Plan of My Talk

- Instabilities of a vicinal face--- bunching and wandering of simple steps: instabilities on a Si(111) vicinal face.
- Step bunching on a Si(001) vicinal face under direct current heating.
- Step wandering on a Si(001) vicinal face under direct current heating.
- Step wandering on a Si(111) vicinal face near $T_c$ during growth.
- Summary

Instabilities of simple steps related to the adatom diffusion on the terraces (1)

Growth or sublimation with the E-S effect (i.e. diffusion barrier at the step)

- Step wandering in growth
  (Bales, Zangwill: Phys. Rev. B 41, 5589 (1990))

- Periodic wandering without evaporation

- Chaotic wandering with evaporation

- Step bunching in sublimation
  (Schwoebel, Shipsey: J. Appl. Phys. 37, 3682)

Boundary conditions at the steps

- Solidification rate = Velocity of the step
  $j_{sed} = j_s(y, \Omega) - j_s(y, c) = K_s(\phi(y, c) - c_{eq}) + K_y(\phi(y, c) - c_{eq})$

- Equilibrium adatom density at the step
  $c_{eq} = c_{eq}^{s}(1 + \frac{\Omega}{k_B T})$
  $c_{eq} = c_{eq}^{s} + \frac{\Omega}{k_B T} + \phi(\frac{c_{eq}^{s}}{k_B T} F_{ad} - \phi)$

Morphological instabilities on a vicinal surface

- In-phase wandering (meandering)

- Bunching

- Banding

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Step Pattern Formation on Si Vicinal Surfaces with Two Coexisting Structures

(Si(111) near $T_c$ and Si(001))
Mechanism of step wandering: A kind of Mullins-Sekerka instability

- Frank-van der Merve
- Volmer-Weber
- Stransky-Krastanov

Diffusion territory of the protrusion of a step

Advancing step is unstable
Receding step is stable

Diffusion length

The contribution of the lower terrace dominates $K_c > K_u$

Instabilities of simple steps related to the adatom diffusion on the terraces (2)

- Drift of adatoms (electromigration) by direct current heating
  - Step wandering with step-down drift
  - Bunching of (impermeable) steps with step-down drift

Experiments on Si(111)

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

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


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


Power law growth if evaporation is negligible.

Mechanism of step pairing on a Si(111) vicinal

Impermeable steps, finite kinetic coefficient

Current on a terrace

$J = -D_i \left( \frac{c_c - c_v}{L} + \frac{c_+ + c_-}{2} \right) v_d$

Step-down drift brings about step pairing

Mechanism of bunch coalescence on a Si(111) vicinal

Current on a terrace

$j = -D_i \left( \frac{c_c - c_v}{L} + \frac{c_+ + c_-}{2} \right) v_d$

Density profile of adatoms
Origin of the growth law of bunches

Current on a terrace
\[ j = -D_i \frac{c_i - c_x}{L} \frac{c_i + c_x}{2} \]

Change of the terrace width
\[ \frac{d\Delta L}{dt} \propto \frac{\Delta L}{N} \propto \frac{D_i}{N} \frac{c_i - c_x}{L^2} \Delta L \]

Collision time
\[ \tau \propto \frac{NL^2}{D_i (c_i - c_x)} \propto L^2 \propto N^2 \]

One can show\[ c_i - c_x \propto N \propto L \] and \[ L \propto N^{-2/(3v+1)} \]

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

- Universal scaling law in bunching as in experiment
\[ L \propto t^{1/2} \]

Alternating structural change of terraces on Si vicinal surfaces

Diffusion anisotropy on a Si(001) vicinal face tilted towards [110]

Two-phase coexistence on a Si(111) vicinal face near the structural phase transition temperature

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

- STM image of a vicinal tilted toward [110]
- Stripes are dimer rows

Si(001) step bunching 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

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.
Si(001) vicinal face tilted toward [110]

- The orientation of dimer rows alternates on consecutive terraces. Diffusion coefficients and drift velocity alternate.

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 the drift of adatoms on a Si(001) vicinal face

- Fast step kinetics is assumed
- Simple steps bunching
- Stable

Pairing of bunches → Formation of large bunches

Simulation of 1D model: drift direction

- $D_{B} = 2D_{A}$
- Step-up drift
- Step-down drift
- Fast TB terraces expand
- Slow TA terraces expand

Density of adatoms in a bunch

- A step pair acts as a simple step
- Si(111) step-down drift
- Si(001) step-up drift

Finite $K$ Infinite $K$


Step distance $l_{B} = N^{-0}$ in a bunch of size $N$ with step repulsion potential → $l^{-0}$

Step-down

Step-up

Empirical exponent: $0 = 3/2(I + 2)$

Growth rate of step bunches

The expected exponent: \( \alpha = 1/(2 + \delta) \)

The growth exponent is not universal.

Comparison with Latyshev's experiment

Assuming the logarithmic and the \( \delta^2 \) repulsion between steps \( \delta = 0.5 \) and \( \alpha = 0.4 \) are obtained.

Drift direction and bunching instability

Average profile of the surface and adatom density

Step bunching on Si(001) vicinal faces

- Large bunches are formed in both drift directions.
- Step pairs and bunches produce a gap in the adatom density and the bunching mechanism is similar to that of simple steps.
- The growth exponent depends on the interaction potential, though weakly.

Si(001) surface after DC heating: Inphase step wandering

- Dampled Si(001) surface heated to 990°C for 18 h with the current along [-110].
- Bunching in both step-up and down current.
- Wandering with step-up current at a large tilt.


Drift direction and instability in MC simulation with strong step repulsion

- **Step down**
- **Step up**

Steady state of step pairs with step-up drift

- Step-up drift
  - Slow TA terraces expand
  - Repulsion produces alternating density gradient.
  - Diffusion current perpendicular to the drift is large on slow TA terraces.

In-phase step wandering induced by the drift without evaporation

- Net diffusion current in x-direction
  \[ J_x^s + J_x^b \propto (D_s - D_b) \Delta \tan \theta \times \frac{\partial \gamma_y(x)}{\partial x} \]
- Restoring current due to the step stiffness
  \[ j_s = -\frac{\beta \mu}{\Delta} \frac{\partial}{\partial x} \left( \frac{\partial^2 \gamma_y}{\partial x^2} \right) \]

Nonlinear effect in conservative systems

- Velocity of a step
  \[ \frac{\partial \gamma_y(x)}{\partial t} = -\frac{\partial}{\partial x} J_s = -\frac{\partial}{\partial x} (J_s^{\text{prop}} + J_s^{\text{visc}}) \]
- Full equation (after scale transformation)
  \[ \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \begin{bmatrix} \frac{\partial \gamma_y}{\partial x} \\ \frac{\partial^2 \gamma_y}{\partial x^2} \end{bmatrix} = \begin{bmatrix} \frac{\partial^2 \gamma_y}{\partial x^2} \\ \frac{\partial \gamma_y}{\partial x} \end{bmatrix} \left( \begin{bmatrix} 1 \\ \left( \frac{\partial \gamma_y}{\partial x} \right)^2 \end{bmatrix} - \left( \frac{\partial \gamma_y}{\partial x} \right) \right) \]

Evolution of wandering pattern---coarsening

- \( t = 2.5 \times 10^5 \)
- \( t = 12.5 \times 10^5 \)

Evolution of wandering ---coarsening exponents

- Wandering amplitude
  \[ W \propto t^{1/2} \]
- Wandering wavelength
  \[ \lambda \propto t^{1/6} \]

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

- The wavelength increases.
- The pattern becomes asymmetric.
- The amplitude growth is slower and saturates.

Effect of impingement $F$ on the wandering

- The wavelength increases.
- The pattern becomes asymmetric.
- The amplitude growth is slower, but the exponent does not change.

Step wandering on Si(001) vicinal faces

With strong step repulsion, bunching is suppressed but in-phase step wandering occurs with step-up drift. Periodic pattern. Imbalance of diffusion current by the step repulsion (in agreement with experiment).

Si(111) step wandering during growth near $T_c$

- Step patterns on vicinal faces of Si(111)

Structure of the vicinal face near $T_c$

- Experimentally, $D_1 c_1 > D_2 c_2$ and the diffusion length in 1x1 phase is larger than that in 7x7.

Two models: diffusion coefficient and lifetime

- Diffusion is faster on the lower terrace
- Evaporation is faster on the upper terrace
- Density is higher on the lower terrace
Simplest model with a gap in diffusion coefficient

\[ d = \frac{l}{2} \]

The terrace is divided into phase 1 (the lower terrace) and phase 2 (the upper terrace) at the center of each terrace.

Adatom current on the terrace during growth without evaporation

- Because of the difference in the diffusion coefficient, adatom current that goes to the upper step is dominant.
- Mass current in x-direction arises.

Nonlinear evolution equation without evaporation

- Velocity of the step

\[ \frac{\partial y(x)}{\partial t} = \frac{\partial}{\partial x} \left( j_x^{\text{mon}} + j_x^{\text{dima}} \right) \]

- Full equation (after scale transformation)

\[ \frac{\partial^2 y(x)}{\partial t^2} = \frac{\partial}{\partial x} \left( \frac{\partial y(x)}{\partial x} \right) - \frac{\partial}{\partial x} \left( x \frac{\partial^2 y(x)}{\partial x^2} \right) \]

Solution of the nonlinear evolution equation and MC simulation result

- The wandering amplitude increases in time as

\[ w \sim t^{1/2} \]

No step repulsion is put in.

- Coarsening also occurs and the wavelength increases as

\[ \sim t^{1/6} \]

Motion of the phase boundary

The phase change is accompanied by a density change.

The density in 1x1 is 6% higher than that in 7x7.

Yang, Williams, Phys. Rev. Lett. 72 (1994) 1862

We regard the phase boundary as a step without height change.

The density gap is much exaggerated.

Elastic interaction between steps and phase boundaries is included.

Comparison of the step patterns in weak evaporation

The pattern is in-phase and periodic if evaporation is weak. In-phase wandering is seen in the different conditions.

Summary for Si(111) near Tc

- Step wandering occurs in growth if diffusion is faster or evaporation is slower in the lower terrace (1×1).
- Wandering pattern in a vicinal face is in-phase and periodic if evaporation is very weak (large diffusion length) as expected in Si(111) near Tc.
- There are several different features in the wandering with the diffusion gap and that with the lifetime gap.

Quantitative comparison with the real system is possible after modifying the model.

Common features of the two systems

- If bunching is suppressed by the repulsion, step wandering occurs due to the difference of the diffusion rate on the two structures. The steps show periodic wandering which grows in the power law $w \propto t^{1/2}$. (This feature is in common with simple vicinals.)
- The repulsive interaction between steps (and the phase boundaries) plays a crucial role to form the stable structure and to produce the current.

Thank you for your attention.