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Evolution of crystal surface by a single screw dislocation with multiple spiral steps

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1. Introduction

This is a preliminary version to the mathematical results on the growth rate of the surface with rotating spiral steps evolving by an eikonal-curvature equation.

The theory of crystal growth with aid of screw dislocations is proposed by [1]. According to the theory spiral steps on the growing crystal surface are proposed by the screw dislocations across with the surface, and the steps evolve with an eikonal-curvature flow

$$V = v_{\infty}(1-\rho_c\kappa), \tag{1.1}$$

where V denotes the normal velocity in the normal direction $\mathbf{n}$ which is a continuous unit normal vector field of the curve Γ_t denoting spirals, κ is the curvature of the spirals in the direction of $-\mathbf{n}$, v_{∞} and ρ_c are constants denoting the mobility and the critical radius of the two dimensional kernel, respectively. The steps evolve on the helical crystal surface going around the screw dislocations, and then the the surface evolves in the vertical direction. Burton, et al. [1] also give some speculations on the growth rate of the evolving crystal surface, in particular by co-rotating pair of spirals. They pointed out if the distance of the pair is enoughly closer than ρ_c, then the growth rate by the pair is twice of that with a single spiral step.

A level set formulation of evolving spirals Γ_t is proposed by [10] or [11]. In the formulation we regard the surface without spiral centers as the bounded domain $W \subset \mathbb{R}^2$. Then, the spirals are described as a zero point set of $u-\theta$ with an auxiliary function u and the predetermined multiple-valued function

$$\theta(x) = \sum_{j=1}^{N} m_j \arg(x-a_j) \tag{1.2}$$

which is introduced by [8] in the Allen–Cahn type equation for evolving spirals, where a_j denotes a center of j-th screw dislocation for $j=1,\dots N$.

The right angle condition between Γ_t and ∂W, i.e.,

$$\Gamma_t \perp \partial W \tag{1.3}$$

is considered in [10] or [11]. Moreover, a simple method reconstructing the surface from solutions to the level set equation is proposed by [11].

In this paper we investigate the vertical growth rate of the surface with $m(\geq 1)$ rotating spiral steps by (1.1)–(1.3). The goal of this paper is to demonstrate that the growth rate of the surface evolving with rotating $m(\geq 1)$ spiral steps by the eikonal-curvature flow is m times of that with a single rotating spiral step under some suitable assumptions.

Ogiwara and Nakamura [9] obtained similar result of the above with the Allen-Cahn type equation introduced by [8]. The crucial difference between ours and the result in [9] is that the solution as in [9] forms $1/m$ times rotational symmetric pattern. The solution in our level set method does not form such a pattern and keep the rotation angle of the curves in whole time.

This paper is organized as follows. We first introduce the level set method for spirals and a way reconstructing the surface with spiral steps in §2. Then we investigate the vertical growth rate of the surface with rotating spiral steps in §3.

2. Preliminaries

We first introduce briefly the level set formulation for spirals by [10] or [11]. Although we consider only a single spiral case in the next section, we here consider the general case: with multiple screw dislocations and multiple spirals. In §2.2 we propose a way reconstructing the surface with spiral steps from the solution to the level set equation, which is introduced by [11].

2.1. Level set formulation for spirals

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain. We here assume that there exist $N \in \mathbb{N}$ spiral centers denoted by $a_j \in \Omega$ for $j = 1, \dots, N$. Let $m_j \in \mathbb{Z} \setminus \{0\}$ be a signed number of spirals associated with a_j; there exist $|m_j|$ spirals associated with a_j rotating with counter-clockwise (resp. clockwise) rotational orientation if $m_j > 0$ (resp. $m_j < 0$) provided that $V > 0$. See [11] for details of signed number of spirals.

As we explained in the previous section, the spirals at time $t \geq 0$, which is denoted by Γ_t, is described as the zero point set of $u - \theta$ with an auxiliary continuous function u. However, we have to remove an open neighborhood U_j of a_j from Ω because of the singularity of θ at a_j. Thus we now set

$W = \Omega \setminus (\bigcup_{j=1}^N \overline{U}_j)$. Assume that $U_i \cap U_j = \emptyset$ if $i \neq j$, $\overline{U}_j \subset \Omega$, and the boundaries ∂U_j for $j = 1, \dots, N$ or $\partial\Omega$ are smooth so that ∂W is smooth. Then, we now give a level set formulation for spirals as

$$\Gamma_t = \{x \in \overline{W};\ u(t,x) - \theta(x) \equiv 0 \mod 2\pi\mathbb{Z}\},\ \mathbf{n} = -\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}. \tag{2.1}$$

Although the above includes a multiple-valued function, (2.1) is locally similar as the usual level set method with locally smooth function $u - \theta$. Then V and κ are represented as

$$V = \frac{u_t}{|\nabla(u-\theta)|}, \quad \kappa = -\mathrm{div}\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}.$$

Thus, we obtain the level set equation for (1.1)–(1.3) as follows.

$$u_t - v_\infty|\nabla(u-\theta)|\left\{\rho_c\mathrm{div}\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|} + 1\right\} = 0 \quad \text{in} \quad (0,T)\times W, \tag{2.2}$$

$$\langle\vec{\nu}, \nabla(u-\theta)\rangle = 0 \quad \text{on} \quad (0,T)\times\partial W, \tag{2.3}$$

where $\vec{\nu} \in S^1$ is the outer unit normal vector field of ∂W. See [5] for details of the level set method.

When we define $\mathbf{n}$ as in (2.1), we have to clarify "interior" and "exterior" of spirals. In [10] or [11] we introduce a covering space of $\overline{W}$ as

$$\mathfrak{X} = \{(x,\xi) \in \overline{W}\times\mathbb{R}^N;\ (\cos\xi_j, \sin\xi_j) = \overline{x - a_j} \text{ for } j = 1,\dots,N\}, \tag{2.4}$$

where $\xi = (\xi_1, \dots, \xi_N)$ and $\bar{x} = x/|x|$ for $x \in \mathbb{R}^2\setminus\{0\}$. Then, the single-valued function

$$\tilde{u}(t,x,\xi) := u(t,x) - \sum_{j=1}^N m_j\xi_j$$

on $[0,\infty)\times\mathfrak{X}$ plays a role of $u - \theta$ on $\mathfrak{X}$, and thus the "interior" $\widetilde{I}_t$ "exterior" $\widetilde{O}_t$, and spirals $\widetilde{\Gamma}_t$ on $\mathfrak{X}$ is defined as

$$\begin{aligned}
\widetilde{I}_t &= \{(x,\xi) \in \mathfrak{X};\ \tilde{u}(t,x,\xi) > 0\},\\
\widetilde{O}_t &= \{(x,\xi) \in \mathfrak{X};\ \tilde{u}(t,x,\xi) < 0\},\\
\widetilde{\Gamma}_t &= \{(x,\xi) \in \mathfrak{X};\ \tilde{u}(t,x,\xi) = 0\}.
\end{aligned}$$

The definition of $\mathbf{n}$ in (2.1) reflects the direction of the interior and exterior as the above.

Much analysis of (2.2)–(2.3) has been done. Note that the equation (2.2) is degenerate parabolic and has singularities at where $\nabla(u-\theta) = 0$, so that the solutions to (2.2)–(2.3) should be considered in viscosity sense; see [3], [2], [4] for details on theory of viscosity solutions. The comparison principle which implies the uniqueness of the viscosity solutions, and the existence of viscosity solutions to (2.2)–(2.3) for a continuous initial data $u_0 \equiv u(0,\cdot)$ globally-in-time are established by [10]. Then, Γ_t is derived with following way.

(i) Construct $u_0 \in C(\overline{W})$ describing Γ_0 in our level set formulation.

(ii) Solve (2.2)–(2.3) with $u|_{t=0} = u_0$.

(iii) Extract Γ_t given by (2.1).

It remains two problems: how to establish (i), and uniqueness of Γ_t with respect to choice of u_0. On (i), the existence of $u_0 \in C(\overline{W})$ describing Γ_0 is proved in [6], and a practical way of the construction u_0 is proposed by [11]. The uniqueness of Γ_t with respect to Γ_0 is also established by [6]. The crucial result is the comparison of interior in $\mathfrak{X}$, which is as follows.

Lemma 2.1 ([6]) *Let u and v be a viscosity sub- and supersolution to* (2.2)–(2.3) *on* $[0,T) \times \overline{W}$ *for some* $T > 0$. *Assume that* $u(0,\cdot)$ *or* $v(0,\cdot)$ *are continuous,* u *and* v *are upper and lower semicontinuous, respectively. If*

$$\begin{aligned}&\{(x,\xi) \in \mathfrak{X};\ \tilde{u}(0,x,\xi) > 0\} \subset \{(x,\xi) \in \mathfrak{X};\ \tilde{v}(0,x,\xi) > 0\}\\ &(\textit{resp. } \{(x,\xi) \in \mathfrak{X};\ \tilde{u}(0,x,\xi) < 0\} \supset \{(x,\xi) \in \mathfrak{X};\ \tilde{v}(0,x,\xi) < 0\}),\end{aligned}$$

then

$$\begin{aligned}&\{(x,\xi) \in \mathfrak{X};\ \tilde{u}(t,x,\xi) > 0\} \subset \{(x,\xi) \in \mathfrak{X};\ \tilde{v}(t,x,\xi) > 0\}\\ &(\textit{resp. } \{(x,\xi) \in \mathfrak{X};\ \tilde{u}(t,x,\xi) < 0\} \supset \{(x,\xi) \in \mathfrak{X};\ \tilde{v}(t,x,\xi) < 0\}),\end{aligned}$$

for $t \in (0,T)$.

Note that only the comparison of interior sets is proved in [6], but the comparison of exterior sets is also derived with parallel argument in [6].

2.2. Height function

A simple way to construct the height function $h(t,x)$ of evolving crystal surface for solution u to (2.2)–(2.3) is introduced by [11].

From the theory of linear elasticity (see e.g. [7]), the crystal surface can be described by the graph of a function $h(t,x)$ which satisfies

$$\begin{cases} \Delta h = 0 \text{ except on } \Gamma_t, \\ h \text{ has jump discontinuities with height } a > 0 \text{ only on } \Gamma_t. \end{cases}$$

The equation for h is represented as

$$\Delta h = -a\mathrm{div}(\delta_{\Gamma_t}\mathbf{n}). \tag{2.5}$$

In [11] the function

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

is introduced instead of solving (2.5) with a suitable boundary condition, where θ_{Γ_t} is a branch of θ whose discontinuities are only on Γ_t. In fact, the above h is a solution to (2.5) by straightforward calculation. A symple way to construct θ_{Γ_t} is proposed by [11]. Let $k = k(t,x) \in \mathbb{Z}$ be such that

$$-\pi \leq u(t,x) - (\Theta(x) + 2\pi k(t,x)) < \pi,$$

where $\Theta = \sum_{j=1}^N m_j\Theta_j(x)$ and $\Theta_j\colon \overline{W} \to [-\pi,\pi)$ is the principal value of $\arg(x-a_j)$. Then,

$$\theta_{\Gamma_t}(x) = \Theta(x) + 2\pi k(t,x) + \pi\vartheta(u(t,x) - (\Theta(x) + 2\pi k(t,x))), \tag{2.6}$$

is our desired function, where $\vartheta\colon \mathbb{R} \to \mathbb{R}$ is the Heaviside function, i.e., $\vartheta(\sigma) = \mathbf{1}_{[0,\infty)}(\sigma) - \mathbf{1}_{(-\infty,0)}(\sigma)$; here $\mathbf{1}_J$ denotes the indicator function for $J \subset \mathbb{R}$. The continuity of θ_{Γ_t} on $\overline{W} \setminus \Gamma_t$ is established from the definition.

To investigate the evolution of the surface by spiral steps we define the mean growth height $H(t)$ of the surface as

$$H(t) = \frac{1}{|W|}\int_W (h(t,x) - h(0,x))\mathrm{d}x. \tag{2.7}$$

3. Surface evolution by multiple spirals associated with a single center

In this section we investigate the surface evolution by a single screw dislocation with multiple spiral steps.

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with smooth boundary. Assume that $0 \in \Omega$ and let $U \Subset \Omega$ be an open neighborhood of $0 \in \Omega$ with smooth boundary. Set $W = \Omega \setminus \overline{U}$ and then ∂W is also smooth.

Assume that $m(\geq 1)$ spirals which are denoted by $\Gamma_0 = \bigcup_{j=0}^{m-1} \Gamma_{j,0}$ associated with a single center $0 \in \Omega$. Let

$$\Gamma_{0,0} = \{P(\sigma) \in \overline{W};\ \sigma \in [0, \sigma_0]\}$$

be a continuous curve which has no self-intersections. Assume that there exists $\alpha_j \in [0, 2\pi)$ for $j = 0, 1, \ldots, m-1$ such that

(A1) $0 = \alpha_0 < \alpha_1 < \alpha_2 < \cdots < \alpha_{m-1} < 2\pi$,

(A2) $R_{\pm\alpha_j}\overline{W} = \overline{W}$ for $j = 0, 1, 2, \ldots, m-1$,

(A3) $\Gamma_{j,0} = R_{\alpha_j}\Gamma_{0,0}$ for $j = 0, 1, 2, \ldots, m-1$,

(A4) $\Gamma_{i,0} \cap \Gamma_{j,0} = \emptyset$ if $i \neq j$,

where R_β is the 2×2 rotation matrix with angle $\beta \in \mathbb{R}$, $R_\beta A = \{R_\beta x \in \mathbb{R}^2;\ x \in A\}$ for $A \subset \mathbb{R}^2$. In this section we consider two kind of the surface evolution:

(E1) by m-spiral steps on Γ_t which evolves with (1.1), (1.3) and the initial condition $\Gamma_t|_{t=0} = \Gamma_0$,

(E2) by only a single spiral step on $\Gamma_{j,t}$ which evolves with the same equations to (E1) and the initial condition $\Gamma_{j,t}|_{t=0} = \Gamma_{j,0}$ for $j = 0, 1, 2, \ldots, m-1$.

We now denote the mean growth height of (E1) or (E2) as $H(t)$ and $H_j(t)$, respectively. The goal of this section is to prove $H(t) = mH_0(t)$.

The situation (E1) is described by our level set formulation as follows.

Step 1. We first construct $u_0 \in C(\overline{W})$ satisfying

$$\Gamma_0 = \{x \in \overline{W};\ u_0(x) - m\theta_0(x) \equiv 0 \mod 2\pi\mathbb{Z}\}, \tag{3.1}$$

where $\theta_0(x) = \arg(x)$. In particular we construct $u_0 \in C(\overline{W})$ satisfying

$$\Gamma_{j,0} = \{x \in \overline{W};\ u_0(x) - m\theta_0(x) \equiv 2\pi j \mod 2\pi m\mathbb{Z}\} \tag{3.2}$$

by the method as in [11].

Step 2. We next solve the level set equation (2.2)–(2.3) with the initial data $u(0, \cdot) = u_0$ and $\theta(x) = m\theta_0$;

$$u_t - |\nabla(u - m\theta_0)| \left\{ \mathrm{div} \frac{\nabla(u - m\theta_0)}{|\nabla(u - m\theta_0)|} + C \right\} = 0 \quad \text{in} \quad (0, T) \times W, \tag{3.3}$$

$$\langle \vec{\nu}, \nabla(u - m\theta_0) \rangle = 0 \quad \text{on} \quad (0, T) \times \partial W. \tag{3.4}$$

Then, Γ_t is extracted as

$$\Gamma_t = \{x \in \overline{W};\ u(t,x) - m\theta_0(x) \equiv 0 \mod 2\pi\mathbb{Z}\}.$$

Step 3. Construct the surface height function h to define the mean growth height H from u as (2.7).

When we consider the situation (E2) in our formulation, rigorously we have to execute the procedure listed above provided that $m = 1$ and $\Gamma_{j,0}$ instead of Γ_0. Hence we consider the equation (3.3), (3.4) with $m = 1$, i.e.,

$$u_t - |\nabla(u-\theta_0)| \left\{ \mathrm{div} \frac{\nabla(u-\theta_0)}{|\nabla(u-\theta_0)|} + C \right\} = 0 \quad \text{in} \quad (0,T) \times W, \tag{3.5}$$

$$\langle \vec{\nu}, \nabla(u-\theta_0) \rangle = 0 \quad \text{on} \quad (0,T) \times \partial W. \tag{3.6}$$

Then $\Gamma_{j,t}$ is described as

$$\Gamma_{j,t} = \{x \in \overline{W};\ v_j(t,x) - \theta_0(x) \equiv 0 \mod 2\pi\mathbb{Z}\}$$

with a solution v_j to (3.5), (3.6) with $v_j(0,\cdot) = v_{j,0}(x)$ satisfying

$$\Gamma_{j,0} = \{x \in \overline{W};\ v_{j,0}(x) - \theta_0(x) \equiv 0 \mod 2\pi\mathbb{Z}\} \tag{3.7}$$

and the same orientation of interior and exterior on $\mathfrak{X}$ as (3.2), i.e.,

$$\{(x,\xi) \in \mathfrak{X};\ \tilde{u}_0(x,\xi) > 2\pi j\} = \{(x,\xi) \in \mathfrak{X};\ \tilde{v}_{j,0}(x,\xi) > 0\}, \tag{3.8}$$

$$\{(x,\xi) \in \mathfrak{X};\ \tilde{u}_0(x,\xi) = 2\pi j\} = \{(x,\xi) \in \mathfrak{X};\ \tilde{v}_{j,0}(x,\xi) = 0\}, \tag{3.9}$$

where $\tilde{u}_0(x,\xi) = u_0(x) - m\xi$, and $\tilde{v}_{j,0}(x,\xi) = v_{j,0}(x) - \xi$. However, our level set formulation enables us to obtain the above situation easily. In fact, $v_j(t,x) := (u(t,x) - 2\pi j)/m$ is also a viscosity solution to (3.5), (3.6) if u is a viscosity solution to (3.3) and (3.4). Moreover $v_{j,0}(x) := (u_0(x) - 2\pi j)/m$ satisfies (3.7), (3.8) and (3.9). Hence we obtain

$$\Gamma_{j,t} = \{x \in \overline{W};\ v_j(t,x) - \theta_0(x) \equiv 0 \mod 2\pi\mathbb{Z}\}$$

by the uniqueness result in [6]. Thus the height of the surface $h_j(t,x)$ and the mean growth height $H_j(t)$ only by $\Gamma_{j,t}$ are defined similarly as h and H by $v_j = (u - 2\pi j)/m$.

We are now in the position to state our main result.

Theorem 3.1 *Assume that (A1)–(A4). Then* $H(t) = mH_0(t)$ *for* $t > 0$.

We here state only the idea of the proof of Theorem 3.1. We first prove the following fundamental result.

Proposition 3.2 *The formula $H(t) = \sum_{j=0}^{m-1} H_j(t)$ holds for $t \geq 0$.*

We here mention the idea of the proof of Proposition 3.2 in a few words. The crucial property is the following description: for $k, k_j \in \mathbb{Z}$ and $t > 0$,

$$\begin{aligned}
&\theta_{\Gamma_t}(x) = m\xi - \pi(2k-1) \\
&\qquad \text{if } (x,\xi) \in \{(y,\eta) \in \mathfrak{X};\ -2\pi k \leq \tilde{u}(t,y,\eta) < -2\pi(k-1)\}, \\
&\theta_{\Gamma_{j,t}}(x) = \xi - \pi(2k_j - 1) \\
&\qquad \text{if } (x,\xi) \in \{(y,\eta) \in \mathfrak{X};\ -2\pi k_j \leq \tilde{v}_j(t,y,\eta) < -2\pi(k_j-1)\},
\end{aligned}$$

where $\tilde{u}(t,x,\xi) = u(t,x) - m\xi$ and $\tilde{v}_j(t,x,\xi) = v_j(t,x) - \xi$. The above implies

$$\theta_{\Gamma_t} = \sum_{j=0}^{m-1} \theta_{\Gamma_{j,t}} + \pi(m-1)$$

and then we obtain $H(t) = \sum_{j=0}^{m-1} H_j(t)$.

Thus, it suffices to prove $H_j(t) = H_0(t)$ for $j = 0, 1, \ldots, m-1$ and $t > 0$. For this purpose we prove the rotational relations between the domain where is not step on Γ_0 and that on Γ_j, i.e.,

$$\begin{aligned}
&\{(x,\xi) \in \mathfrak{X};\ -2\pi k < \tilde{v}_{j,0}(x,\xi) < -2\pi(k-1)\} \\
&\quad = \widetilde{R}_{\alpha_j}\{(x,\xi) \in \mathfrak{X};\ -2\pi k < \tilde{v}_{0,0}(x,\xi) < -2\pi(k-1)\} \\
&\quad := \{(R_{\alpha_j}x, \xi + \alpha_j) \in \mathfrak{X};\ -2\pi k < \tilde{v}_{0,0}(x,\xi) < -2\pi(k-1)\} \\
&\quad = \{(x,\xi) \in \mathfrak{X};\ -2\pi k < \tilde{v}_{0,0}(R_{-\alpha_j}x, \xi - \alpha_j) < -2\pi(k-1)\}.
\end{aligned}$$

Note that

$$\tilde{v}_{0,0}(R_{-\alpha_j}x, \xi - \alpha_j) = \frac{u_0(R_{-\alpha_j}x)}{m} + \alpha_j - \xi,$$

which is well-defined by (A2). Then, the function

$$v_j(t, R_{-\alpha_j}x) + \alpha_j = \frac{u(t, R_{-\alpha_j}x)}{m} + \alpha_j$$

is also well-defined by (A2), and a viscosity solution to (3.5)–(3.6) with initial data $v_j(0, R_{-\alpha_j}x) + \alpha_j = u_0(R_{\alpha_j}x)/m + \alpha_j$ by the rotation invariance on (3.5)–(3.6). Then, by Lemma 2.1 we obtain

$$\begin{aligned}
&\{(x,\xi) \in \mathfrak{X};\ -2\pi k < \tilde{v}_j(t,x,\xi) < -2\pi(k-1)\} \\
&\quad = \{(x,\xi) \in \mathfrak{X};\ -2\pi k < \tilde{v}_0(t, R_{-\alpha_j}x, \xi - \alpha_j) < 2\pi(k-1)\}. \qquad (3.10)
\end{aligned}$$

Thus we obtain $h_j(t,x) = h_0(t, R_{-\alpha_j}x) + a(\ell + \alpha_j/2\pi)$ with a constant $\ell \in \mathbb{Z}$, which implies

$$\begin{aligned} H_j(t) &= \frac{1}{|W|}\int_W (h_j(t,x) - h_j(t,x))\mathrm{d}x \\ &= \frac{1}{|W|}\int_W (h_0(t, R_{-\alpha_j}x) - h_0(t, R_{-\alpha_j}x))\mathrm{d}x \\ &= \frac{1}{|W|}\int_W (h_0(t,x) - h_0(t,x))\mathrm{d}x = H_0(t) \end{aligned}$$

for $j = 0, 1, \ldots, m-1$ and $t > 0$. Hence we obtain Theorem 3.1.

Remark 3.3 It is known that (2.2)–(2.3) is derived from asymptotic expansion of the Allen-Cahn type equation due to [8]. It is obtained in [9] that solutions to the Allen-Cahn type equation converges to the solution describing a stationary rotating spirals with $1/m$-rotational symmetric pattern, which is different behavior of that the rotational relation (3.10) expresses.

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