A level set method for spiral crystal growth and growth rate of crystal surface

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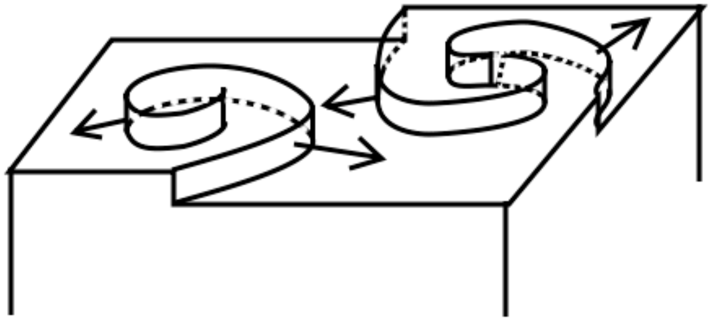
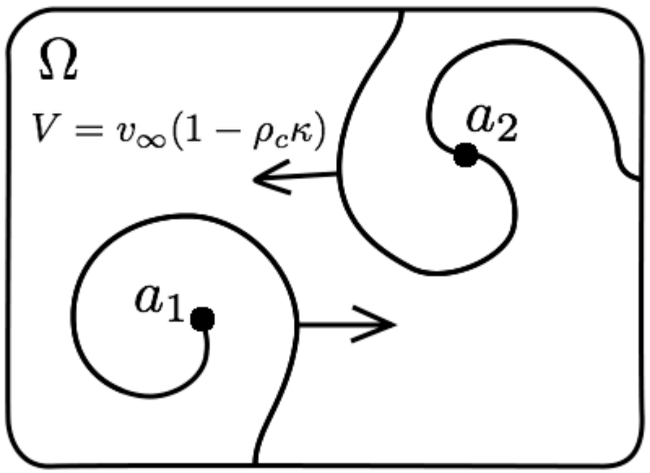
Spiral Crystal growth

Growth of a crystal with aid of screw dislocations. (1949, Frank)



Screw dislocation intersecting a surface provides steps.



<u>Burton-Cabrera-Frank(1951)</u>:

Steps evolve by

$$V = v_\infty(1 - \rho_c \kappa)$$

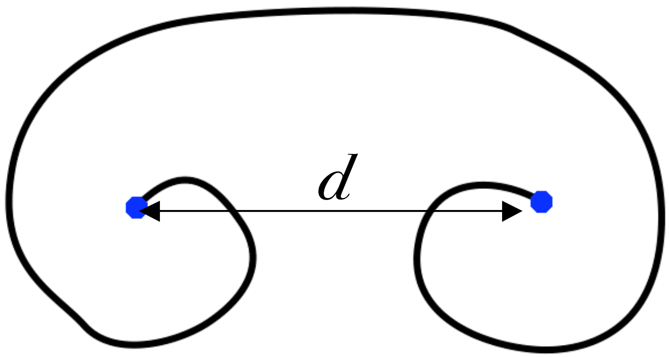
v_∞: velocity of straight line step

ρ_c: critical radius for 2D kernel

Growth of surface by a pair of screw dislocations

Burton-Cabrera-Frank also pointed out:

By an opposite pair:



- $d < 2\rho_c \Rightarrow$ Surface does not evolve(inactive pair)
- $d >> 2\rho_c \Rightarrow$ Grow as single spiral.

AIM: To clarify the relation between the growth rate and the distance of a pair.

Problems: formulation of (1)motion of spirals, (2)height function from spirals, (3)Growth rate, and (4)numerical simulations.

Models for multiple spirals

Difficulty: Evolving spirals, Curvature flow(degenerate parabolic PDE)

●Allen-Cahn type equation('98 Karma-Plapp, Kobayashi)

Phase field model approximating of mean curvature flow

(Multiple-well potential + Sheet structure function)

●Level set method('00 Smereka, '03 Ohtsuka)

Smereka: System of two mean curvature flow equations with auxiliary functions describing the location and existence of steps

Ohtsuka: Single equation with auxiliary function and sheet structure function(given)

Level set formulation ('03 O)

● θ is firstly introduced by Karma-Plapp. or Kobayashi in Allen-Cahn type equation model.

$$\Gamma_t := \bigcup_{k\in\mathbb{Z}} \{x \in \overline{W} \mid u(t,x) - \theta(x) = 2\pi k\}, \quad \vec{\mathbf{n}} = -\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}$$

$$\theta(x) = \sum_{j=1}^{N} m_j \arg(x - a_j)$$

m_j: Strength of s.d.($0,\ \pm 1,\ \pm 2,\ \ldots$)

a_j: Center of s.d.

$$\Rightarrow V = \frac{u_t}{|\nabla(u-\theta)|}, \quad \kappa = \operatorname{div}\left(-\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}\right)$$

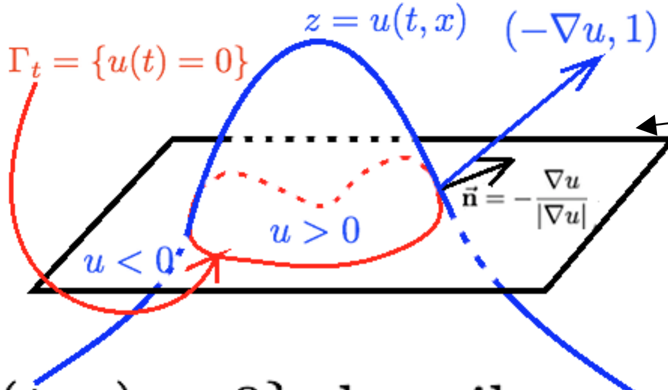
Level set equation:

$$u_t - v_\infty |\nabla(u-\theta)| \left\{1 + \rho_c \operatorname{div} \frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}\right\} = 0$$

$$\text{in } (0,T) \times \overline{W}$$

Idea of the formulation

Usual level set:

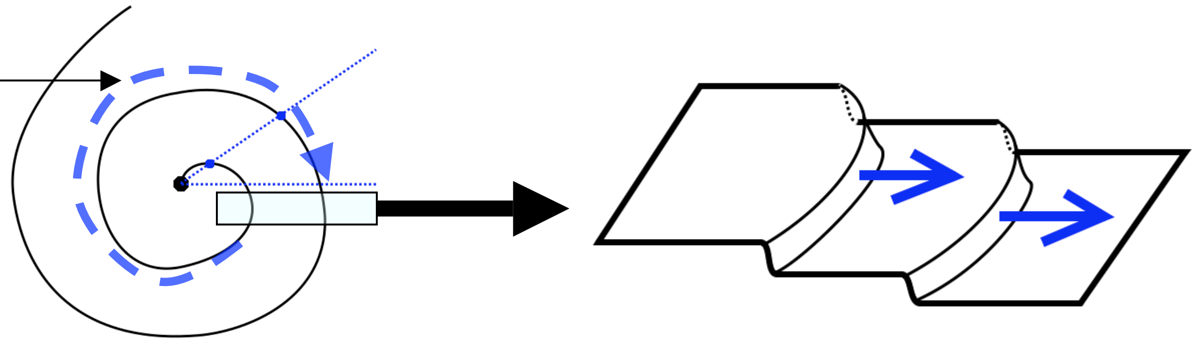


The level surface is the plane.

$\Gamma_t = \{x|\ u(t,x) = 0\}$ describes a closed curve.

Thus, at least usual level set does not work well.

We need decreasing u along to the curve.



$\Rightarrow \Gamma_t = \{x|\ u(t,x) \equiv \arg x\}$

The helical surface plays the role of level surface.

(We regard the spiral curve as the curve on the helical surface.)

Height function

Assumption: Displacement of lattice by screw dislocations is only in vertical direction.

$$\Delta h = -h_0 \mathrm{div} \delta_{\Gamma_t} \vec{\mathbf{n}} = \begin{cases} -h_0 \mathrm{div}(\vec{\mathbf{n}}) & \text{on } \Gamma_t \\ 0 & \text{otherwise} \end{cases}$$

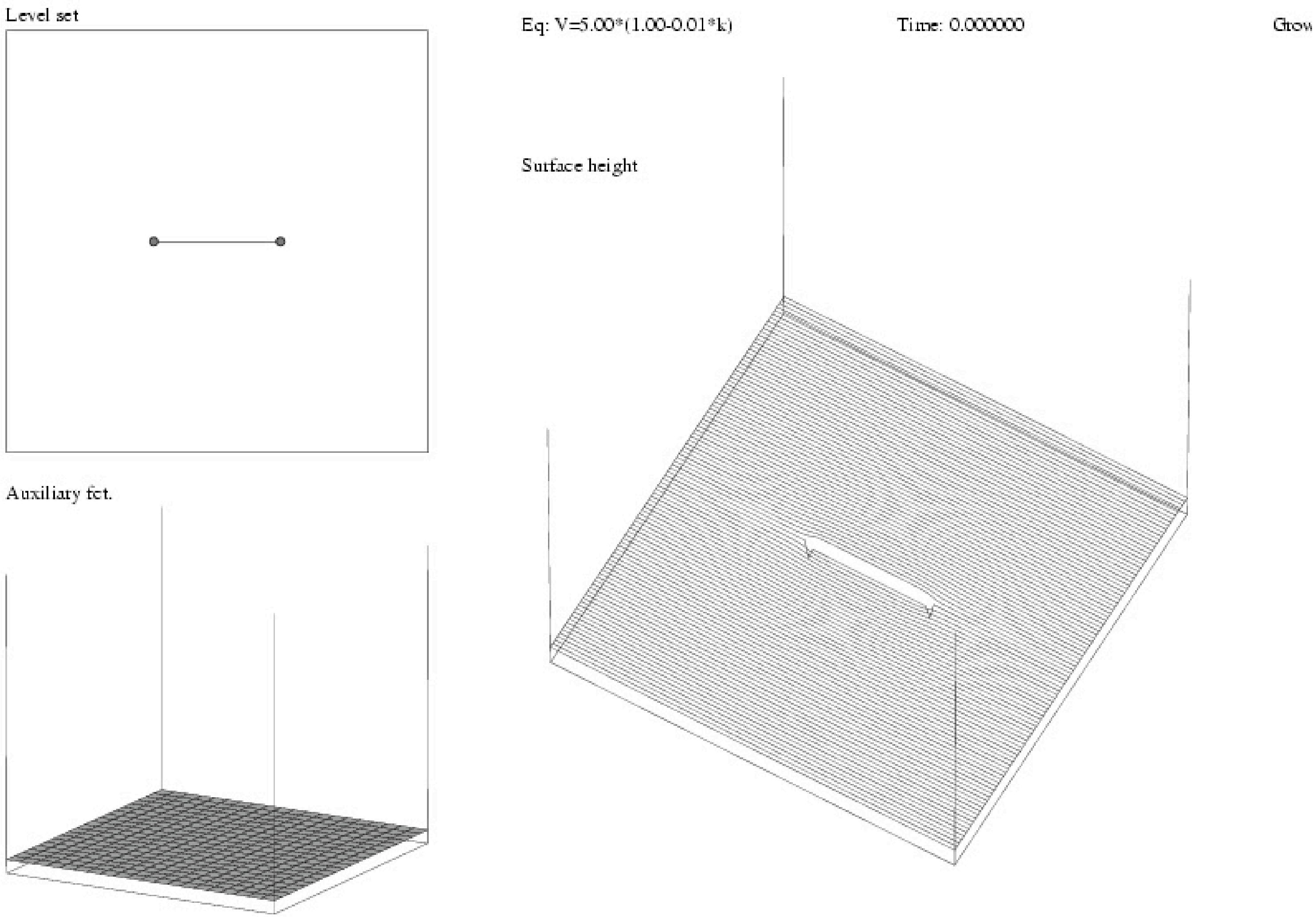
From the theory of dislocation(see Hirth-Lothe),

$$h(x) = \arg(x) \quad \text{if } \Gamma_t = \{(x,0) |\ x > 0\}$$

$$\Rightarrow h(t,x) = \frac{h_0}{2\pi} \theta_{\Gamma_t}(x)$$

Branch of θ whose discontinuities are only on Γ_t.

Sample of simulation



Growth rate

$$R = h_0 \frac{\omega}{2\pi} = \omega_1 \frac{v_\infty}{\rho_c}$$

(ω: angle velocity of rotating spiral)

Rotating number = number of sheets piling up on the surface

Mean height: $R_h(t;t_0) := \frac{1}{|W|}\int_W [h(t,x) - h(t_0,x)]dx$

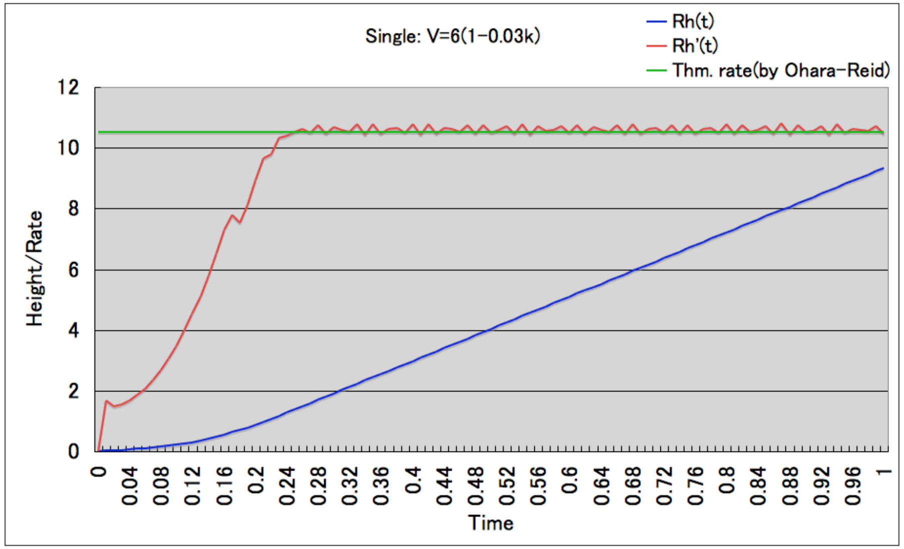
Growth rate: $R_h'(t;t_0)$ (or slope of lin. approx. of $R_h(t;t_0)$).

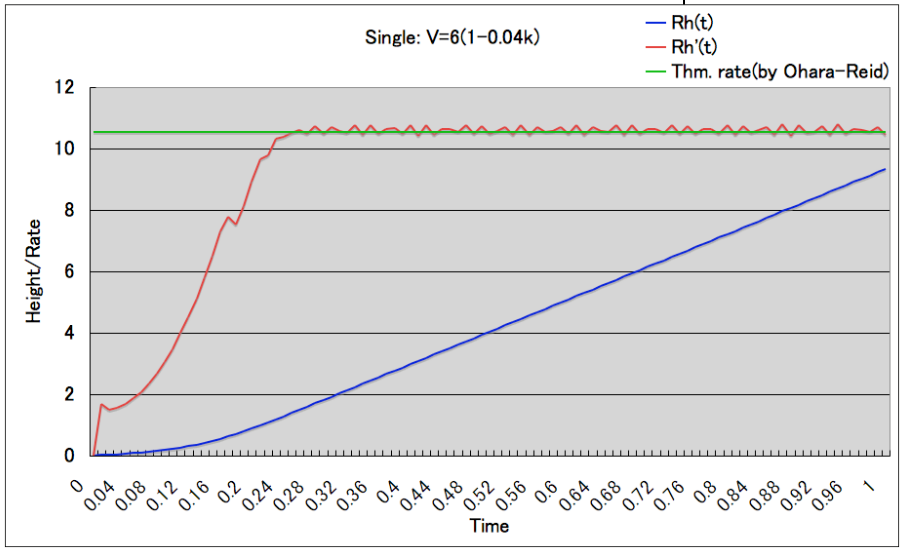
ω_1: 0.315(BCF, approximation by rotating spiral),

0.330958061(Ohara-Reid, shooting method).

Single spiral

$$\theta(x) = \arg(x)$$





ρ_c=0.03

Thm. rate=10.534722

Slope of linear approx.

(0.3≦t≦1)=10.59968608

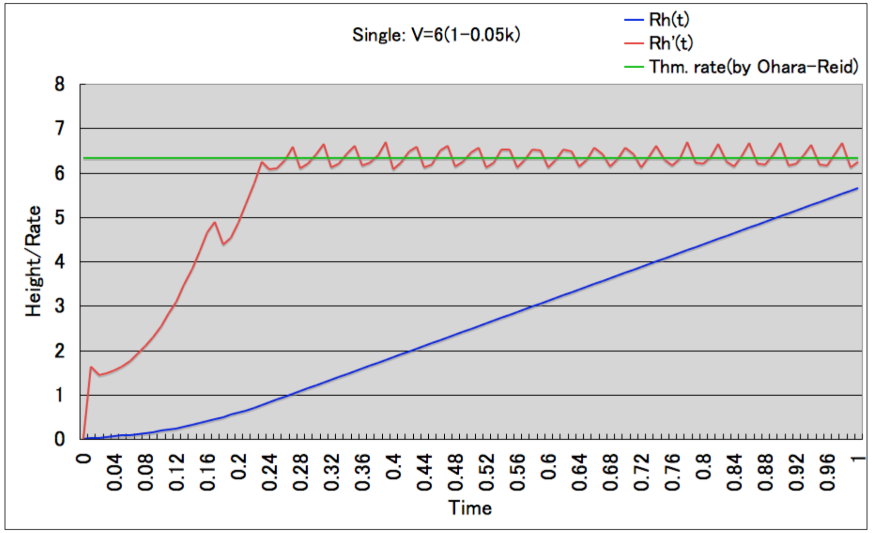
ρ_c=0.04

Thm. rate=7.901042

Slope of linear approx.

(0.3≦t≦1)=7.945823514

Single spiral(2)

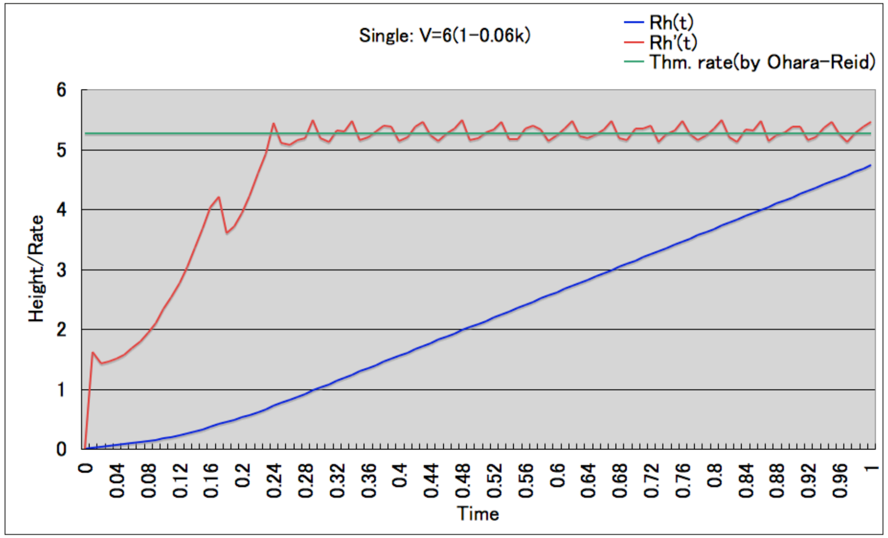


ρ_c=0.05

Thm. rate=6.320833

Slope of linear approx.

(0.3≦t≦1)=6.35231272



ρ_c=0.06

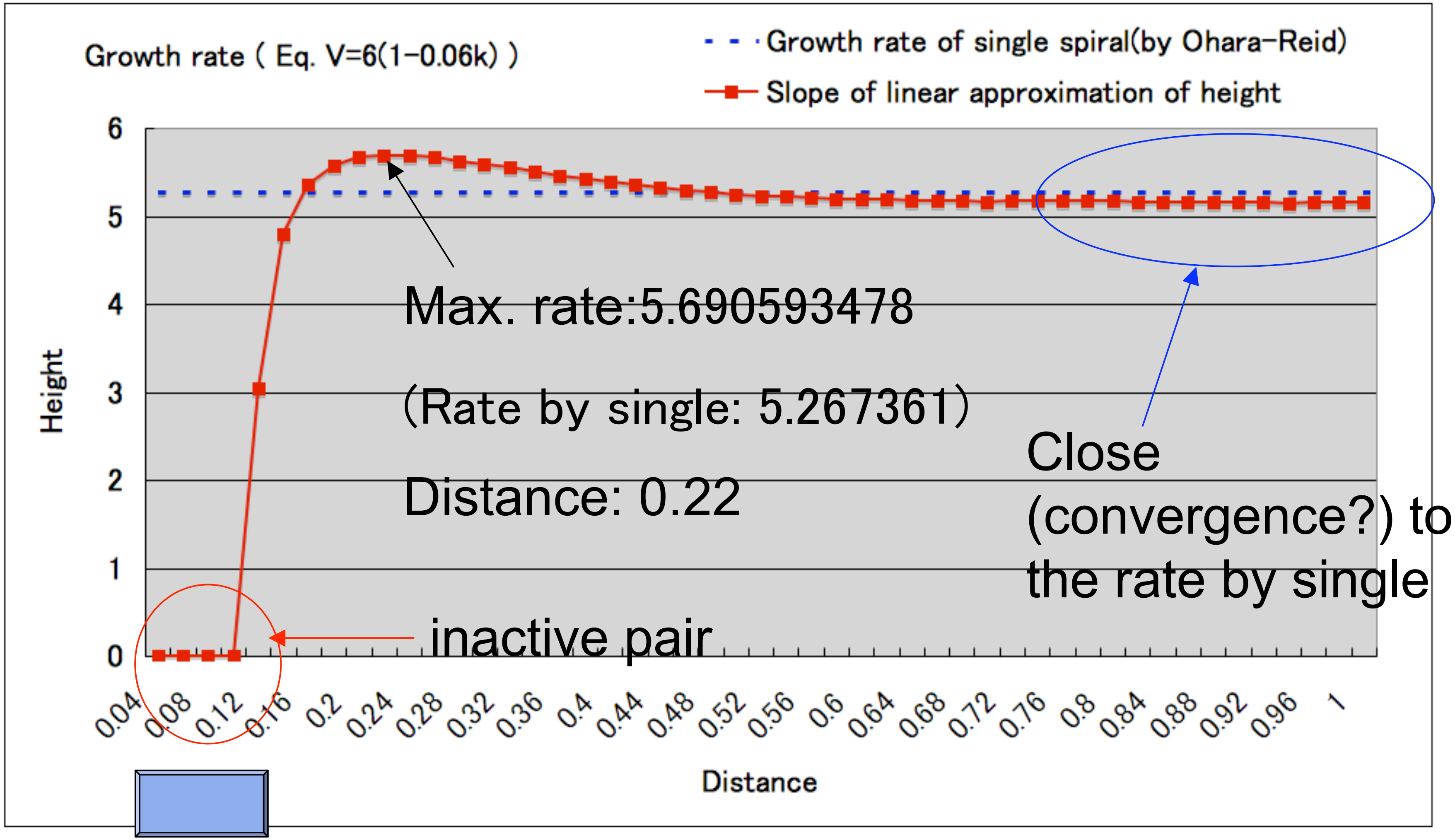
Thm. rate=5.267361

Slope of linear approx.

(0.3≦t≦1)=5.288160184

Opposite pair

$$\theta(x) = -\arg(x - a_1) + \arg(x - a_2),$$
$$a_1 = (-a, 0),\ a_2 = (a, 0)$$



Relation between distance and growth rate

Burton-Cabrera-Frank: Critical distance = “order of 3 ρ_c”.

Critical radius	By single	Maximum growth rate	Distance
0.03	10.534722	11.35638563	0.10
0.04	7.901042	8.519515442	0.14
0.05	6.320833	6.820273597	0.18
0.06	5.267361	5.690593478	0.22
0.07	4.514881	4.874485818	0.26
0.08	3.950521	4.296473992	0.30
0.09	3.511574	3.798435471	0.34
0.10	3.160417	3.454963363	0.38

Numerically, critical distance is close to 4 ρ_c.

Summary

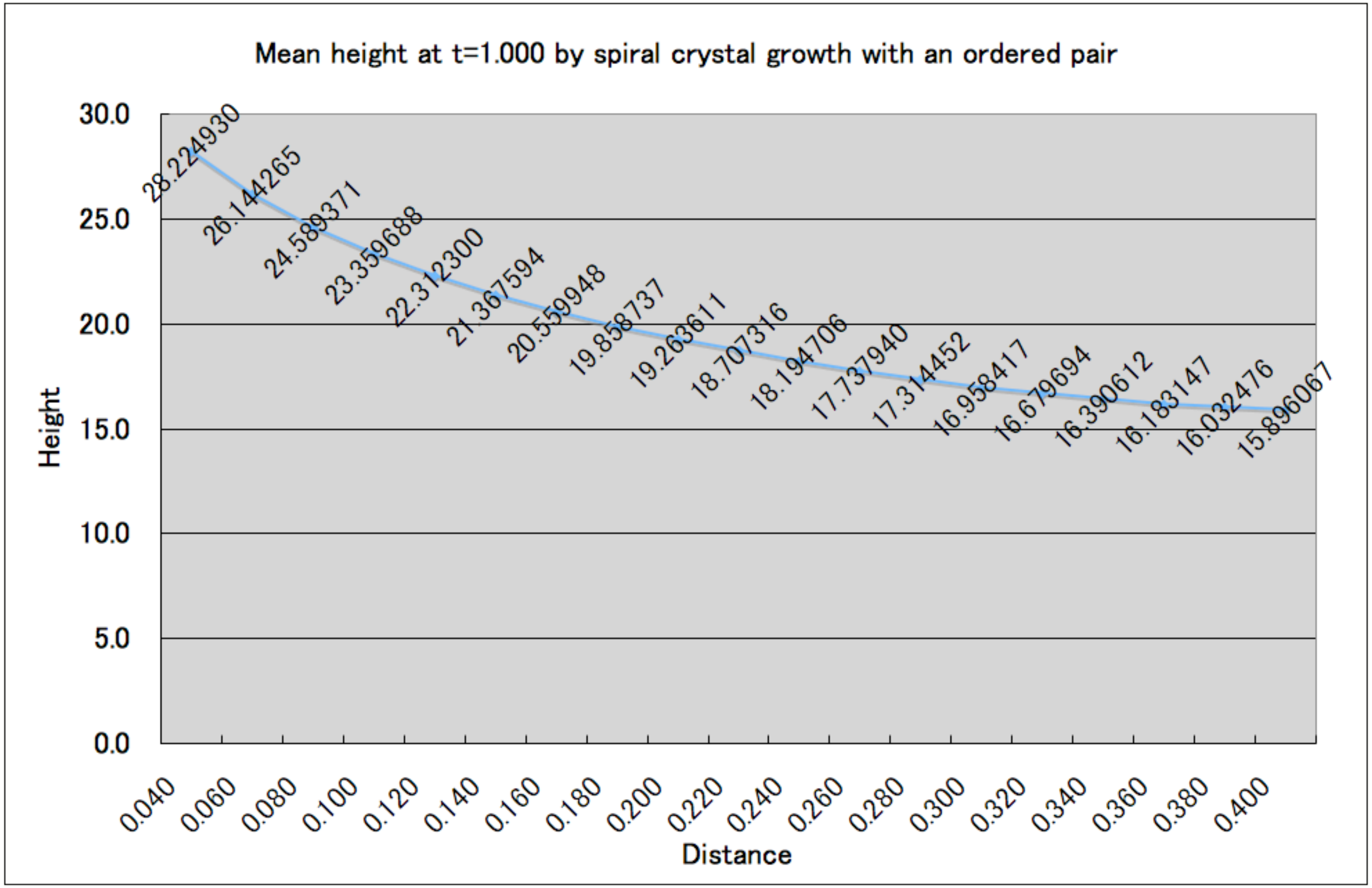
1. Introduction of level set formulation for spirals. (Basically, level set method or phase field model are mathematical formulation for motion of interfaces.)
2. Introduction of growth rate in numerical simulation.
3. Numerical simulation of the growth by an opposite pair.
   1. One can find the existence of inactive pairs, and critical distance giving an maximum growth rate, which is faster than the growth by single spiral.
   2. Critical distance is close to $4\rho_c$. (BCF pointed out that is $3\rho_c$.)

Continue to the poster session

There are numerical simulations

- with impurity
- interlaced spirals
- variable driving force
    - wisker type
    - hollow core type

Ordered pair



Existence of upper bound for inactive pair

Theorem. Assume that N=2, m_1=$-m_2$=1, and $\rho_1 = \rho_2$. If $|a_1 - a_2| < 2/C$, then there exists M>0 such that for any Γ_0 and $u_0 \in C(\overline{W})$ satisfying

$$\Gamma_0 = \{x \in \overline{W};\ u_0(x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\},$$

$$z < M \quad \text{for any } (t,x,z) \in [0,\infty) \times \mathfrak{X}$$

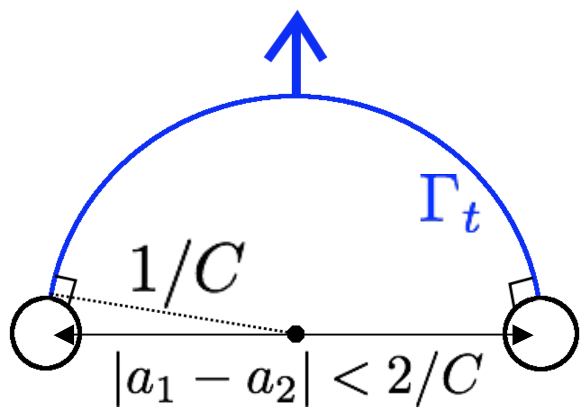
$$\text{satisfying } u(t,x) - z > 0,$$

where $u(t,x)$ is a viscosity solution to (LV) with $u|_{t=0} = u_0$.

Idea of the proof: There exists a Γ which is a part of the circle $|x|=1/C$ satisfying $\Gamma \perp \partial W$.

Let $v(x) = \theta_\Gamma(x) \equiv \arg(x - a_1) - \arg(x - a_2)$ whose discontinuity is only on Γ.

⇒Then $v(x)$ is a viscosity supersolution to (LV).



Inactive pair(Simulation)