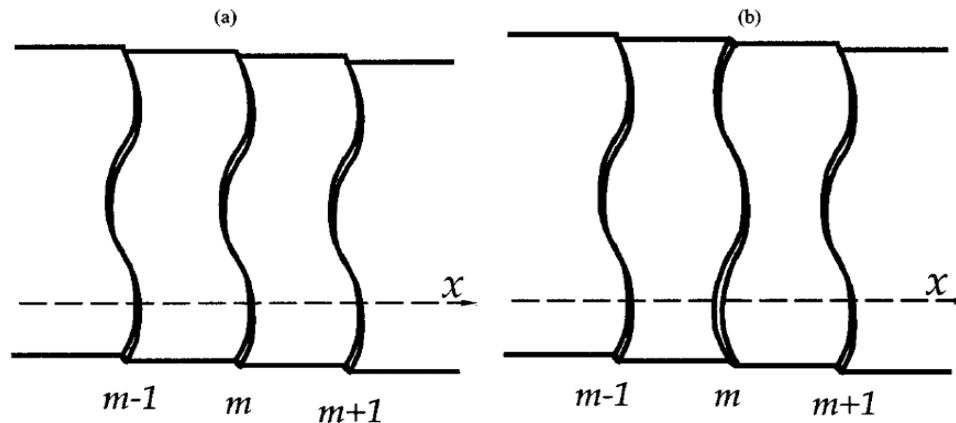
Sinuous or meandering   Varicose

Mathematical Formulation

$$D\nabla\rho^- \bullet \mathbf{n} = k^-(\rho^- - \rho_o - \beta\kappa)$$

$$\frac{\partial\rho}{\partial t} = D_s\nabla^2\rho + V_o\frac{\partial\rho}{\partial x} - \frac{1}{\tau_v}\rho + F$$

y

x

V_o

$$-D\nabla\rho^+ \bullet \mathbf{n} = k^+(\rho^+ - \rho_o - \beta\kappa)$$

$\mathbf{n}$

x

ℓ
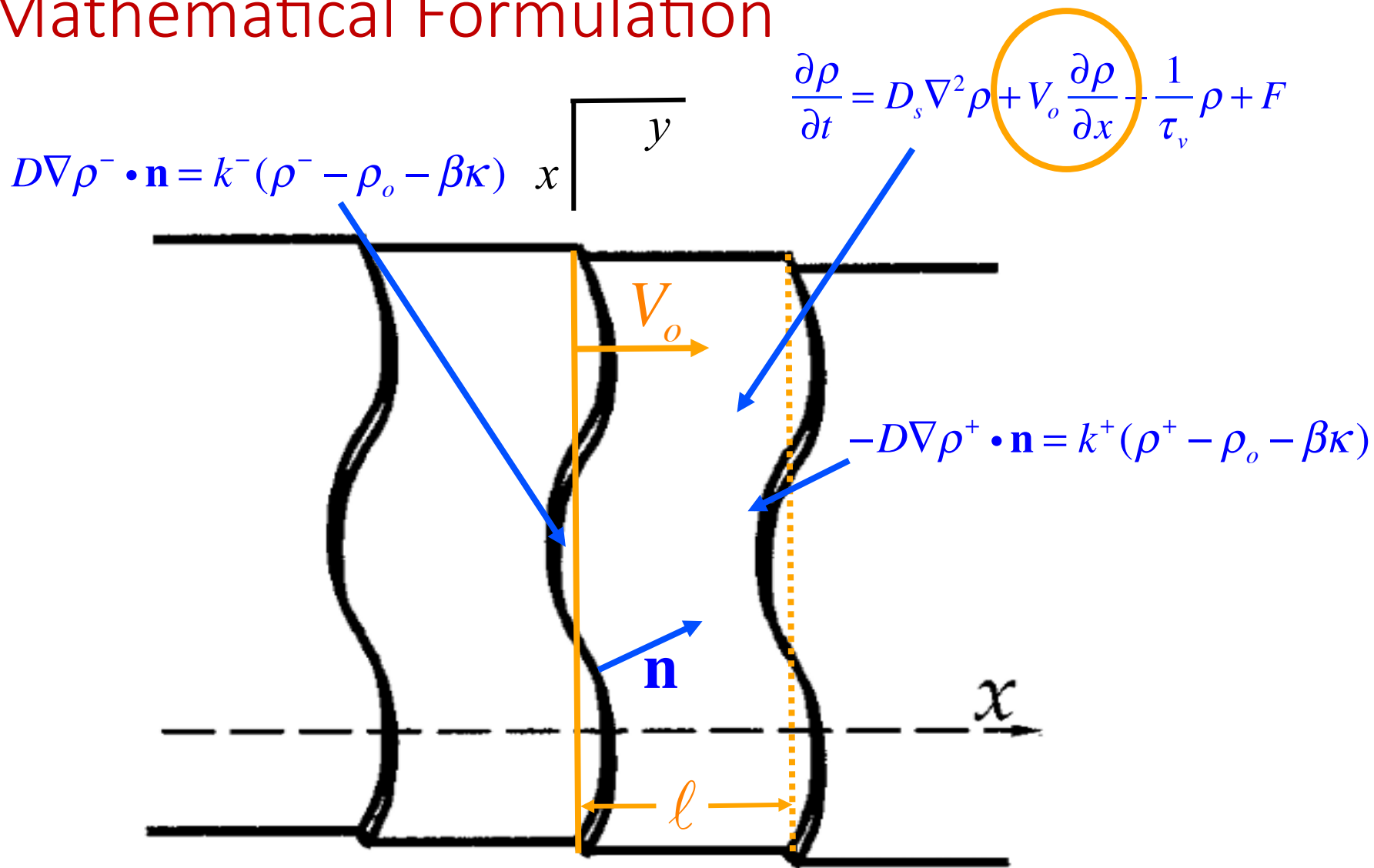
$$V = \Omega\left(D_s\nabla\rho^+ \cdot \mathbf{n} - D_s\nabla\rho^- \cdot \mathbf{n}\right) = k^+\rho^+ - k^-\rho^- - 2\rho_e$$

Linear Stability Analysis

- To avoid numerical simulations, consider very small perturbations about the flat step

- This yields two problems, one for straight edges propagating at a constant velocity V (order zero), one for the evolution of the perturbation (order 1)

- For the interface:

$$y = h(x,t) = 0 + \epsilon \exp(\sigma t + ikx) \qquad \left(\epsilon \ll 1\right)$$

- For the concentration field

$$\rho(x,y,t) = \rho^{(0)}(y) + \epsilon \rho^{(1)}(y) \exp(\sigma t + ikx)$$

- Goal: determine if the perturbation grows or shrinks, and the phase

$$\sigma = \sigma_R + i\sigma_I$$

Linear Stability

Sinuous or meandering

Varicose

$$\sigma_I = 0$$
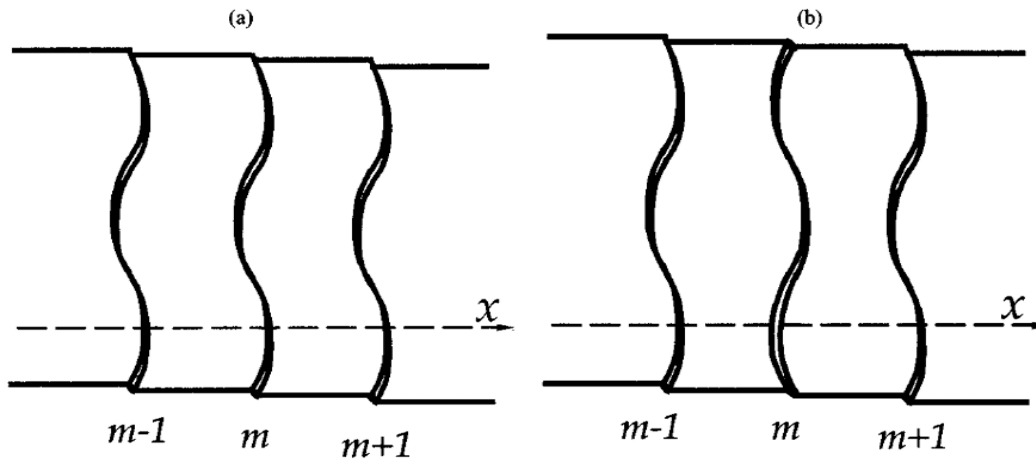
$$\sigma_I = \pi$$

- Field equation is linear: same in basic and perturbed states

- Not true for the boundary conditions, for example

$$\kappa = -\frac{h_{xx}}{\left(1 + h_x^2\right)^{3/2}} = -\frac{\epsilon h_{xx}^{(1)}}{\left(1 + \epsilon^2 (h_x^{(1)})^2\right)^{3/2}} = -\epsilon h_{xx}^{(1)} = \epsilon k^2 \exp(\sigma t + ikx)$$

Linear Stability

- At the interface we need quantities such as

$$\rho(x, \epsilon h^{(1)}(x,t)) = \rho^{(0)}(x,0) + \epsilon \left.\frac{\partial \rho^{(0)}}{\partial y}\right|_{0} h^{(1)}(x,t) + \epsilon \rho^{(1)}(x,0,t)$$

- Use these two ideas to linearize all the boundary conditions

- Result is an order (1) problem where the field equations are solved in a fixed domain with a flat interface, but with boundary conditions that vary with position along the step edges

- Algebraically messy!

Dispersion relation

- One finds a dispersion relation:

$$\sigma_R(k,\sigma_I) = g(k,\sigma_I) - k^2 f(k,\sigma_I)$$

Edge energy

Diffusion

$$\sigma_R(k,\sigma_I) = \Omega\Delta F(d^- - d^+)N(k,\sigma_I) - k^2 f(k,\sigma_I)$$

- Where the supersaturation is

$$\Delta F = F - \rho_o / \tau_v$$

- Which is positive for growth and negative for evaporation

$$d = D_s / k$$

- In most cases there is an ES barrier, $k^+ > k^-$ and thus $d^- - d^+ > 0$

- f is always positive, so as expected line tension is stabilizing

- Need to examine the sign of N

Dispersion relation: Single Step

- Let $\ell \longrightarrow \infty$

- Thus $\sigma_I = 0$

- For large k, $f(k)$ dominates, for small k, $f(k)$ goes to a constant, and thus the edge energy term goes to zero

- For small k,

$$g(k) = \Omega \Delta F k^2 \left(d^- - d^+\right) \frac{\left(d^- + d^+\right) + 1/\kappa}{\left(\kappa d^- + 1\right)^2 \left(\kappa d^+ + 1\right)^2}$$

where $\kappa = (D_s \tau_v)^{-1/2}$

- Thus,
  - If there is no ES barrier, the step is stable, why?

Dispersion relation: Single Step

Zero Ehrlich-Schwoebel barrier

Point effect of diffusion on upper and lower terraces in opposite direction: no driving force force for instability

Positive Ehrlich-Schoewbel barrier

Point effect of diffusion only on lower terraces: can have an instability

(Bales and Zangwill, PRB, 1990)
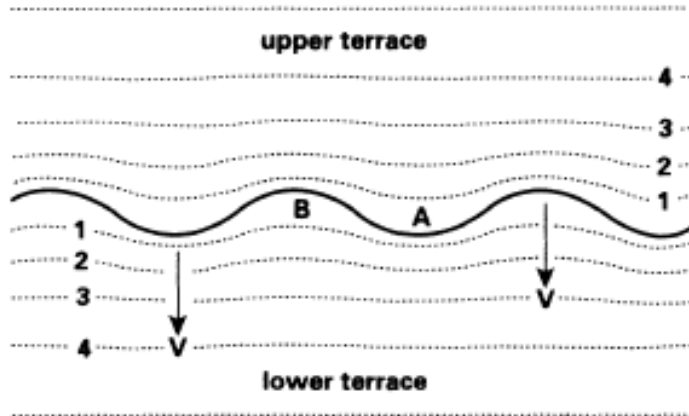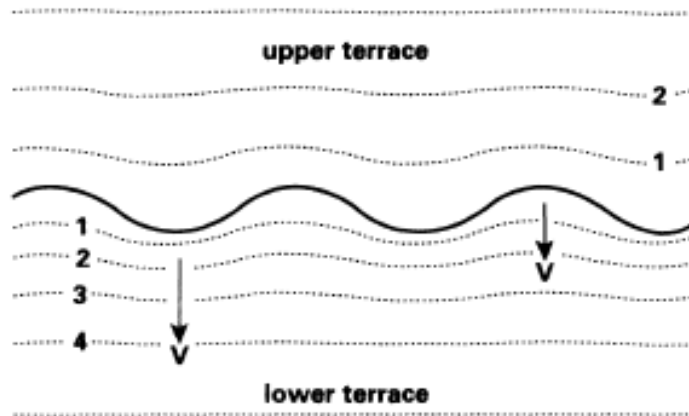
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where $\kappa = (D_s \tau_v)^{-1/2}$

- Thus,
  - If there is no ES barrier, the step is stable, why?
  - In most cases, $d^- - d^+ > 0$ and $\Delta F > 0$, and thus $g(k) > 0$
  - $g(k) \sim k^2$, so for sufficiently large prefactor,

Dispersion relation: Single Step

We obtain a dispersion relation:
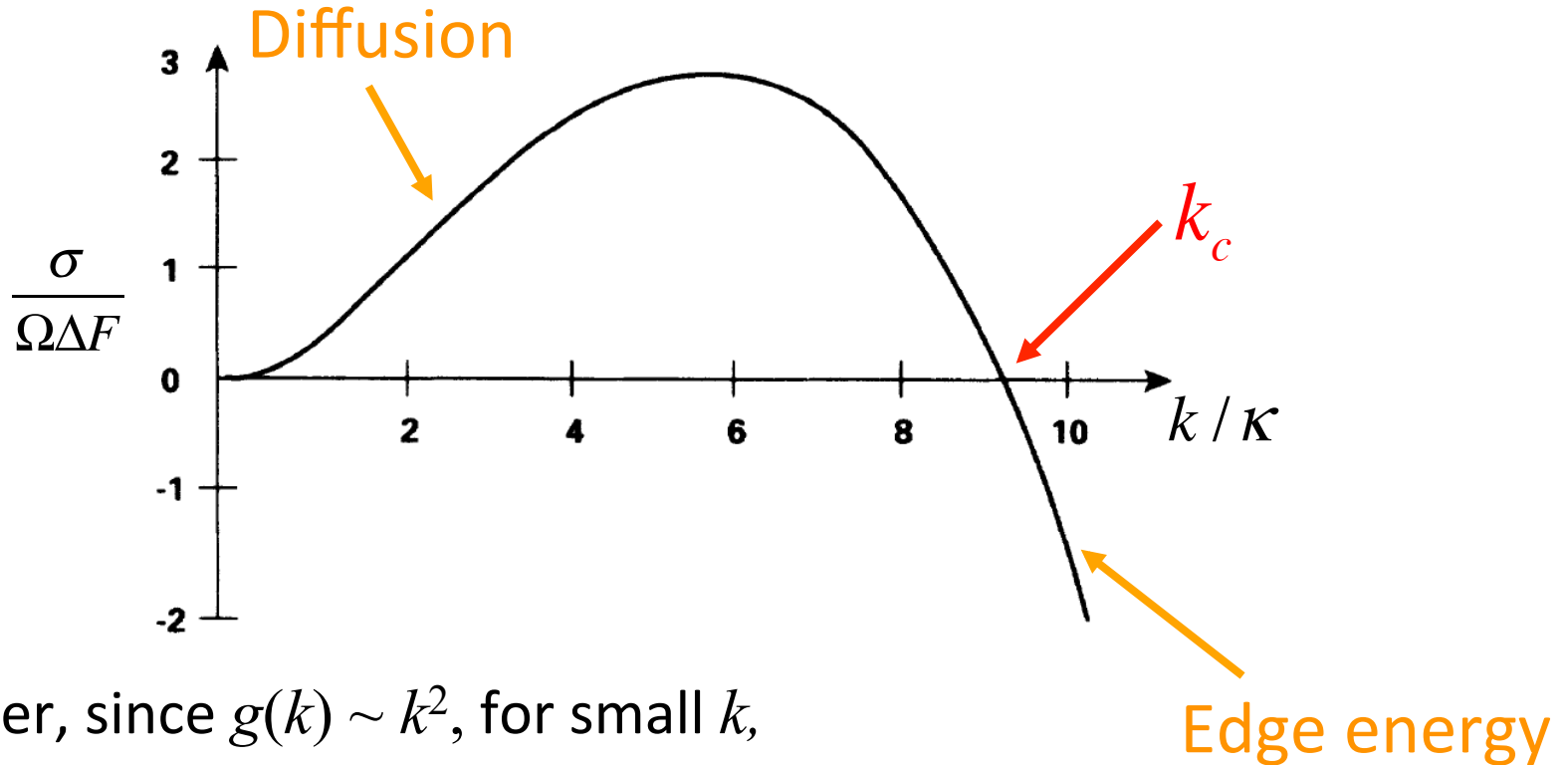
However, since $g(k) \sim k^2$, for small k,

$$\sigma_R = \left[\Omega \Delta F k^2 \left(d^- - d^+ \right) \frac{\left(d^- + d^+ \right) + 1/\kappa}{\left(\kappa d^- + 1 \right)^2 \left(\kappa d^+ + 1 \right)^2} - f \right] k^2$$

Dispersion relation: Single Step

$$\sigma_R = \left[\Omega \Delta F k^2 \left(d^- - d^+ \right) \frac{\left(d^- + d^+ \right) + 1/\kappa}{\left(\kappa d^- + 1 \right)^2 \left(\kappa d^+ + 1 \right)^2} - f \right] k^2$$

- So there exists a critical supersaturation below which the step remains planar

- For sufficiently small step energy an isolated step will be unstable

Dispersion relation: Multiple Steps

- Consider the limit suggested by MBE (Si, Ge)
- No evaporation $\tau_v \rightarrow \infty$
- Mode with the largest σ_R has $\sigma_I = 0$
- In this limit,

$$g(k, \sigma_I = 0) = \Omega\left(d^- - d^+\right)\frac{\ell^2 k^2}{2\left(d^- + d^+ + \ell\right)}$$

$$f(k, \sigma_I = 0) = \frac{\Omega \ell D_s \beta}{k_b T} k^2$$

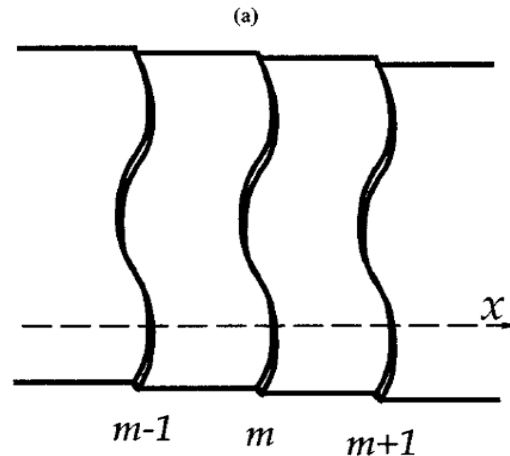- Since,

$$\sigma_R(k, \sigma_I) = g(k, \sigma_I) - k^2 f(k, \sigma_I)$$

- The train of steps is always unstable to a long wavelength ($k \rightarrow 0$) mode

Dispersion relation: Multiple Steps

- So step flow during MBE with an ES barrier is unstable to meandering:

(a)

$m-1$ m $m+1$

- Large literature examining the evolution beyond linear theory, one finds cells dendrites etc.

Role of Beam Fluctuations

- Do fluctuations in the beam intensity induce a rough surface?

- Competition between "healing" (surface diffusion), and randomness of the deposition process

- Why does surface diffusion heal?

- Consider a surface above T_R (isotropic)

$$\mu = \mu_o + V_m \gamma \kappa$$

- Mass balance at the surface:

$$\rho_v V = -\nabla_s \bullet \mathbf{J}_s$$

Capillarity Driven Surface Diffusion

- The flux along the surface:

$$\mathbf{J}_s = -D_s \nabla_s \mu$$

- Substituting into the above,

$$\rho_v V = \nabla_s^2 \mu$$

- Using the expression for the chemical potential, ields an evolution equation for the surface,

$$V = \alpha \nabla_s^2 \kappa \qquad \text{(Mullins ca. 1960)}$$

- Consider a small perturbation about a flat interface $y(x,t) = \epsilon h(x,t)$

$$h_t = -\alpha h_{xxxx}$$

- Assume,

$$h = h_o \exp(\sigma t + ikx)$$

Capillarity Driven Surface Diffusion

- One obtains,

$$\sigma = -\alpha k^4$$

- Thus, all perturbations decay:

capillarity driven surface diffusion smooths
or heals the surface

Surface Roughness

- As we saw, the surface is considered rough when the height-height correlation function diverges for large r, t.

$$G(\mathbf{r},t) = \left\langle \left(z(\mathbf{r},t) - z(\mathbf{r}+\mathbf{r}',t) \right)^2 \right\rangle$$

- At $t = 0$, the surface is flat, $G(\mathbf{r},t) = 0$

- Does beam noise lead to a rough surface?

- Consider a deposition of h atomic layers

- Surface diffusion smooths the surface on a distance ℓ_s

- Average number of atoms deposited $\ell_s^2 h$

- Since the deposition is random (0,1), the mean square deviation is also $\ell_s^2 h$. Thus,

$$\delta h \approx \sqrt{h} / \ell_s$$

Surface Roughness

$$\delta h \approx \sqrt{h} / \ell_s$$

- If $\ell_s \approx 100$, then $h > 10^4$ for $\delta h > 1$

- So, in most cases beam fluctuations are not important

- However, there is much beautiful physics still to be done. No variational principle!

- Edwards-Wilkinson. Take the surface diffusion model and make it a Langevin equation,

$$h_t = -\alpha h_{xxxx} + f(x,t)$$

- Where $f(x,t)$ is the random beam deposition

- The correlation length $\xi \sim t^{1/4}$

Karder-Parisi-Zhang Equation

- Include a lower order term to the Edwards-Wilkinson equation

- Connection to MBE not clear

- Inspired by models for deposition at very low temperatures

$$h_t = a(h_x)^2 - \alpha h_{xxxx} + f(x,t)$$

- Huge literature on this topic (KPZ paper has over 4000 citations)