On growth speed of a birth-spread model for two-dimensional nucleation on a crystal surface

Yoshikazu Giga (University of Tokyo)
Joint work with
Hiroyoshi Mitake (Hiroshima University)
Hung V. Tran (University of Wisconsin)
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1. Introduction
1.1 Models (for growth of a crystal surface)

**Two-dimensional nucleation:** A flat crystal surface grows by adatoms over the surface. How should one model this phenomenon to measure the growth rate?

There are several models. A typical one is “Birth and Spread Model” (cf. M. Ohara – R. C. Reid (1973))
Birth and Spread Model

1. Birth
Adatoms touch to the crystal surface on a set $E$. The set $E$ is a set of nucleation centers. The height is assumed to be $h > 0$. 

\[
\text{birth}\quad E \rightarrow R^2
\]
2. Spread / propagation

Each layer (step) moves horizontally with horizontal normal speed:

\[ V = v_\infty (\rho_c \kappa + 1). \]

Here \( \kappa \) : the mean curvature (sum of principal curvature)
\( v_\infty > 0 \) : step velocity
\( \rho_c > 0 \) : critical radius

spread

Birth and Spread Model (continued)
Birth and Spread Model (continued)

3. Repeat the Step 1 (Forming the second layer)

4. Repeat the Step 2

and repeat 3 and 4 successively.

Step 3
Birth and Spread Model (continued)

Step 4

Step 5
Derivation of PDE model

Let \( w = w(x, t) \) be the height function at the place \( x \in R^2 \) and the time \( t > 0 \).

1. Birth (with speed \( c > 0 \))

\[
u(x, t) = c \mathbf{1}_E t, \quad \mathbf{1}_E (x) = \begin{cases} 1, & x \in E \\ 0, & x \notin E \end{cases}
\]

or \( u_t = c \mathbf{1}_E \)

2. Spread

\[
u_t = v_\infty \left( \rho_c \ \text{div} \left( \frac{Du}{|Du|} \right) + 1 \right) |Du|
\]

Repeating these processes alternatively with the time grid \( \tau \) and sending \( \tau \to 0 \) to get the equation

\[
w_t - v_\infty \left( \rho_c \ \text{div} \left( \frac{Dw}{|Dw|} \right) + 1 \right) |Dw| = c \mathbf{1}_E
\]

( Trotter-Kato product formula )
Problem

Consider

\[ \begin{cases} \frac{w_t - v_\infty}{\rho_c \text{ div } \left( \frac{Dw}{|Dw|} \right) + 1} |Dw| = c_1 E \\ w|_{t=0} = 0. \end{cases} \]

What is the large time behavior of \( w \)? For example, investigate the asymptotic speed (growth rate)

\[ \lim_{t \to \infty} \frac{w(x, t)}{t} = ? \]

( The value may not be \( c \). )
2. The case of no curvature and spherical symmetric case

2.1 The case $\rho_c = 0$

Equation becomes

$$\begin{cases} w_t - v_\infty |Dw| = c1_E \ (E : \text{bounded closed set}) \\ w \bigg|_{t=0} = 0 \end{cases}$$

The unique “envelope” solution is

$$w(x, t) = c(t - v_\infty \\text{dist}(x, E))_+$$

so that $w/t \to c$ as $t \to \infty$. The set $E$ can be a point or a discrete set, so we need a notion of an envelope solution (Y. G. – N. Hamamuki (2013))
Asymptotic speed in the case $\rho_c = 0$

\[
\begin{cases}
  w_t - v_\infty |Dw| = \sum_{i=1}^{m} c_i 1\{a_i\}, & c_i > 0 \\
  w \big|_{t=0} = 0
\end{cases}
\]

The unique envelope solution is given

\[
w(x, t) = \max_{1 \leq i \leq m} c_i (t - v_\infty |x - a_i|)_+
\]


The problem is **coercive** so general growth rate can be obtained. (N. Hamamuki (2014))

2.2 Spherical symmetric case

From now on, we assume $\rho_c = 1, v_\infty = 1$.
Consider the level-set flow equation of the eikonal-curvature flow $V = \kappa + 1$ with source term $f$:

\[
\begin{cases}
  w_t - \left( \text{div} \left( \frac{Dw}{|Dw|} \right) + 1 \right) |Dw| = f(x) & \text{in } R^n \times (0, \infty), \\
  w \bigg|_{t=0} = w_0 & \text{in } R^n.
\end{cases}
\]
Assumptions on $f$ and $w_0$

Here $f$ is bounded and $f \geq 0$, supp $f$ is compact, $w_0$ is continuous, supp $w_0$ is compact.

Basic properties

• Even if $f$ is discontinuous, there exists a global-in-time viscosity solution, which may not be unique (Y. G. – Mitake – Tran)

• Weak comparison principle holds.
Spherical symmetric case

A non-coercive equation:

\[ w_t - \left(1 - \frac{n-1}{r}\right)w_r = c1_{B(0,R_0)}. \]

Assume that \( E = B(0,R_0) \) a closed ball of radius \( R_0 \) centered at zero. Let \( w \) be the maximum solution of (P) with \( f = c1_E, w_0 = 0 \). The solution \( w \) can be obtained by an explicit calculation.

- \( R_0 < n - 1 \Rightarrow \) the growth is completed in finite time
- \( R_0 > n - 1 \Rightarrow \) the growth rate equals \( c \)
- \( R_0 = n - 1 \Rightarrow w(x,t) = tc1_{B(0,R_0)} \)
  It grows with speed \( c \) in \( B(0,R_0) \) but never grows outside \( B(0,R_0) \)
Spherical symmetric case

**Theorem 2.1.** (i) If $R_0 < n - 1$, then

$$w(x, t) = \min(ct, \varphi(r))$$

$\varphi$: stationary solution

(ii) If $R_0 > n - 1$, then

$$\lim_{t \to \infty} \frac{w(x, t)}{t} = c \quad (\text{locally uniformly})$$

(There is an explicit formula for $w$)

(iii) If $R_0 = n - 1$, $w(x, t) = t \ c1_{B(0,R_0)}$

Here $w$ is the maximal viscosity solution.

Note that even if $E = \partial B(0, R_0)$ with $R_0 > n - 1$, we get $\frac{w(x,t)}{t} \to c$. 

3. Existence of asymptotics speed for a Lipschitz source term (work in progress)

Consider

\[
\begin{cases}
    w_t - \left( \text{div} \left( \frac{Dw}{|Dw|} \right) + 1 \right)|Dw| = f(x) & \text{in } \mathbb{R}^n \times (0, \infty) \\
    w \bigg|_{t=0} = w_0 & \text{in } \mathbb{R}^n
\end{cases}
\]

\(f: \text{bounded, } f \not\equiv 0, \text{supp } f: \text{compact}\)

\(w_0: \text{continuous, supp } w_0: \text{compact}\)

(There is a unique viscosity solution if \(f\) is Lipschitz.)

**Theorem 3.1.** Assume that \(f\) is Lipschitz. Let \(w\) be the viscosity solution of (P). Then \(\lim_{t \to \infty} \frac{w(x, t)}{t} = a\) exists and the convergence is locally uniform.
What is the growth rate $a$?

Let $\phi(t)$ be the maximum value of $w$ at time $t$, i.e.,

$$\phi(t) := \max_{x \in \mathbb{R}^n} w(x, t)$$

**Theorem 3.2 (Subadditivity of $\phi$).** $\phi(t + s) \leq \phi(t) + \phi(s)$ for all $t, s > 0$

**Proof.** Set $v(x, t) := w(x, t + s) - \phi(s)$ so that $v(x, 0) \leq 0$. By the comparison principle, $v(x, t) \leq w(x, t)$, which implies

$$w(x, t + s) \leq w(x, t) + \phi(s)$$

for all $x \in \mathbb{R}^n$. 


What is the growth rate \( a \)\? (continued)

**Lemma 3.3.**

\[
\begin{align*}
  a &= \lim_{t \to \infty} \frac{\phi(t)}{t} = \inf_{t > 0} \frac{\phi(t)}{t}
\end{align*}
\]

**Proof.** Fekete’s lemma on subadditivity says that \( \phi(t)/t \) is nonincreasing. Thus \( \lim_{t \to \infty} \phi(t)/t \) exists.

The growth rate in Theorem 3.1 must be \( \inf \phi(t)/t \).
Idea of the proof of Theorem 3.1

Lemma 3.4 (Lipschitz bound). There exists $C > 0$ depending on $f$ and $w_0$ such that

$$\|w_t\|_{L^\infty(R^n \times [0, \infty))} + \|Dw\|_{L^\infty(R^n \times [0, \infty))} \leq C$$

Proof of Theorem 3.1. For any fixed $R > 0$ we have, by Lemma 3.4,

$$|w(x, t) - \phi(t)| = |w(x, t) - \max_{y \in [-d, d]^n} w(y, t)| \leq L(R + d)$$

where $d$ is taken so that $\text{supp } f, \text{supp } w_0 \subset [-d, d]^n$. Thus

$$\lim_{t \to \infty} \sup_{|x| < R} \left| \frac{w(x, t) - \phi(t)}{t} \right| = 0,$$

which yields Theorem 3.1.
Bernstein’s argument to get a Lipschitz bound (formal proof of Lemma 3.4)

We recall that our equation can be written as

\[ w_t - \sum_{i,j} a_{ij} (Dw) w_{x_i x_j} - |Dw| - f = 0 \]

with \( a_{ij}(p) = \delta_{ij} - p_i p_j / |p|^2 \). We set \( U = |Dw|^2 / 2 \) and differentiate in \( x_k \) the above equation and multiply \( w_{x_k} \) to get

\[
2U_t - \sum_{i,j,k,\ell} a_{ij} \left( U_{x_i x_j} - w_{x_i x_k} w_{x_j x_k} \right) - f_{x_k} w_{x_k} \\
- \left\{ (a_{ij})_{p_\ell} w_{x_i x_j} + \frac{2w_{x_\ell}}{|Dw|} \right\} U_{x_\ell} = 0
\]
Take max point \((x_0, t_0) \in R^n \times (0, T]\) of \(U\), i.e.,

\[
U(x_0, t_0) = \max_{R^n \times [0,T]} U.
\]

(We may assume that \(t_0 > 0\).) At this point \(U_t \leq 0\), \(DU = 0\), \(D^2 U \leq 0\). Thus

\[
\sum_{i,j,k} a_{ij} w_{x_i x_k} w_{x_j x_k} - f_{x_k} w_{x_k} \leq 0. \quad (*)
\]

Note that \(0 \leq A \leq I\) for \(A = (a_{ij})\).

A linear algebra inequality \((\text{tr } AB)^2 \leq \text{tr } A \text{ tr } AB^2\) for \(A \geq 0\) implies

\[
\left(\sum a_{ij} w_{x_i x_j}\right)^2 \leq n \sum a_{ij} w_{x_i x_k} w_{x_j x_k}.
\]
Formal proof continued 2

Note that
\[
\left( \sum a_{ij} w_{x_i x_j} \right)^2 = (w_t - |Dw| - f)^2 \geq \frac{1}{2} |Dw|^2 - \exists M_0
\]
provided that \( |w_t| \leq M_1 \) (since \( f \) is Lipschitz).

Thus (*) implies
\[
\frac{1}{2n} |Dw|^2 - Df \cdot Dw \leq M_2 \quad \text{at } (x_0, t_0).
\]

This implies a bound for \( |Dw| \) (or \( U \)). (The bound for \( |w_t| \leq M_1 \) is easier.)

Actual proof needs approximation of the equation so that the equation is parabolic e.g. \( |Dw| \) is approximated by \((|Dw|^2 + \epsilon^2)^{1/2}\).
4. Estimate for asymptotic speed
(Y. G. – H. Mitake – H. Tran, preprint)

Problem. If $f(x) = c1_E$, in what $E$

$$\limsup_{t \to \infty} \frac{w(x, t)}{t} < c \quad \text{and} \quad \liminf_{t \to \infty} \frac{w(x, t)}{t} > 0?$$

We have studied this problem when $E$ is a ball. In this case

$$\frac{w(x, t)}{t} \to 0 \quad \text{or} \quad \frac{w(x, t)}{t} \to c.$$ 

Are there any intermediate situation?
4.1 In the case of square

Assume that \( E = \{(x_1, x_2) ||x_i| \leq d, i = 1, z\} \). Let \( w \) be the maximal solution of

\[
\begin{align*}
  w_t - \left( \text{div} \frac{Dw}{|Dw|} + 1 \right) |Dw| &= c1_E, \\
  w\big|_{t=0} &= 0.
\end{align*}
\]

\( d < 1/\sqrt{2} \)

\( 1/\sqrt{2} < d < 1 \)

\( d > 1 \)
Intermediate situation

**Theorem 4.1 (Y. G. – H. Mitake – H. Tran, preprint).**
Assume that $\frac{1}{\sqrt{2}} < d < 1$. Then there exists $\alpha$ and $\beta$ such that $0 < \alpha < \beta < c$ at

$$
\alpha \leq \liminf_{t\to\infty} \frac{w(x, t)}{t} \leq \limsup_{t\to\infty} \frac{w(x, t)}{t} \leq \beta
$$

locally uniformly for $x \in \mathbb{R}^2$.

Growth speed seriously depends on the shape of $E$. 
4.2 Motion of the top – flow with obstacle

We consider

\[ w_t - \left( \text{div} \frac{Dw}{|Dw|} + 1 \right) |Dw| = c1_E, \quad w\big|_{t=0} = 0 \]

for a general compact set \( E \) in \( R^n \).

By comparison, \( w^*(x, t) \leq ct \) in \( R^n \times (0, \infty) \).

Notation:

\[ A_{\text{max}}(t) = \{ x \in R^n | w^*(x, t) = ct \}. \]
Curvature flow with obstacle

Lemma 4.2. The set $A_{\text{max}}(t)$ is a set theoretic solution of $V = \kappa + 1$ (i.e., $h(x, t) = 1_{A_{\text{max}}(t)}(x)$) is a viscosity subsolution of

$$h_t - \left( \text{div} \frac{Dh}{|Dh|} + 1 \right) |Dh| = 0.$$

Moreover, $A_{\text{max}}(t) \subset E$.

Actually, $h$ is a subsolution of the obstacle problem

$$\max \left\{ h_t - \left( \text{div} \frac{Dh}{|Dh|} + 1 \right) |Dh|, h - 1_E \right\} = 0 \text{ in } R^n \times (0, \infty)$$

Curvature flow with an obstacle: G. Mercier......
Note that
\[ w_c(x, t) := w(x, t) - ct \]
is a viscosity subsolution of (L) and \( w_c \leq 0 \). Moreover, \( A_{max}(t) = \{ x \in R^n | w^*_c(x, t) = 0 \} \). Thus \( A_{max} \) is a set theoretic subsolution (cf. Y. G., Surface Evolution Equations, 2006).

**Proof for** \( A_{max} \subset E \). If not, \( \exists x_0 \in A_{max}(t_0) \cap E^c \) with some \( t_0 > 0 \). Then \( \varphi(x, t) = ct \) is a test function of \( w^* \) from above. This is a contradiction

\[
c = \varphi_t - \left( \text{div} \frac{D\varphi}{|D\varphi|} + 1 \right) \left| D\varphi \right| \mid_{(x_0, t_0)} \leq c1_E(x_0) = 0.
\]
4.3 Upper estimate

Lemma 4.3. Assume that a flow \( V = \kappa + 1 \) with obstacle \( E \) starting from \( E \) vanishes at \( t = t_0 \). Then there exists \( b \in (0, c) \) such that \( \max_x w(x, t_0) \leq bt_0 \).

Proof. Since \( A_{\max}(t_0) = \phi \), we have
\[
\max_x w(x, t_0) < ct_0.
\]
We set
\[
b = \max_x \frac{w(x, t_0)}{t_0}
\]
to get the desired result.
**Global upper estimate**

**Theorem 4.4.** Under the assumption of Lemma 4.3 with \( t_0 \). There exists \( b \in (0, c) \) such that

\[
w(x, t) \leq bt + (c - b)t_0, \quad (x, t) \in \mathbb{R}^n \times (0, \infty).
\]

In particular,

\[
\limsup_{t \to \infty} \frac{w(x, t)}{t} \leq b.
\]
Since

\[ \max_x w(x, t_0) \leq b t_0, \]

by induction we have

\[ w(x, mt_0 + t) \leq w(x, t) + mbt_0 \quad \text{on } R^n \times (0, \infty) \]

In particular, \( w(x, mt_0) \leq mbt_0 \). Thus for \( t \in (mt_0, (m + 1)t_0) \), \( m \in \mathbb{N} \), we observe that

\[
    w(x, t) \leq w(x, mt_0) + c(t - mt_0) \leq bmt_0 + c(t - mt_0) \\
    = bt + (c - b)(t - mt_0) \leq bt + (c - b)t_0
\]

Estimate from below is similar. Theorem 4.1 now follows.
4.4 In the case of square of medium size

Lemma 4.5. If $D > 1$ with $d < 1$, $D = \sqrt{2}d$, then there exists $t_0 > 0$ such that $A_{\text{max}}(t_0) = \phi$. 
Obstacle problem

We shall construct a supersolution of the obstacle problem

\[
\max \left\{ y_t - \frac{y_{xx}}{1 + y_x^2} - (1 + y_x^2)^{1/2}, y - g(x) \right\} = 0
\]

in \((-D, D) \times (0, \infty)\)

where \(g(x) = -|x|, D = \sqrt{2}d\).

To simplify the work, we seek a self-similar solution of form

\[
y(x, t) = \lambda(t)Y \left( \frac{x}{\lambda(t)} \right), \quad \lambda'(t) = \frac{1}{\lambda(t)} - 1.
\]
Idea of the proof of Theorem 4.1

\[
\frac{1}{\sqrt{2}} < d < 1 \text{ yields an intermediate speed }
\]

Lemma 4.5 together with Theorem 4.4 yields an upper bound for \( w \).

We construct a supersolution for the obstacle problem outside \( E \) for \( V = \kappa + 1 \) which leads the estimate for \( w/t \) from below.
Open issues

• **Growth rate.** If $f = c1_E$, we do not know the existence of the growth rate $\lim_{t \to \infty} w/t$. (One has to be careful that in the case of $E = B(0, n - 1)$ critical size the growth rate depends on the place.)

• **Dependence.** does the growth rate depend on $f$ or $E$ continuously?

• **The value of the growth rate.** Is it possible to characterize this quantity?
5. More examples (work in progress)

Consider for \( 1/2 < R_0 < 1, \ a > 0 \)

\[
E = B((-a, 0), R_0) \cup B((a, 0), R_0)
\]

**Corollary 5.1.**  
(i) If \( a > 0 \) is small enough to satisfy \( a + R_0 < 1 \), then \( w \) is bounded in \( R^2 \).

(ii) If \( a > 0 \) a middle length, more precisely, \( 1 < a + R_0 < 2R_0 \). Then there exists \( 0 < \alpha \leq \beta < c \) such that

\[
\alpha \leq \liminf_{t \to \infty} \frac{w(x, t)}{t} \leq \limsup_{t \to \infty} \frac{w(x, t)}{t} \leq \beta.
\]

(iii) If \( a > 0 \) is large enough so that \( R_0 < a \), then \( w \) is bounded.
Figure of two disks

(i) \[ 2a \] 

(ii) \[ a \]

(iii) 

1 < a + R_0 < 2R_0
Other examples

Time dependent source term $c_1 E(t)$

First example

\[ E(t) = \begin{cases} 
B(a_1, R_1) & \text{for } 0 \leq t \leq t_1 \\
B(a_1, R_1) \cup B(a_2, R_2) & \text{for } t_1 \leq t \leq t_2 \\
B(a_1, R_1) \cup B(a_2, R_2) \cup B(a_3, R_3) & \text{for } t_2 \leq t \leq t_3 
\end{cases} \]

Corollary 5.2. If there exists $i$ such that $R_i > 1$, then

\[ w(x, t)/t \to c \quad \text{as} \quad t \to \infty. \]

If $B(a_i, R_i) \cap B(a_j, R_j) = \emptyset$ for all $i, j, i \neq j$, then $w(x, t)$ is bounded if $R_i < 1$ for all $i$. 

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Open problem

If \( B(a_iR_i) \cap B(a_jR_j) \neq \emptyset \) for some \( i, j \) with \( i \neq j \) and \( R_i < 1 \) for all \( i \), what is the growth rate?

Second example

The source term is

\[
c_1^{1_B(0,R(t))}
\]

with a continuous function \( t \mapsto R(t) \).
Corollary 5.3. Assume that there exists

\[
\lim_{T \to \infty} \frac{|\{t \in [0, T] | R(t) < 1\}|}{T} =: \alpha_-
\]

\[
\lim_{T \to \infty} \frac{|\{t \in [0, T] | R(t) = 1\}|}{T} =: \alpha
\]

\[
\lim_{T \to \infty} \frac{|\{t \in [0, T] | R(t) > 1\}|}{T} =: \alpha_+
\]

Then

\[
\lim_{t \to \infty} \frac{w(x, t)}{t} = c(\alpha + \alpha_+) \quad \text{for } x \in B(0,1)
\]

\[
= c(1 - \alpha_-)
\]

\[
\lim_{t \to \infty} \frac{w(x, t)}{t} = c\alpha_+ \quad \text{for } x \in R^2 \setminus B(0,1).
\]
Summary

We have studied asymptotic speed for the level-set equation of the eikonal curvature flow equation with source term.

• Spherical symmetric case: asymptotic speed is computable.
• Lipschitz source term: existence of asymptotic speed
• Case of intermediate speed: application of eikonal curvature flow equation with obstacle.