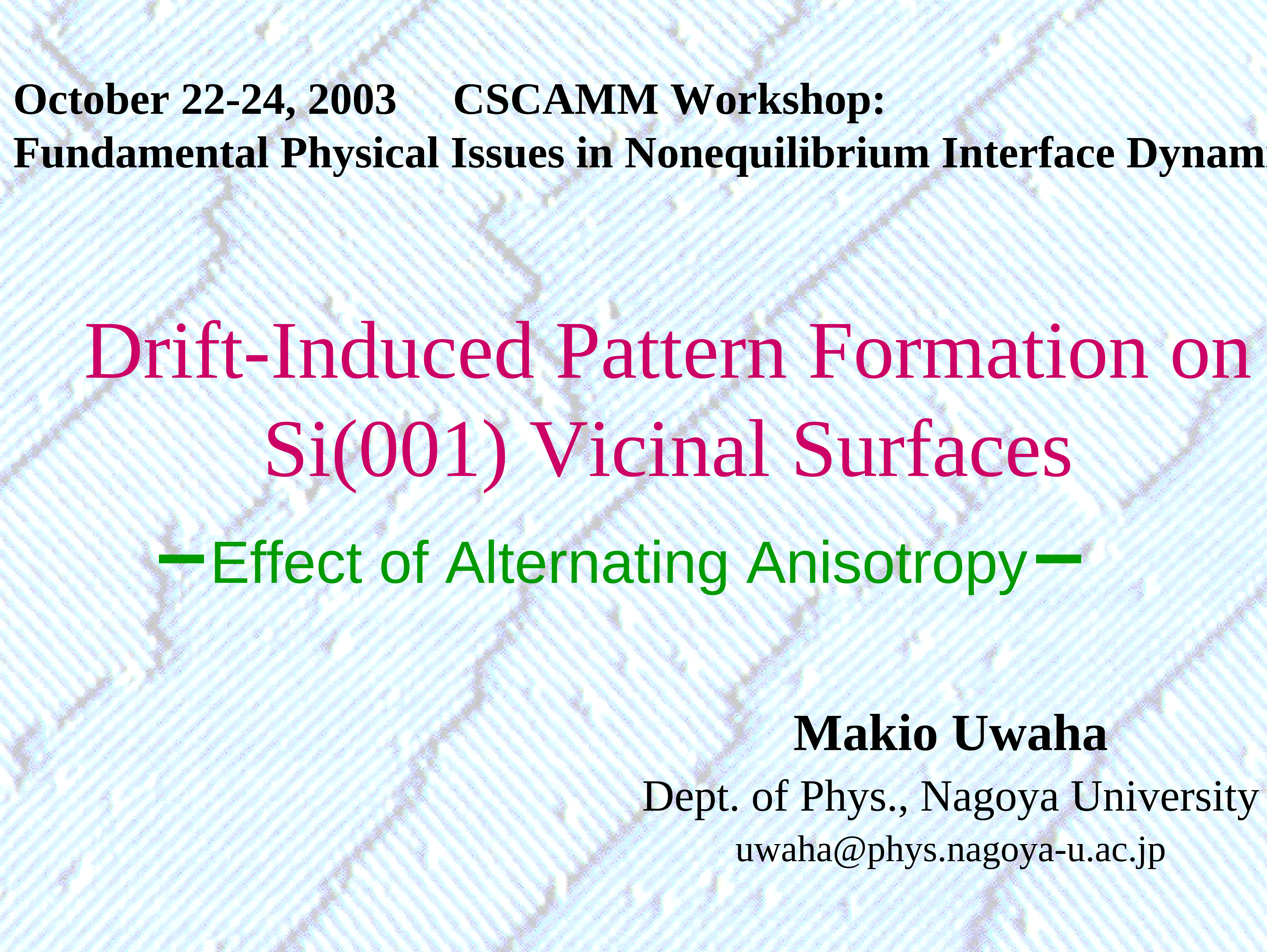

October 22-24, 2003 CSCAMM Workshop:
Fundamental Physical Issues in Nonequilibrium Interface Dynam

Drift-Induced Pattern Formation on Si(001) Vicinal Surfaces

−Effect of Alternating Anisotropy−

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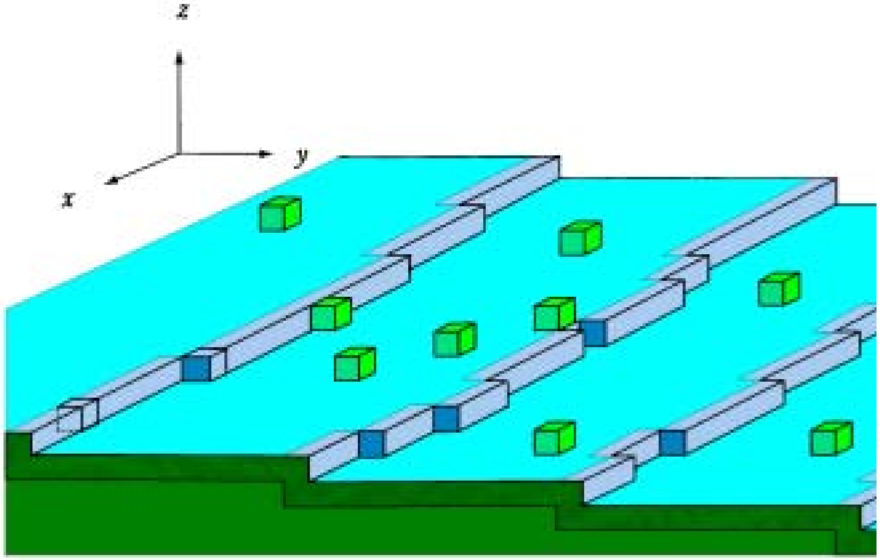
Plan of My Talk

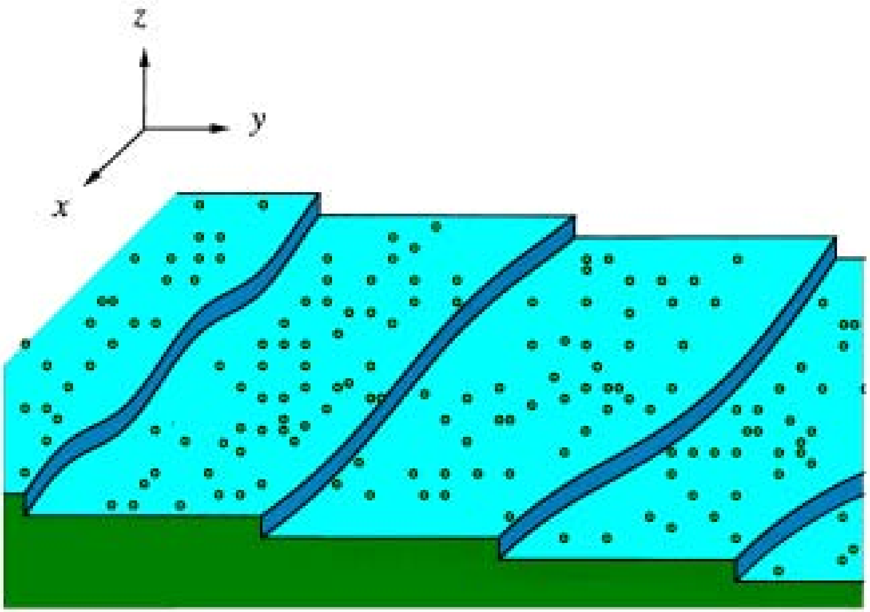
- Preliminaries: models, instabilities of a vicinal face---step bunching and step wandering on Si(111) vicinal faces.
- Characteristics of the Si(001) vicinal face and experimental observations of instabilities under direct current heating.
- Our theoretical study and Monte Carlo simulation: mechanism of step bunching and a new kind of wandering instability

Lattice model and continuum step model

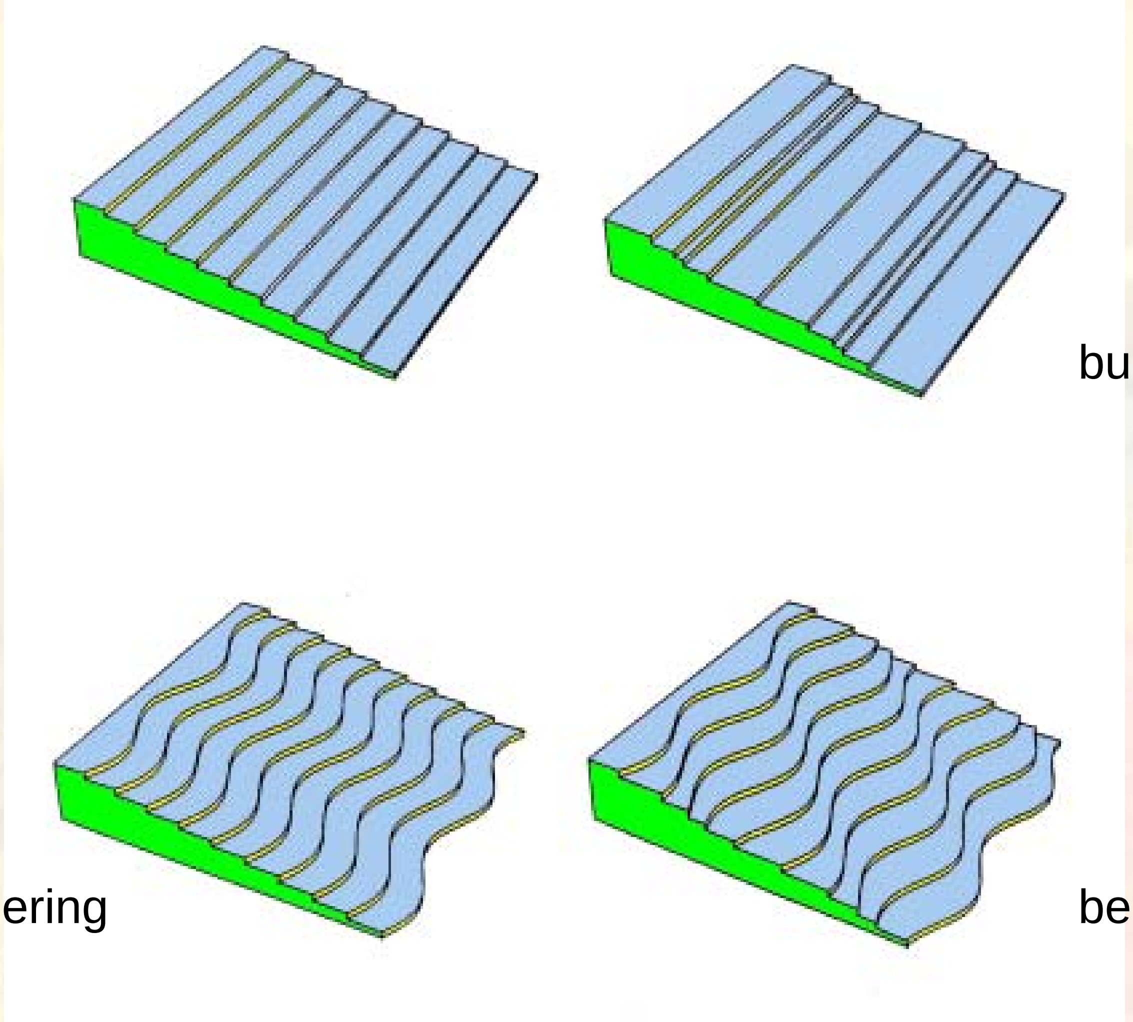
Lattice model:
- Monte Carlo simulation

Continuum model：
- Mathematical Analysis
- Simulation in 1D





Morphological instabilities on a vicinal surface



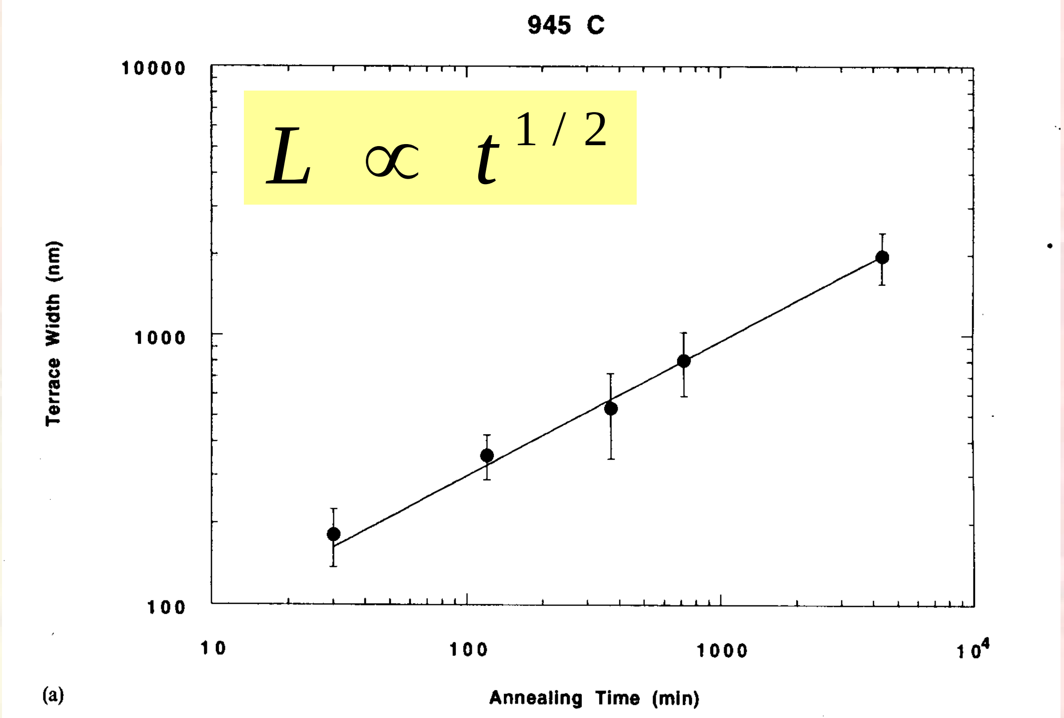
vicinal face

bunching

In-phase wandering

bending

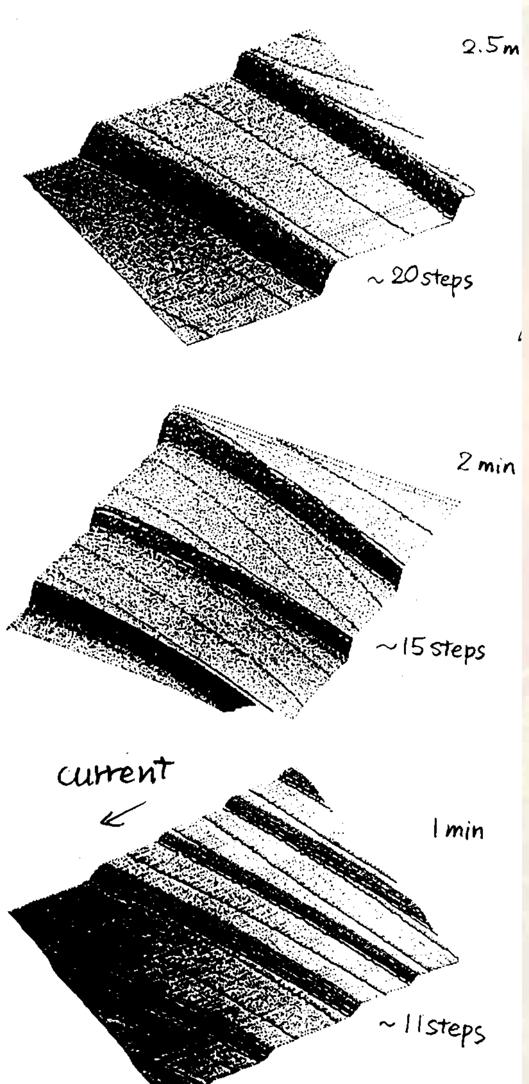
Step bunching on a Si(111) vicinal face under direct current heating



$L \propto t^{1/2}$

Yang, Fu, Williams: Surf. Sci. 356 (1996) 101

Fu, Liu, Johnson, Weeks, Williams:
Surf. Sci. 385 (1997) 259



Theoretical study on growth of step bunches in Si(111) with drift

- C. Misbah, O. Pierre-Louis: Phys. Rev. E **53** (1996) R4319
- M. Sato, M. Uwaha: J. Phys. Soc. Jpn. **65** (1996) 1515

  Step bunches (during evaporation) are described by Benney equation →Steady State of bunches.

- H. Dobbs, J. Krug： J. Phys. I France **6** (1996) 413

  MC simulation of SOS lattice model → $t^{1/4}$(1D), $t^{1/2}$ (2D)

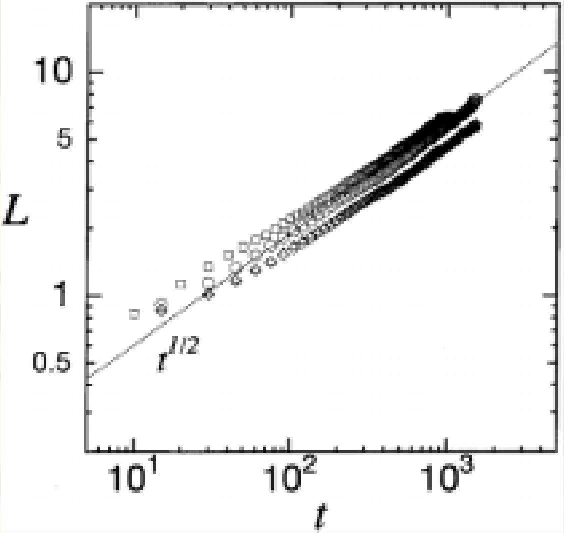
- D.-J. Liu, J. D. Weeks： Phys. Rev. B **53** (1998) 14891

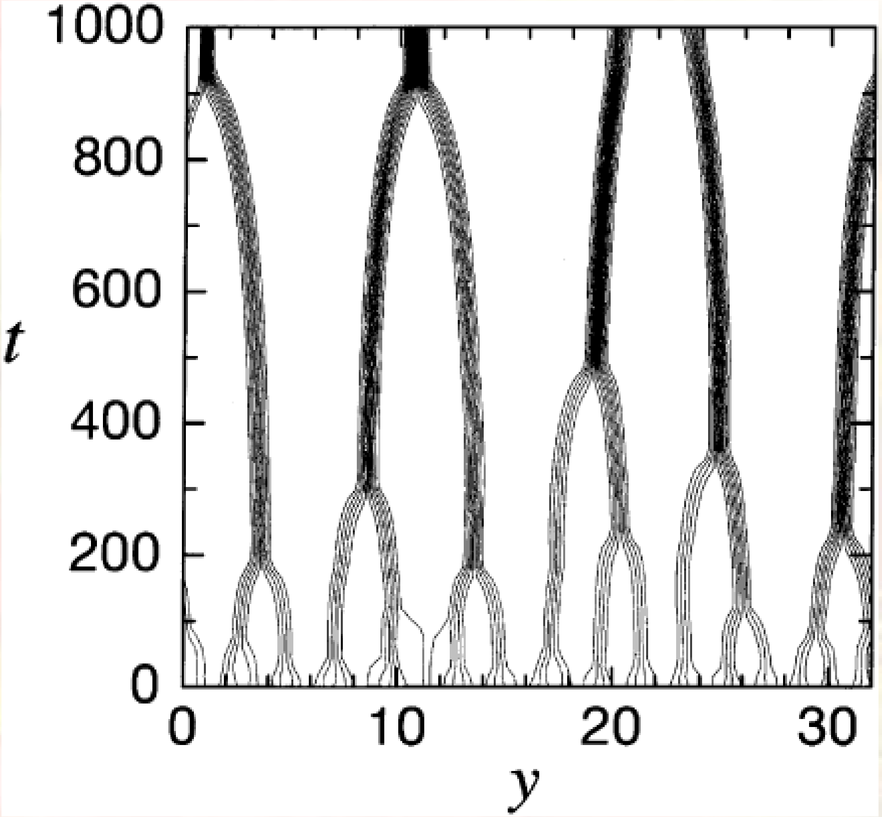
  Continuum model + scaling hypothesis → $t^{1/2}$ growth(1D)

Step bunching on a Si(111) vicinal face under direct current heating—1D model

- Instability with step-down drift
  → Formation of step pairs
- Equidistant pairs are also unstable → Hierachical pairing
- Scaling laws in bunching

$$L = t^{1/2}$$





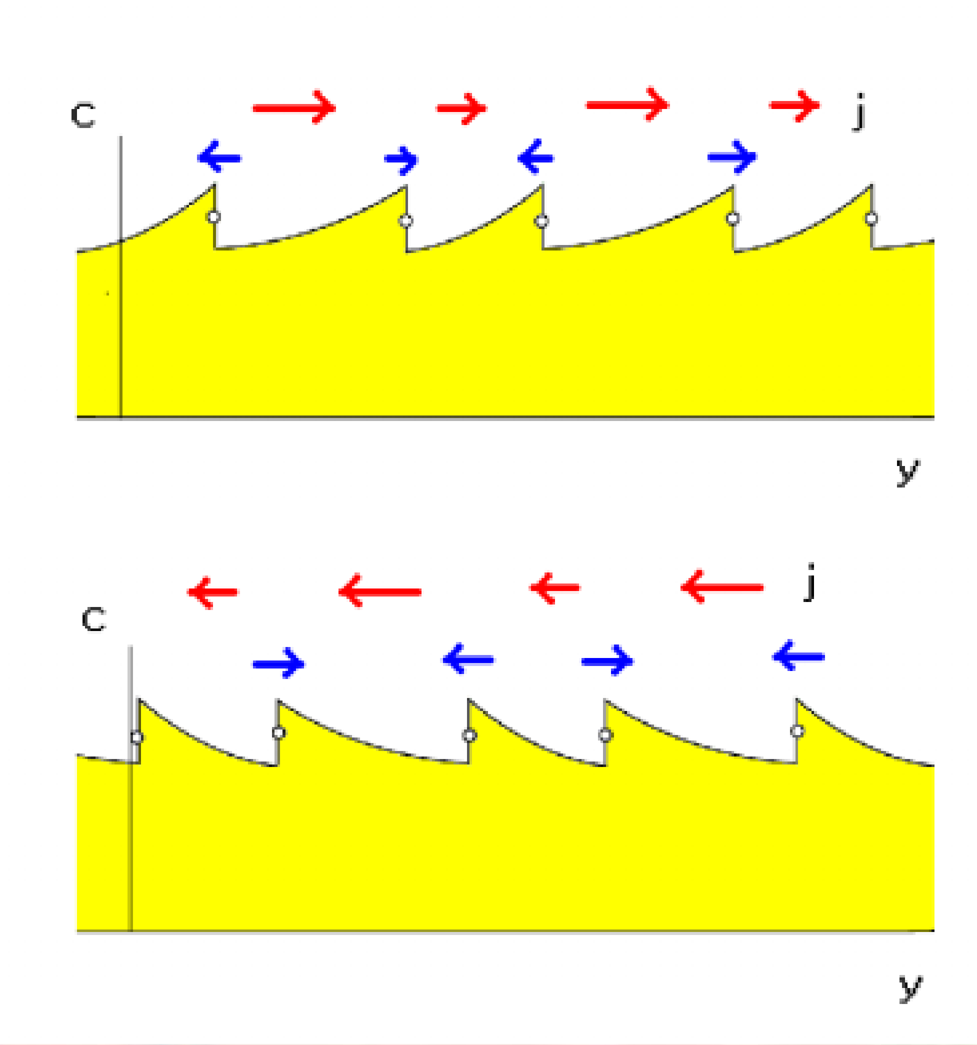
Sato, Uwaha: J. Phys. Soc. Jpn. 67 (1998) 367

Mechanism of step pairing in a Si(111) vicinal

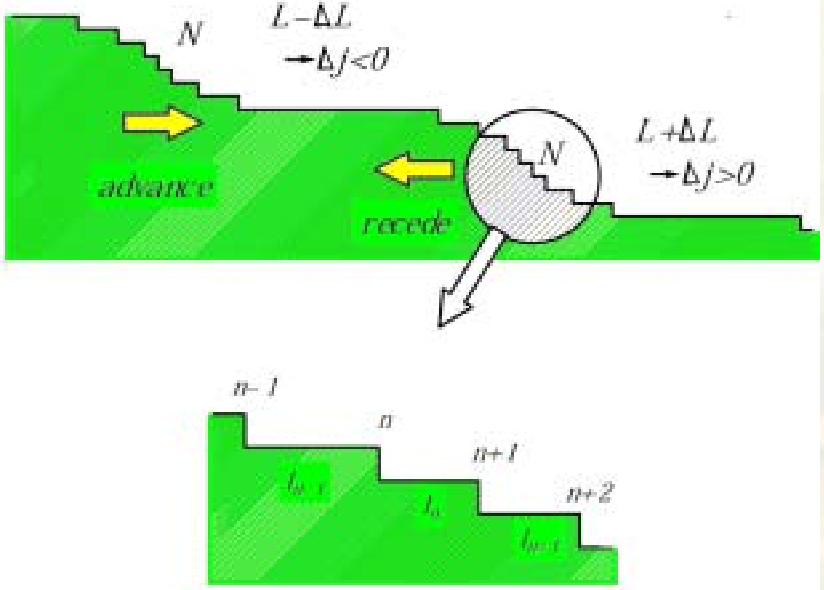
Current on a terrace

$$j \approx -D_s \frac{c_- - c_+}{L} + \frac{c_- + c_+}{2} v_d$$

Density profile of adatoms



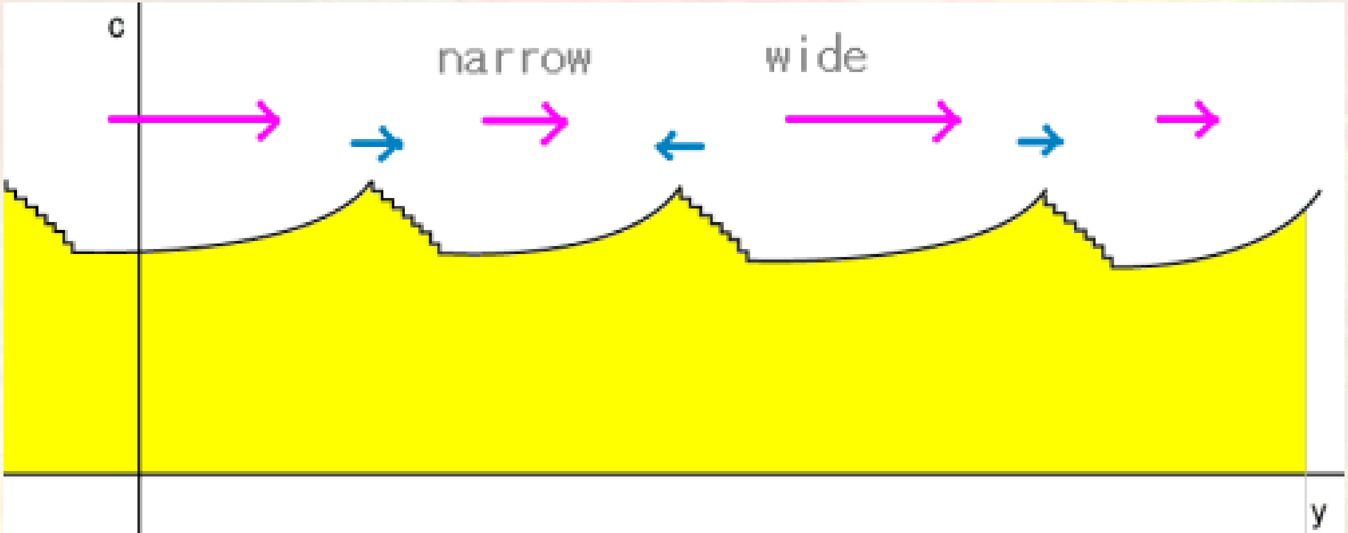
Mechanism of bunch coalescence on a Si(111) vicinal



Current on a terrace

$$j \approx -D_s \frac{c_1 - c_N}{L} + \frac{c_1 + c_N}{2} v_d$$

Density profile of adatoms



Origin of the growth law of bunches

Current on a terrace

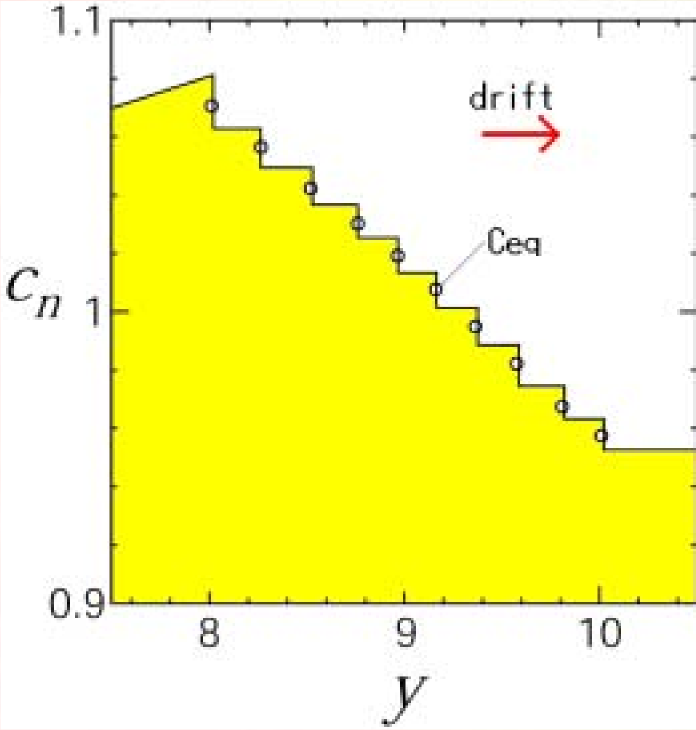
$$j \approx -D_s \frac{c_1 - c_N}{L} + \frac{c_1 + c_N}{2} v_d$$

Change of the terrace width

$$\frac{d\Delta L}{dt} \propto \frac{\Delta j}{N} \propto \frac{1}{N} \frac{c_1 - c_N}{L^2} \Delta L$$

Collision time

$$\tau \propto \frac{L^2}{v_d} \propto N^2$$



Step repulsion potential $\propto l^{-\nu}$

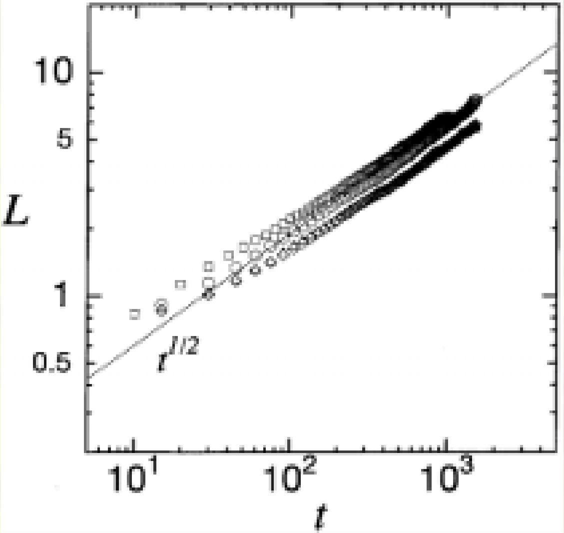
One can show $c_1 - c_N \propto N$

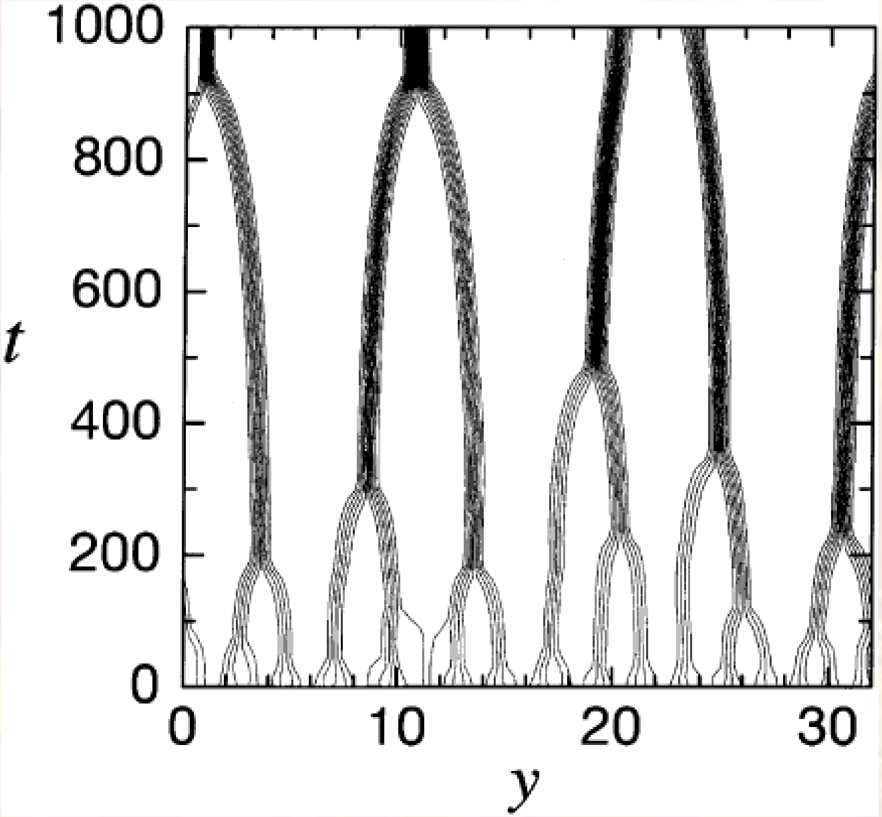
And $l_b \propto N^{-2/(\nu+1)}$

Step bunching on a Si(111) vicinal face under direct current heating—1D model

- Instability with step-down drift
  → Formation of step pairs
- Equidistant pairs are also unstable → Hierachical pairing
- Scaling laws in bunching

$$L = t^{1/2}$$





Sato, Uwaha: J. Phys. Soc. Jpn. 67 (1998) 367

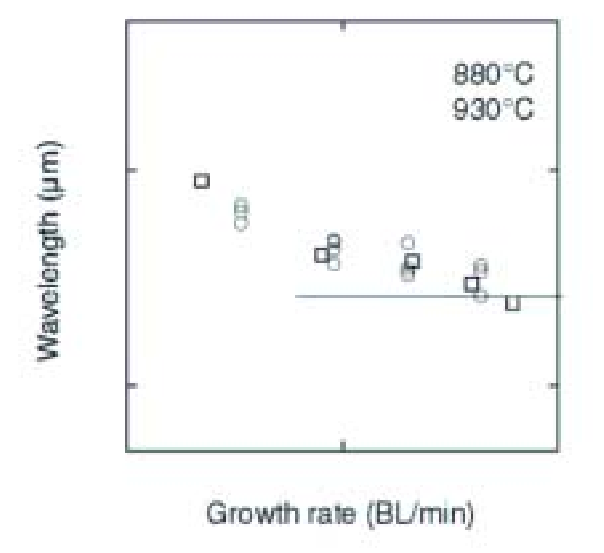
Causes of step wandering instability

Asymmetry of the diffusion filed in front and in back of the step

Mechanisms

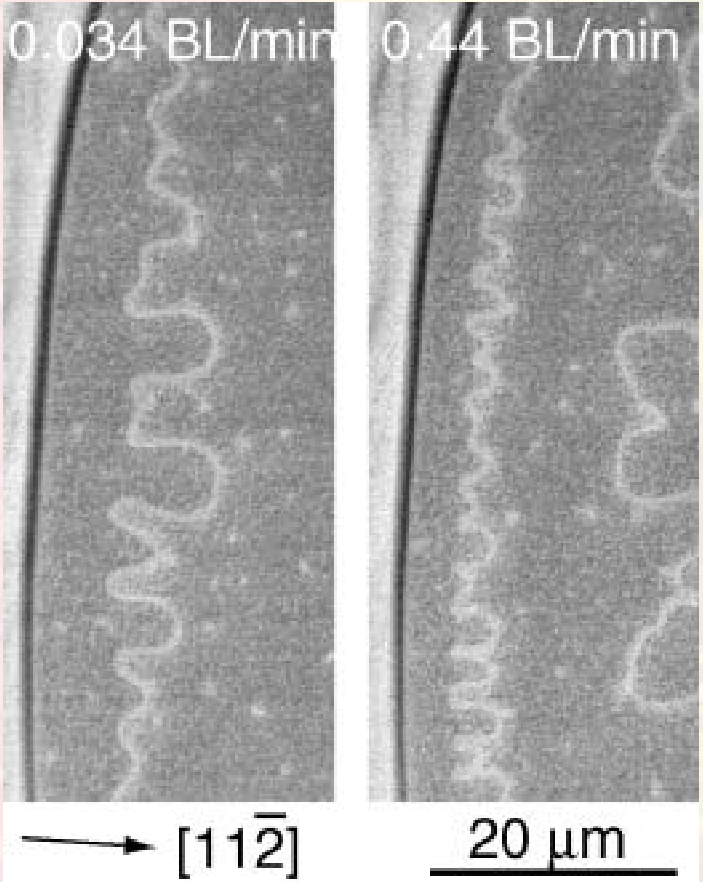
- Ehrlich-Schwoebel (ES) effect (Bales, Zangwill 1990)
- Kink Schwoebel effect (Pierre-Louis, D'Orsogna, Einstein 1999)
- Drift flow of adatoms by an external field (Sato, Uwaha 1996)
- Difference of the terrace width in front and in back of the step

Step wandering due the difference of the terrace width



- Wandering wave number in the one-sided model

$$k_{\max} = \sqrt{\frac{k_B T V_0}{3\Omega^2 \tilde{\beta} c_{eq}^0 D_s}}$$



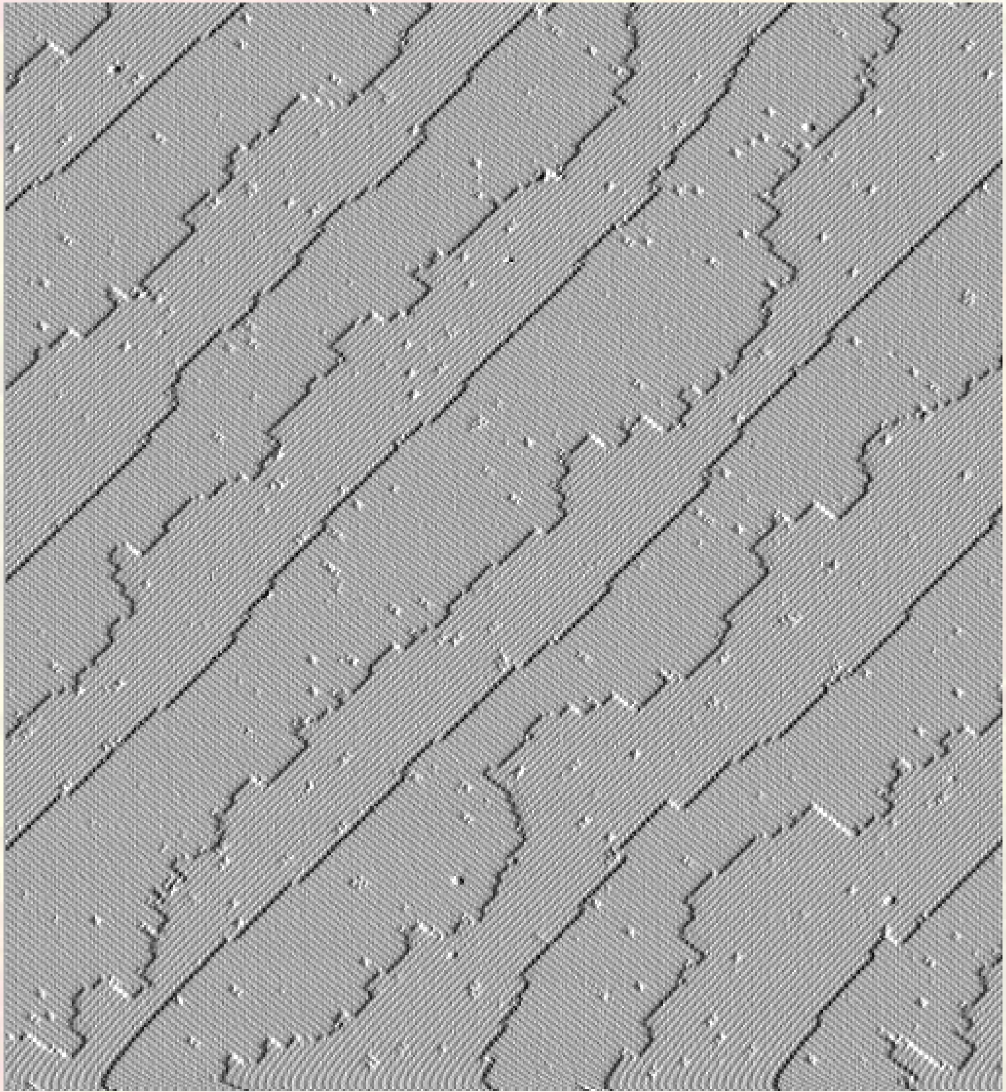
Homma, Finnie, Uwaha: Surf. Sci. 492 (2001) 125

Two kinds of steps and terraces on a Si(001) vicinal face

- STM image of a vicinal tilted towards [110]

- A-step with few kinks
- B-step with many kinks

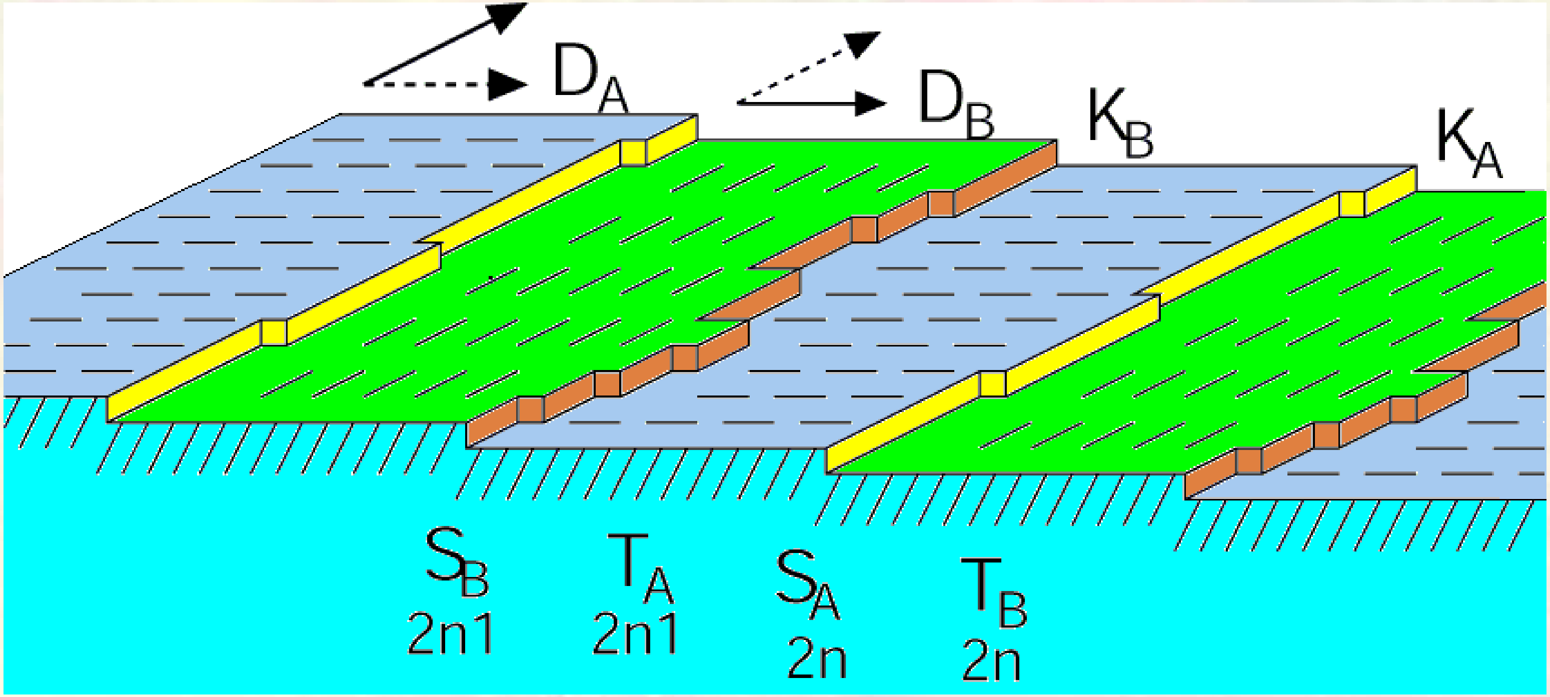
- Stripes are dimer rows



(STM image taken by Swartzentruber et al.)

Si(001) vicinal face tilted to [110]

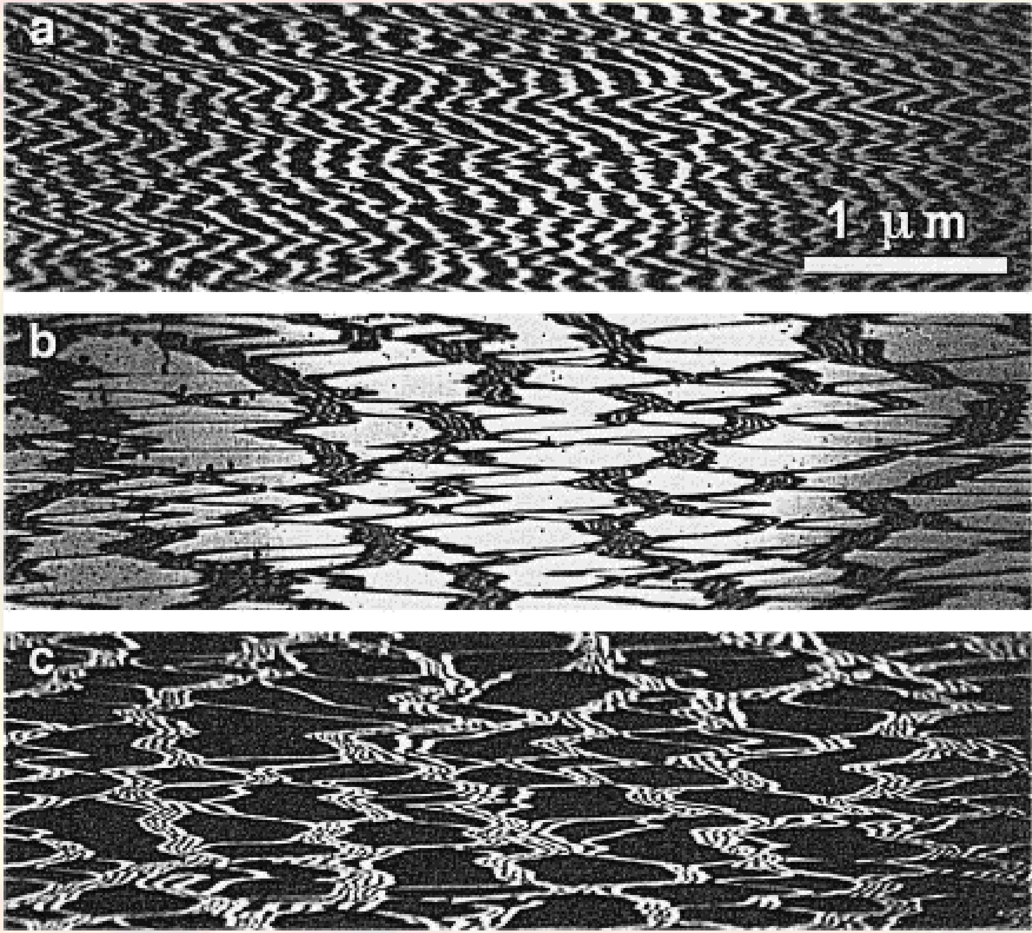
- The orientation of dimer rows alternates on neighboring terraces.



Si(001) step pairing with drift

REM images of the stepped Si(001) surface.

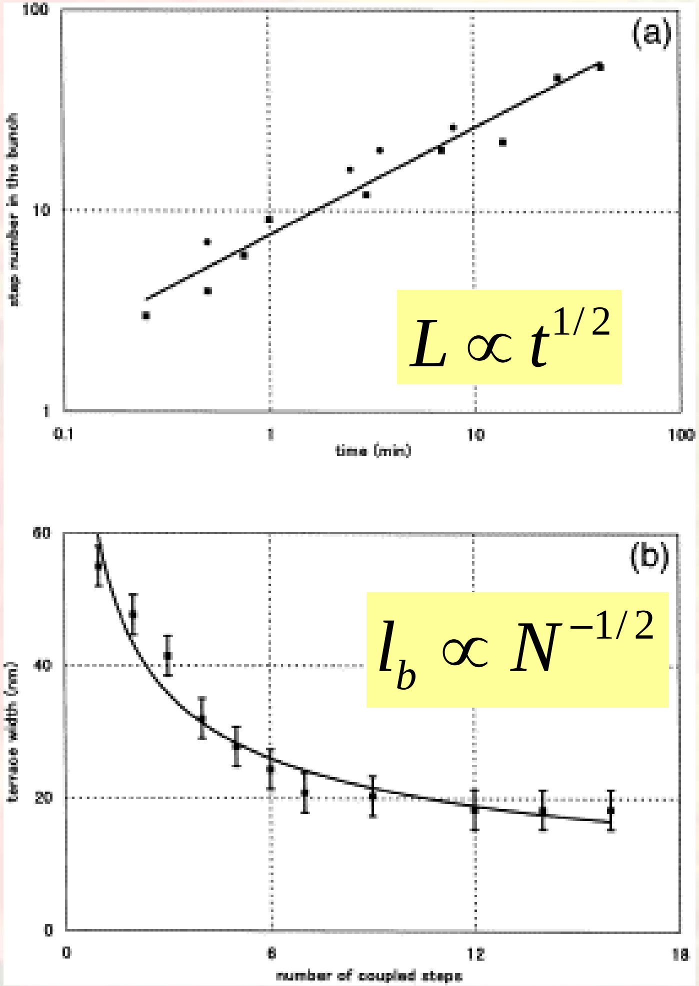
- (a) After AC heating.
- The same surface after DC heating at 1150 ° C for 2 min: (b) in the step-up, (c) in the step-down directions



Latyshev, Lytvin, Aseev: Appl. Surf. Sci. **130-132** (1998) 139

Si(001) step bunching with drift

- (a) Change of the average distance between bunches. The power-law with an exponent 0.5.
- (b) Average distance between the steps in a bunch vs. the number of steps in the bunch. The exponent is -0.5.



$$L \propto t^{1/2}$$

$$l_b \propto N^{-1/2}$$

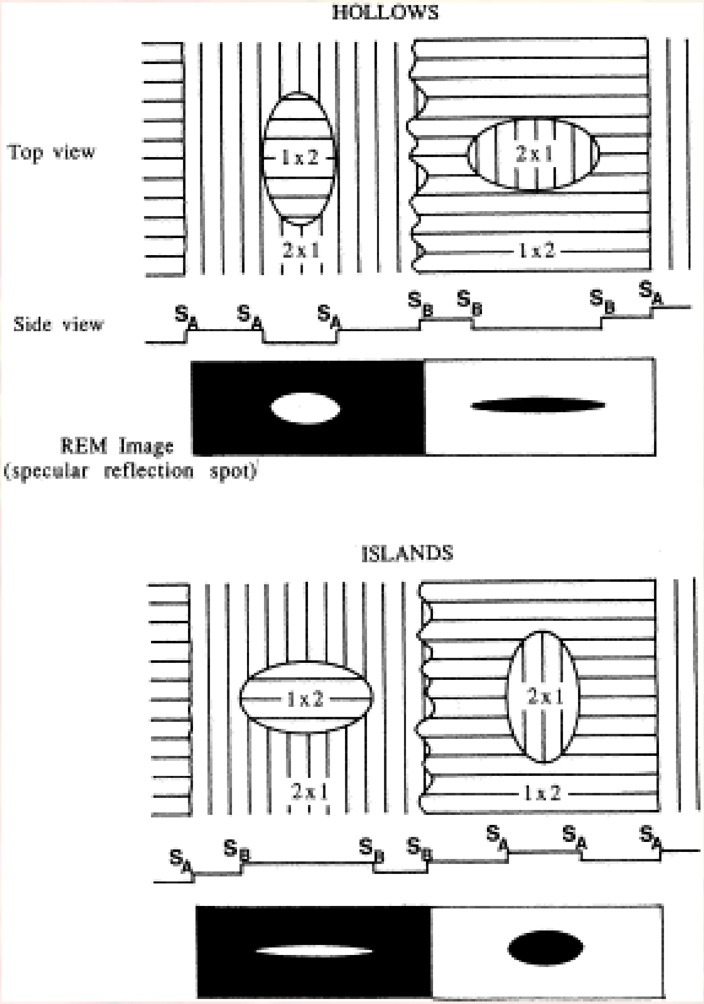
Latyshev, Lytvin, Aseev: Appl. Surf. Sci. **130-132** (1998) 139

Si(001) island motion with drift

A stepped Si(001) surface with hollows and islands.

- The analysis of the island motion is consistent with the positive effective charge of adatoms.

Métois, Heyraud, Pimpinelli:
Surf. Sci. **420** (1999) 250



Originally found by Ichikawa and Doi: Appl. Phys. Lett. 60, 1082 (1992)

Theoretical study on bunching in Si(001)

- S. Stoyanov: Jpn. J. Appl. Phys. **29** (1990) L659
  1D model → Formation of step pairs due to the difference in adatom mobility (diffusion coefficient)
- A. Natori, H. Fujimura, H. Yasunaga: Jpn. J. Appl. Phys. **31** (1992) 1164
  Numerical simulation of 1D model (repulsion, impermeable steps) →Formation of large bunches with step-up drift only.
- M. Sato, M. Uwaha, and Y. Saito： J. Cryst. Growth **237-239** (2002) 43
  Stability analysis of 1D model． Monte Carlo simulation of 2D lattice model → bunching in both drift direction

Vicinal face of Si(001)

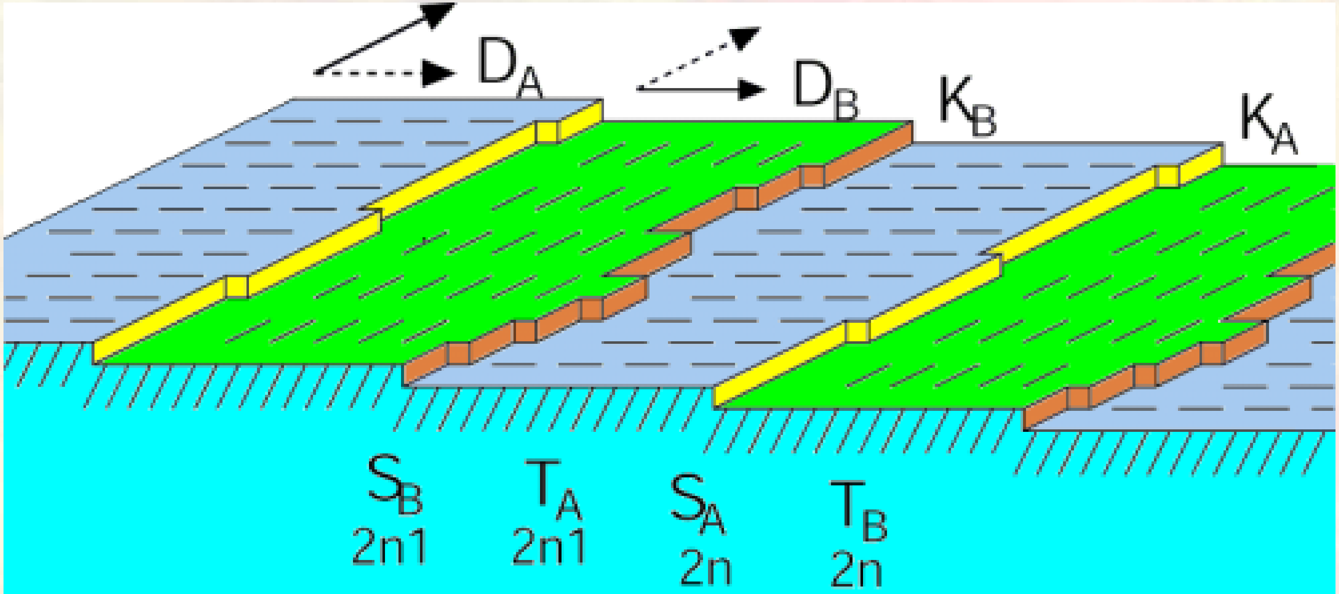
- Alternating dimer row direction on consecutive terraces

→ Diffusion coefficients and drift velocity alternate.

$$D_B > D_A$$

$$v_{A,B} = \frac{D_{A,B}}{k_B T} Z_{eff} eE$$

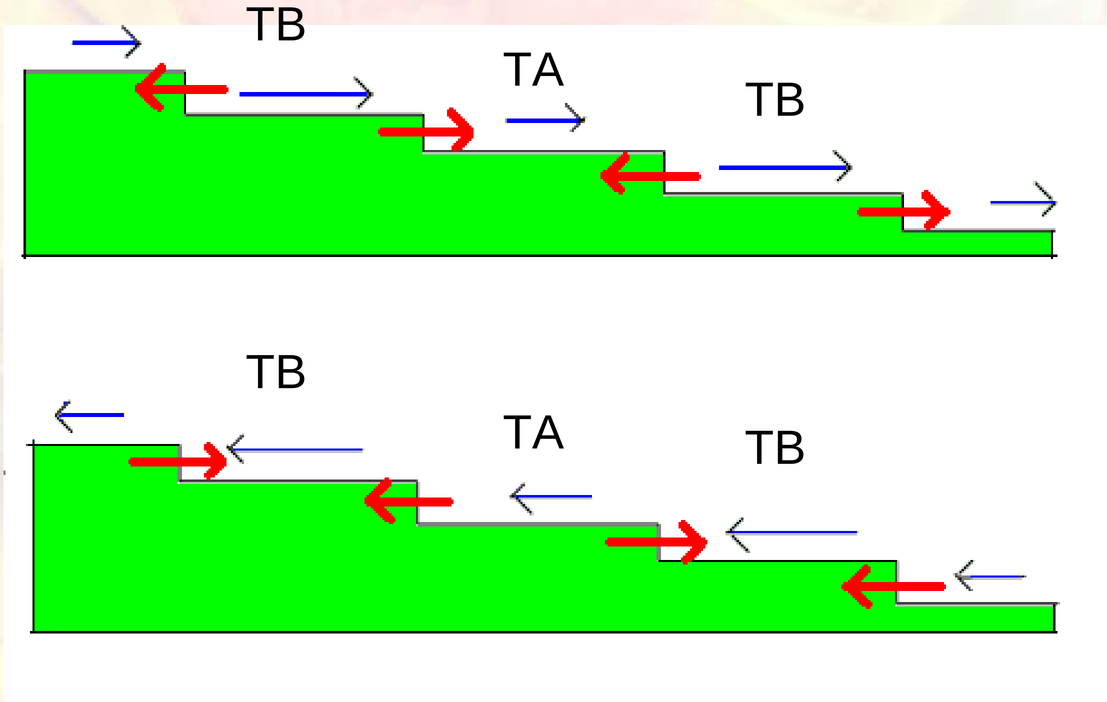
Assume fast step kinetics



Formation of step pairs by the drift of adatoms on a Si(001) vicinal face (Stoyanov 1990)

- Step-down drift
  ↓
  Fast TB terraces expand

- Step-up drift
  ↓
  Slow TA terraces expand



Pairing of steps → Formation of large bunches?

Formation of large bunches by drift of adatoms on a Si(001) vicinal face

- Step-down drift

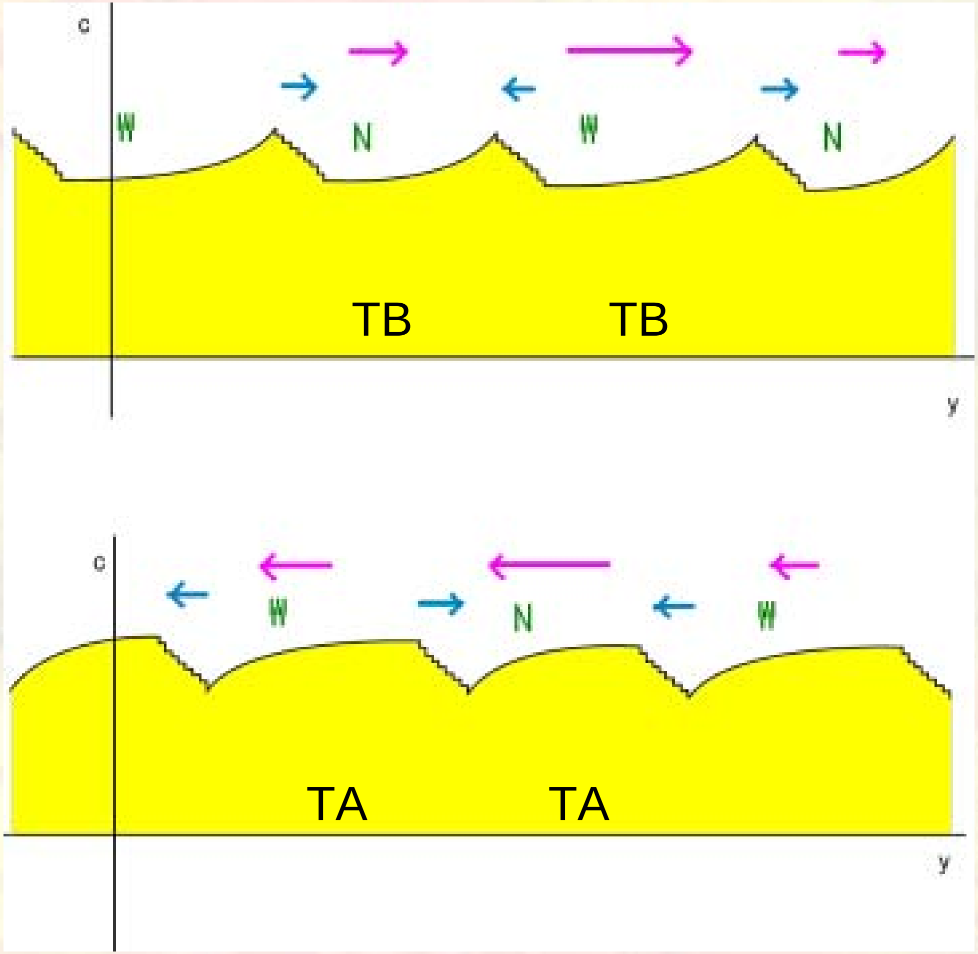
  ↓

  Fast TB terraces expand

- Step-up drift

  ↓

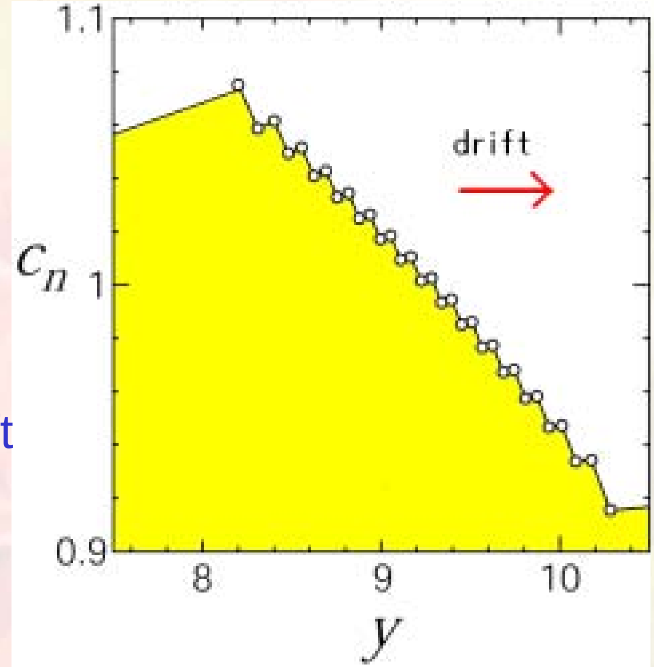
  Slow TA terraces expand



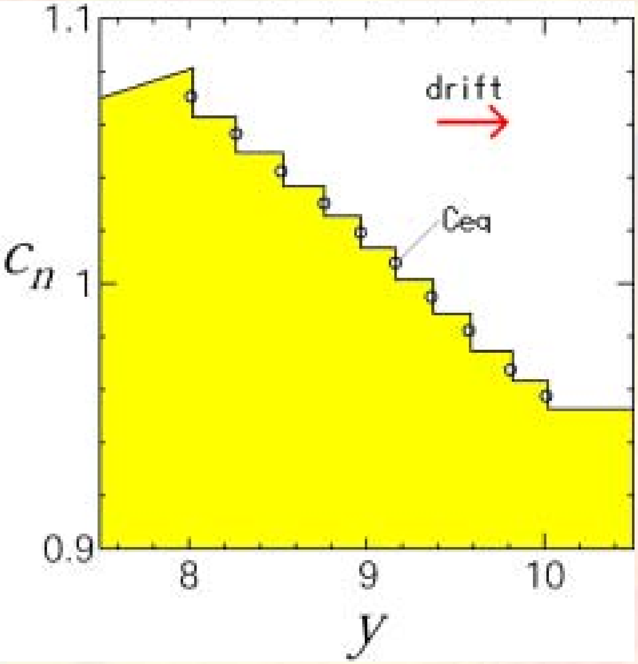
Pairing of steps → Formation of large bunches

Density of adatoms in a bunch

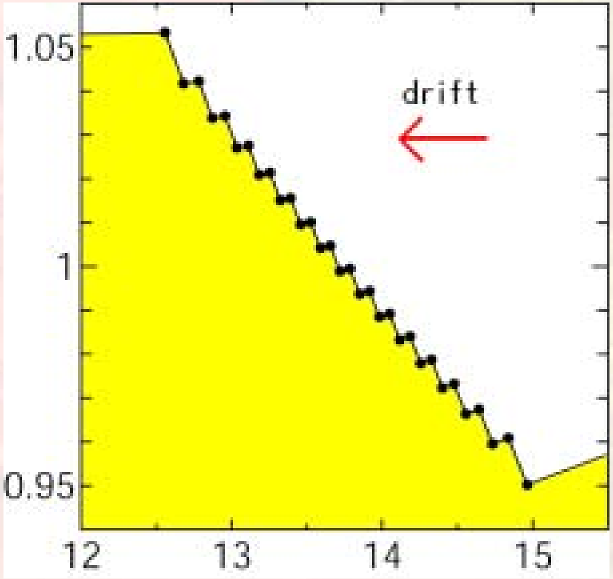
Si(001)
step-down drift



Si(111) step-down drift

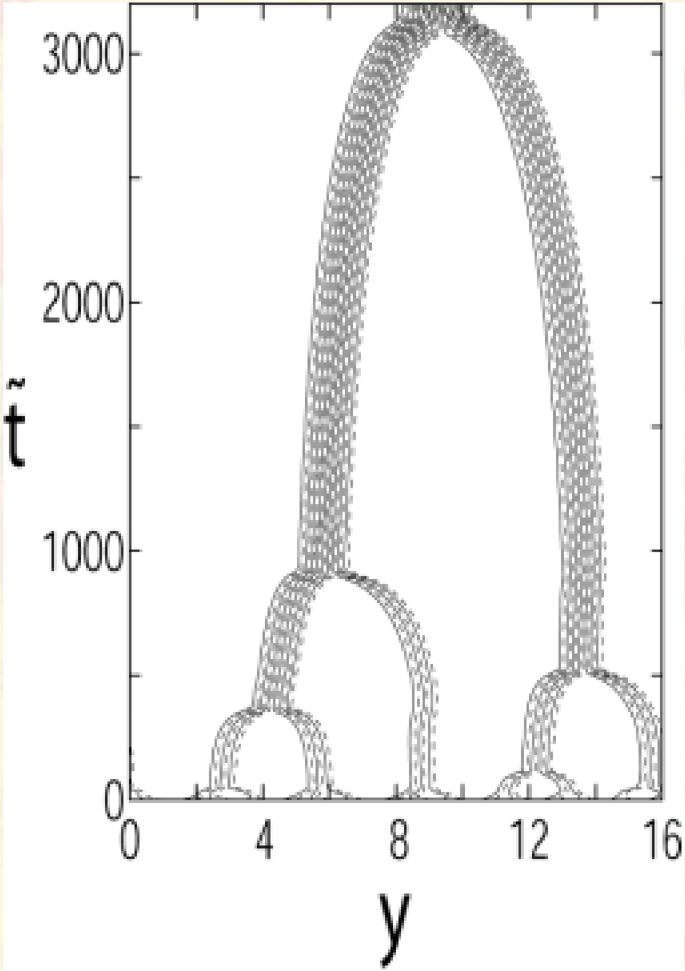


Si(001)
step-up drift

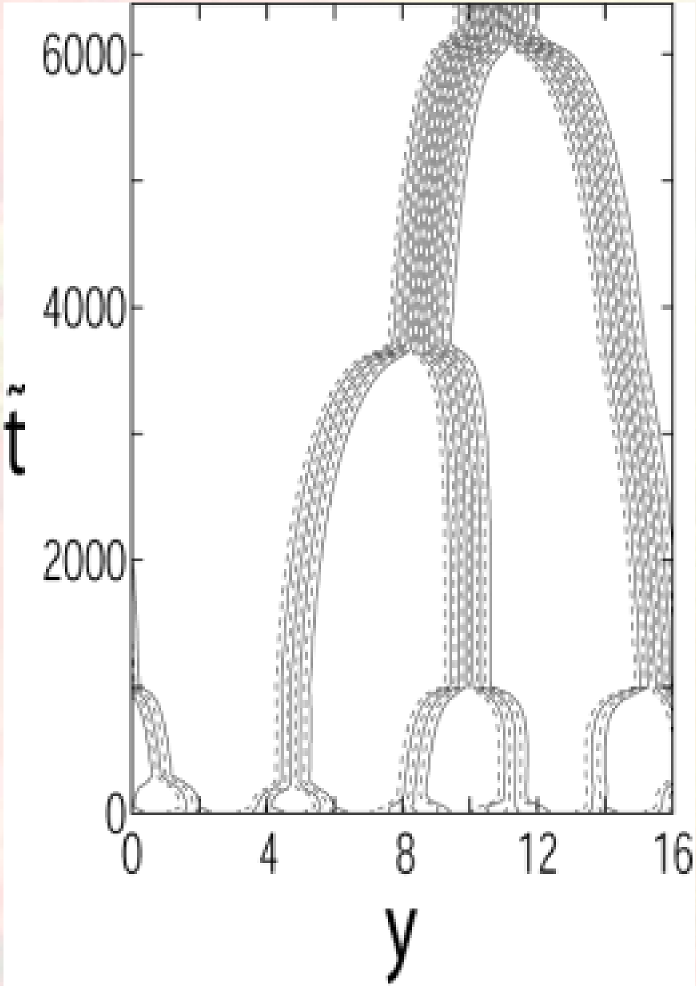


Drift direction and bunching Instability

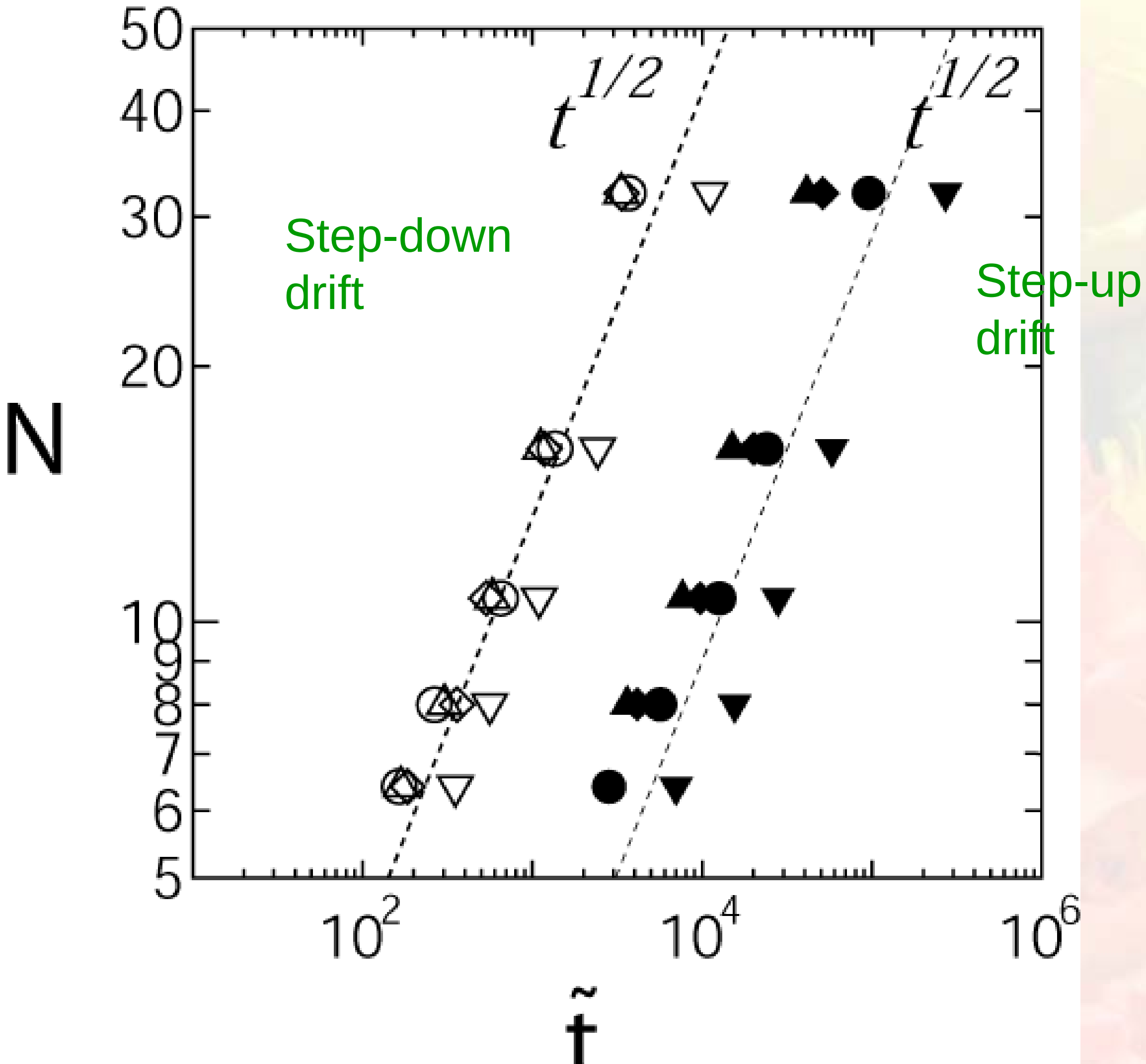
Step-down



Step-up



Growth rate of step bunches

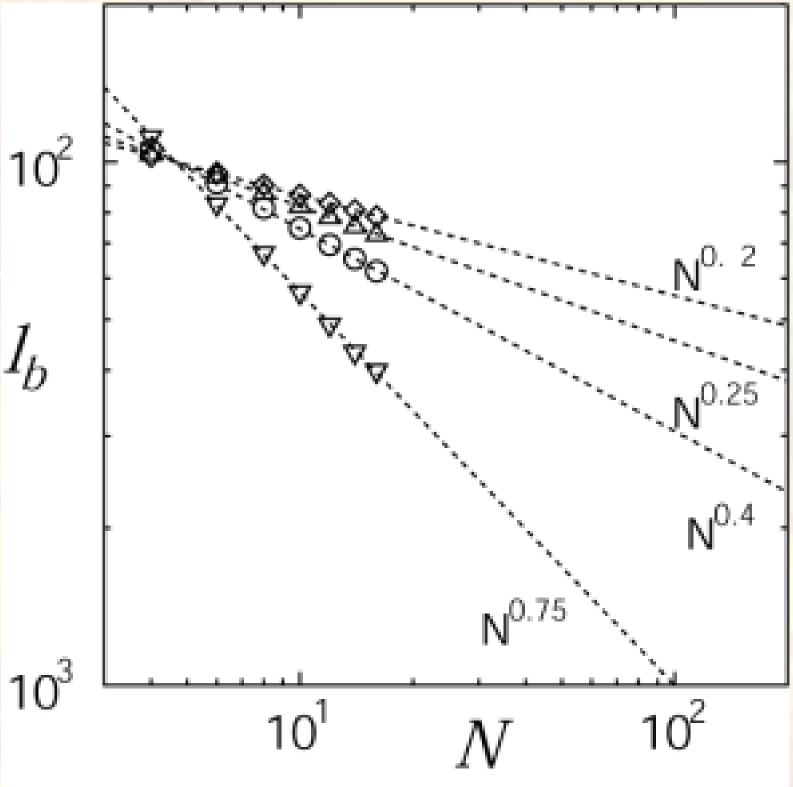


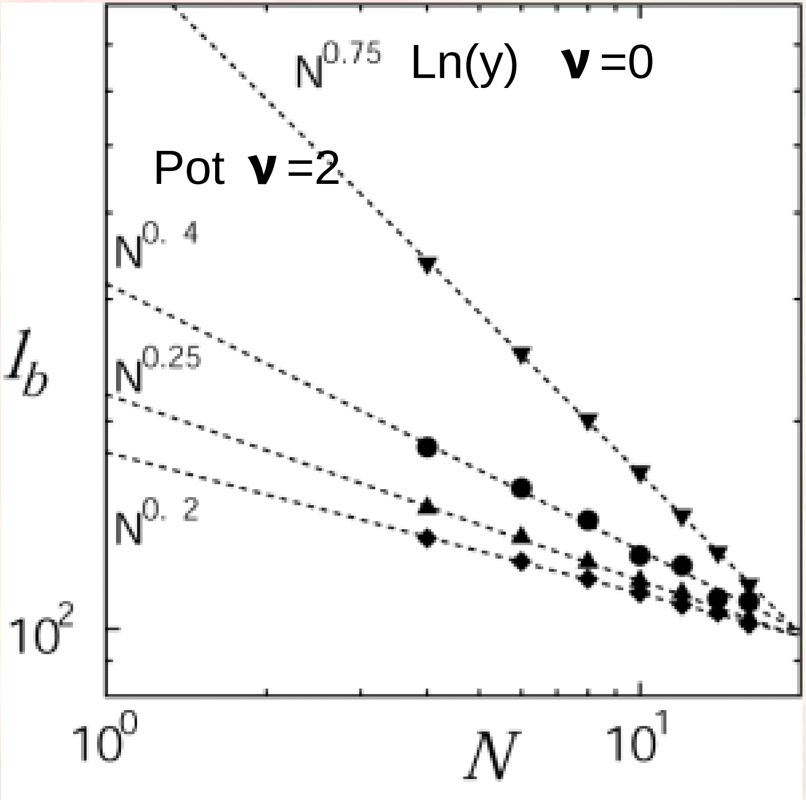
Step distance l_b in a bunch of size N with step repulsion potential $\propto l^{-\nu}$

Step-down

Exponent=3/2(ν+2)

Step-up





Anisotropic diffusion and drift in the Monte Carlo simulation

$$\mathrm{Pr}_{move} = \frac{1}{4} p \left(1 \pm \frac{Z_{eff} eEa}{2k_B T} \right)$$

- Choose an atom

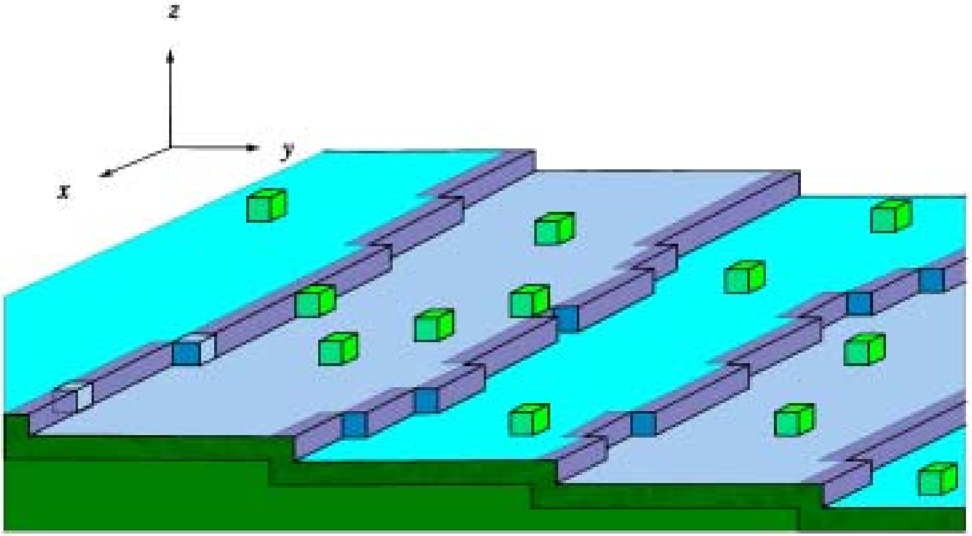
  ↓

  Terrace: A or B

  ↓

  Reduction factor for diffusion if the motion is in the slow direction

Drift is taken account as a biased diffusion.



Drift direction and bunching instability

Step-down

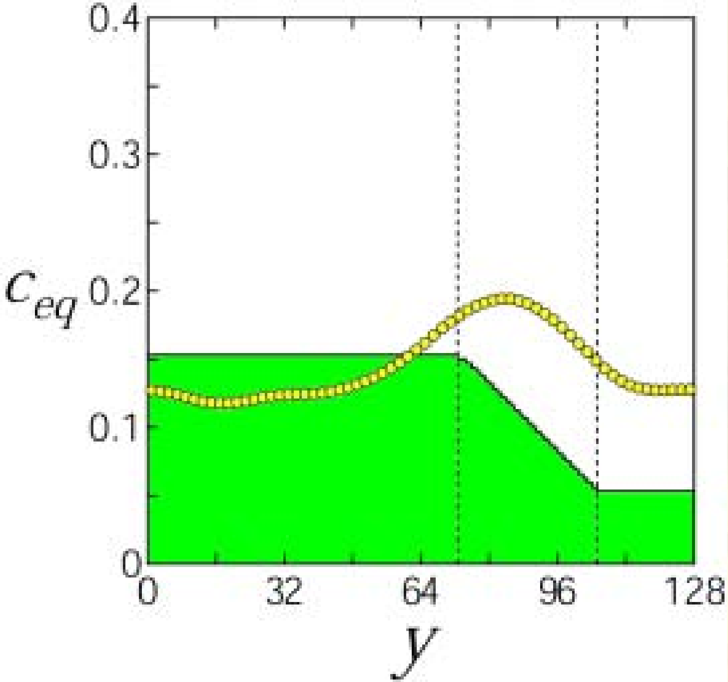
Step-up

Heavy figures deleted. See

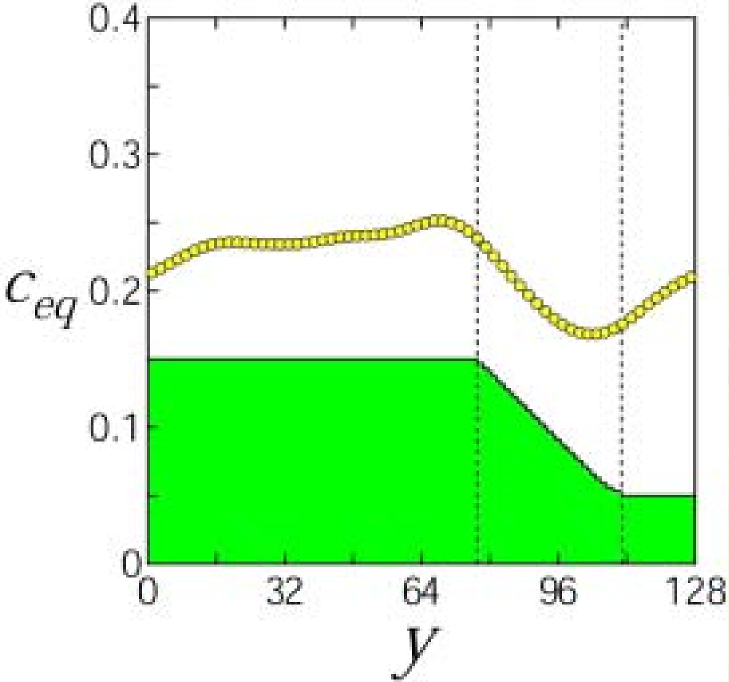
M. Sato, M. Uwaha, and Y. Saito：J. Cryst. Growth **237-239** (2002) 43

Average profile of the surface and adatom density

Step-down



Step-up



Drift →

← Drift

Drift direction and growth rate of bunches

Step-down

$$N_{bunch} \propto t^{1/2}$$

Step-up

Heavy figures deleted . See
M. Sato, M. Uwaha, and Y. Saito：J. Cryst. Growth **237-239** (2002) 43

Drift direction and bunching instability

Step-down

Step-up

Heavy figures deleted . See

M. Sato, M. Uwaha, and Y. Saito：J. Cryst. Growth **237-239** (2002) 43

Drift direction and instability in MC simulation with strong step repulsion

Step down

Step up

Heavy figures deleted. See

M. Sato, M. Uwaha, Y. Saito and Y. Hirose, Phys. Rev. B 67, 125408 (2003)

Steady state of step pairs with step-up drift

- Step-up drift

  ↓

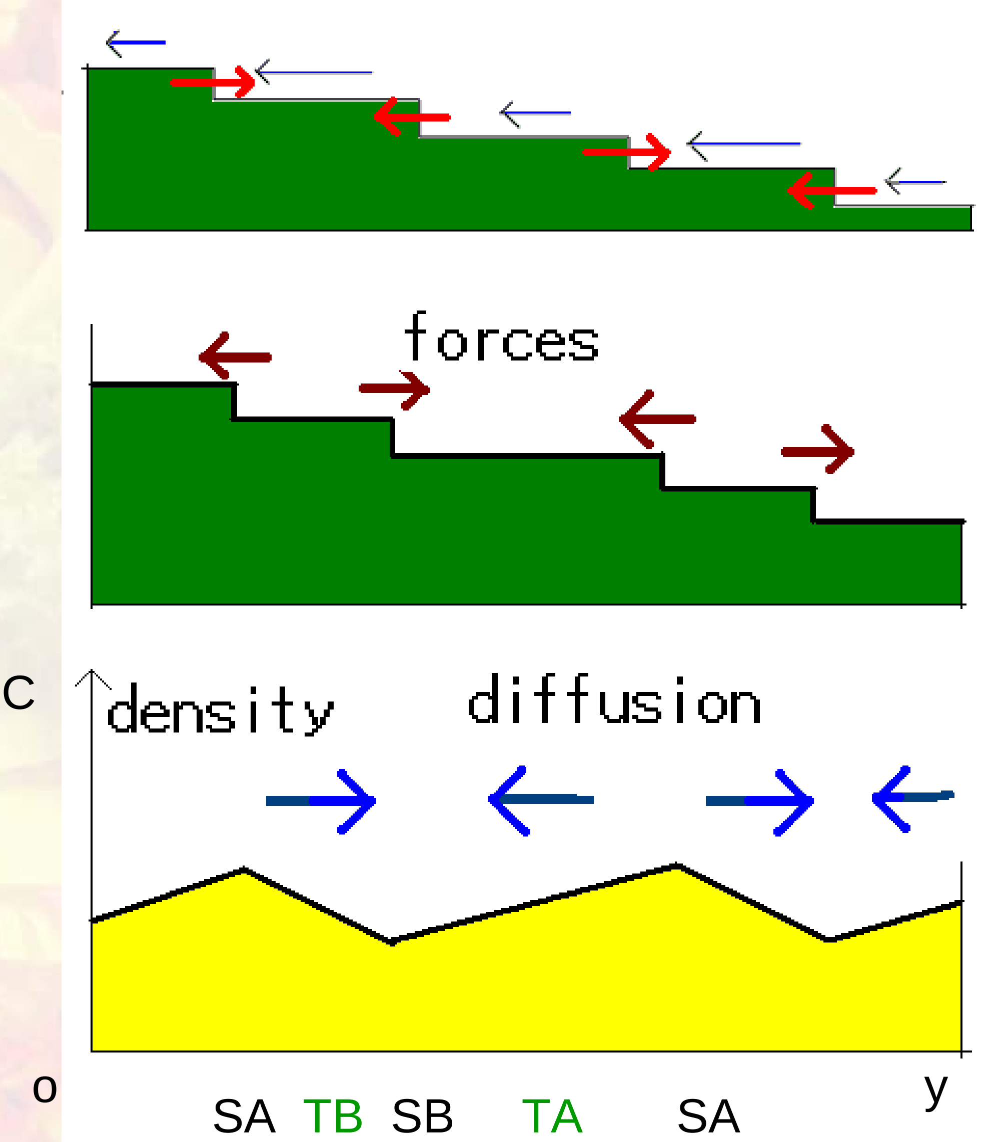
  Slow TB terraces expand

  ↓

  Repulsion produces alternating density gradient

  ↓

  Diffusion current perpendicular to the drift is large on slow TB terraces



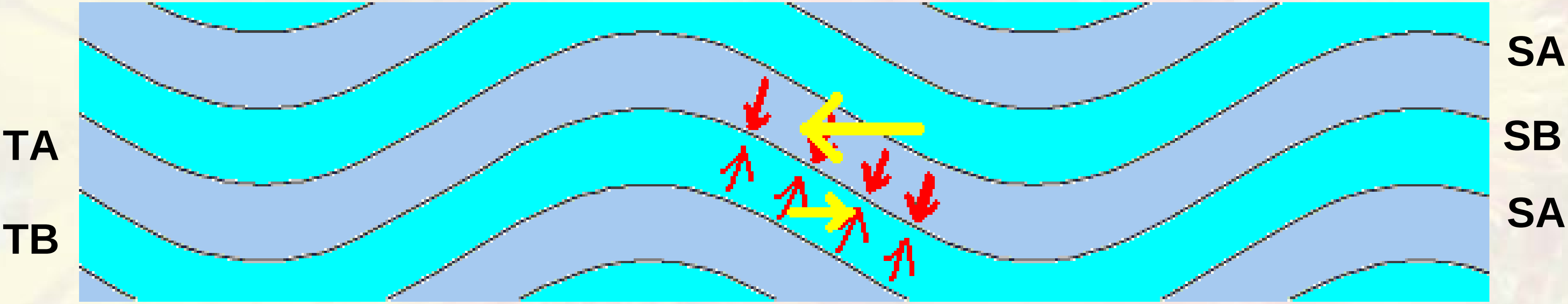
In-phase step wandering induced by the drift without evaporation

- Net diffusion current in x-direction

$$J_x^A + J_x^B \propto (D_\perp - D_{II})\Delta c \tan\theta \propto \frac{\partial y_s(x)}{\partial x}$$

- Restoring current due to the step stiffness

$$j_x \propto -\frac{\partial \mu}{\partial x} \propto -\frac{\partial}{\partial x}\left(\tilde{\beta}\frac{\partial^2 y_s}{\partial x^2}\right)$$



Wandering motion by the transverse currents

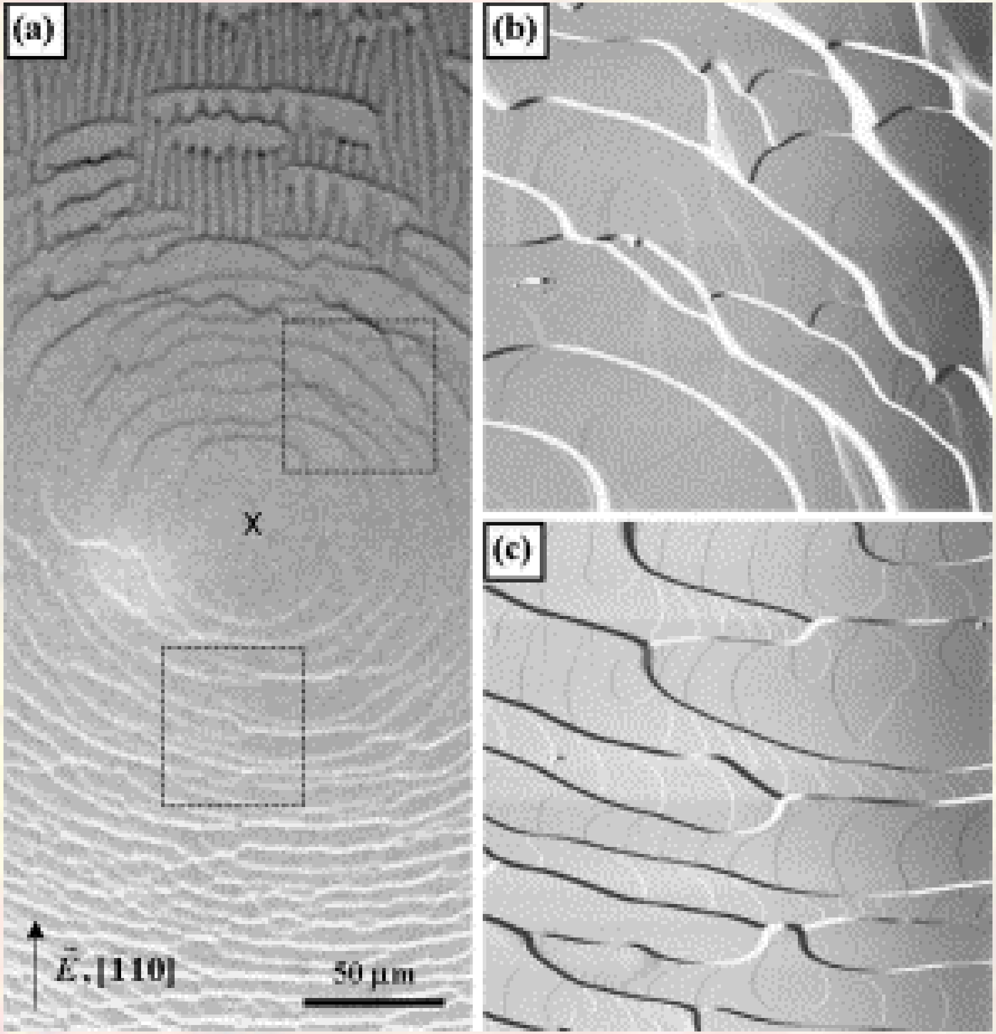
- The balance of adatom currents in *x*-direction

$$
\begin{aligned}
&\frac{\partial y_s}{\partial t} \propto -\nabla \cdot J \\
&= -\frac{\partial}{\partial x}(J_x^A + J_x^B + J_x^{relax}) \\
&\propto -\frac{\partial}{\partial x}\left(\frac{\partial y_s(x)}{\partial x} - \frac{\partial}{\partial x}\left(\frac{\partial^2 y_s(x)}{\partial x^2} \right)\right) \\
&= -\frac{\partial^2 y_s(x)}{\partial x^2} + \frac{\partial^4 y_s(x)}{\partial x^4} \\
&\propto (k^2 - k^4) y_s(k)
\end{aligned}
$$

Si(001) surface after CD heating

- Dimpled Si(0 0 1) surface heated to 990 ° C for 18 h with the current along [-110].
- (b)and(c) ”Illuminated” from the left.

Nielsen, Pettersen, Pelz,
Surf. Si. **480** (2001) 84



Nonlinear effect in conservative systems

- Velocity of a step

$$\frac{\partial y_s(x)}{\partial t} = -\frac{\partial}{\partial x} J_x = -\frac{\partial}{\partial x}\left(J_x^{growth} + J_x^{relax}\right)$$

- Full equation (after scale transformation)

$$\frac{\partial y_s}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{1}{1+\left(\frac{\partial y_s}{\partial x}\right)^2}\left(\frac{\partial y_s}{\partial x} + \frac{\partial}{\partial x}\left(\frac{\frac{\partial^2 y_s}{\partial x^2}}{\left(1+\left(\frac{\partial y_s}{\partial x}\right)^2\right)^{3/2}}\right)\right)\right]$$

Pierre-Louis, Misbah, Saito, Krug, Politi: Phys. Rev. Lett. 80 (1998) 4221

Instabilities by drift in MC simulation with strong step repulsion

Step down

Step up

Heavy figures deleted See
M. Sato, M. Uwaha, Y. Saito and Y. Hirose, Phys. Rev. B 67, 125408 (2003)

Evolution of wandering pattern---coarsening

t =2.5x10^5

t =12.5x10^5

Heavy figures deleted See
M. Sato, M. Uwaha, Y. Saito and Y. Hirose, Phys. Rev. B 67, 125408 (2003)

Evolution of wandering ---coarsening exponents

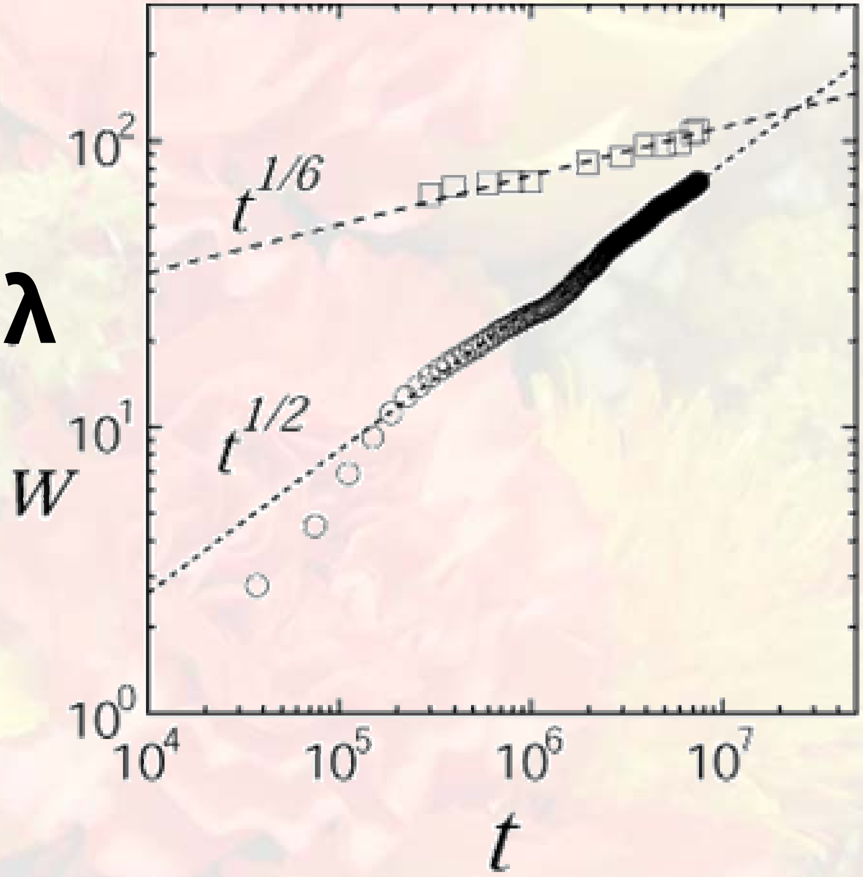
Wandering amplitude

$$w \propto t^{1/2}$$

Wandering wavelength

$$\lambda \propto t^{1/6}$$

Agree with the result of numerical integration of the continuum equation (Paulin, Gillet, Pierre-Louis, Misbah, Phys. Rev. Lett. 86 (2001) 5538)



Summary

- Formation of large bunches in both drift directions is explained by a simple picture.

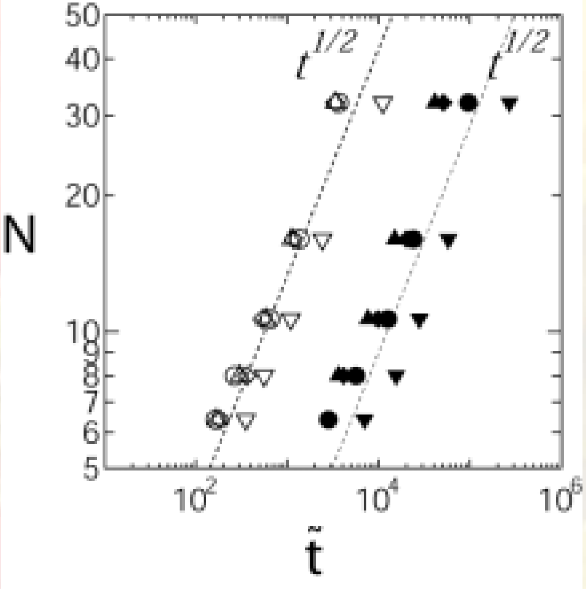
- Under strong step repulsion, bunching is suppressed but in-phase step wandering occurs with step-up drift → Periodic growing pattern appears.

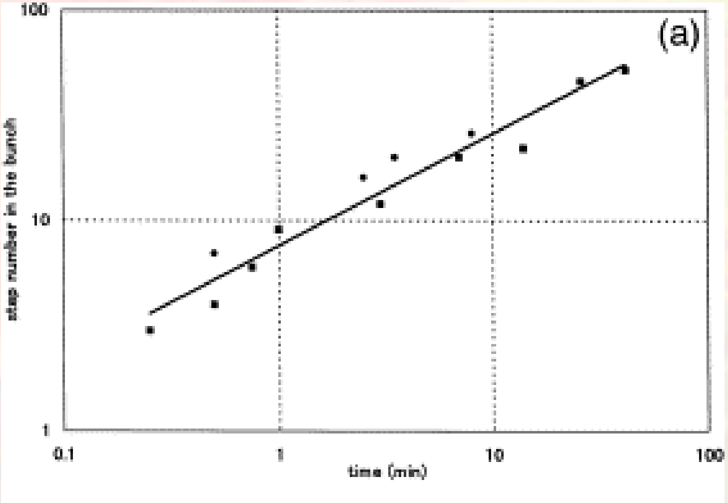
  ↑ Imbalance of diffusion current by the step repulsion (many-body effect!)

  (in agreement with experiment)

Remaining problem

- Why is the time scale for bunch growth independent of the drift direction?





Thanks to CSCAMM