On the role of kinetic and interfacial anisotropy in the crystal growth theory

Mi-Ho Giga
Graduate School of Mathematical Sciences
University of Tokyo
3-8-1 Komaba Meguro-ku
Tokyo 153-8914, Japan
mihogiga@ms.u-tokyo.ac.jp

Yoshikazu Giga
Graduate School of Mathematical Sciences
University of Tokyo
3-8-1 Komaba Meguro-ku
Tokyo 153-8914, Japan
labgiga@ms.u-tokyo.ac.jp

Abstract

A planar anisotropic curvature flow equation with constant driving force term is considered when the interfacial energy is crystalline. The driving force term is given so that a closed convex set grows if it is sufficiently large. If initial shape is convex, it is shown that a flat part called a facet (with admissible orientation) is instantaneously formed. Moreover, if the initial shape is convex and slightly bigger than the critical size, the shape becomes fully faceted in a finite time provided that the Frank diagram of interfacial energy density is a regular polygon centered at the origin. The proofs of these statements are based on approximation by crystalline algorithm whose foundation was established a decade ago. Our results indicate that the anisotropy of interfacial energy plays a key role when crystal is small in the theory of crystal growth. In particular, our theorems explain a reason why snow crystal forms a hexagonal prism when it is very small.

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1 Introduction

In a growing crystal it often appears a flat surface called a facet. We are interested in explaining in what way such a facet is formed using a macroscopic model based on thermomechanics [Gu]. When
a crystal is very small, it is sometimes observed that all surfaces of crystals are facets. Such a shape is often called **fully faceted**. In other words, it is a polytope. A typical example is a beautiful hexagonal prism of a snowflake. Formation of facets as well as fully faceted shapes is due to anisotropy of crystals since without anisotropy no facet is expected like fluid drops. There are at least two types of anisotropies – interfacial anisotropy and kinetic anisotropy. The role of these two anisotropies is often confused. In this paper we intend to clarify its role by giving several theorems which can be proved by development of the theory of very singular diffusion equations.

We consider an anisotropic curvature flow equations for an evolving (hyper)surface \( \{ \Gamma_t \}_{t \geq 0} \) (physically a crystal surface) in \( \mathbb{R}^n \) \((n \geq 2)\) of the form

\[
V = M(\vec{n})(\kappa_\gamma + \sigma) \quad \text{on} \quad \Gamma_t, \tag{1.1}
\]

where \( V \) denotes the normal velocity of \( \Gamma_t \) in the direction of unit normal \( \vec{n} \) of \( \Gamma_t \). The function \( M \) is called a **mobility**. It is a positive function defined on a unit sphere. In many models it is considered as a given function. The quantity \( 1/M \) is called a **kinetic coefficient** [Gu]. The quantity \( \kappa_\gamma \) is a weighted mean curvature or anisotropic mean curvature. It is the first variation of the interfacial energy \( I \) of the hypersurface \( \Gamma \):

\[
I(\Gamma) = \int_\Gamma \gamma_0(\vec{n})d\mathcal{H}^{n-1}, \tag{1.2}
\]

where \( \gamma_0 \) is a given positive function depending on the normal (orientation) called the **interfacial energy density** and \( d\mathcal{H}^{n-1} \) denotes the area element. We may write

\[
\kappa_\gamma = -\frac{\delta I}{\delta \Gamma}
\]

in a symbolic way. Its explicit form is formally as

\[
\kappa_\gamma = -\text{div}_\Gamma \left[ (\nabla_p \gamma)(\vec{n}) \right] \quad \text{on} \quad \Gamma, \tag{1.3}
\]

where \( \gamma(p) = |p|\gamma_0(p/|p|) \) is the 1-homogeneous extension of \( \gamma_0 \) to \( \mathbb{R}^n \) and \( \text{div}_\Gamma \) is the surface divergence and \( \nabla_p \gamma \) is the gradient of \( \gamma \). If \( \gamma_0 \) is identically equal to 1 so that \( \gamma_0 \) is isotropic, the interfacial energy \( I \) is nothing but the surface area of \( \Gamma \). In this case \( \gamma(p) = |p| \) and \( \kappa_\gamma = -\text{div}_\Gamma \vec{n} \) which is \((n-1)\) times mean curvature. The function \( \gamma_0 \) is determined by a crystal lattice structure. At least in very low temperature it is theoretically computable [K], [H], [KK]. It seems that there is no reasonable way to calculate mobility \( M \). The anisotropy in \( \gamma_0 \) is called interfacial anisotropy while the anisotropy in \( M \) is called kinetic anisotropy. If both \( \gamma_0 \) and \( M \) are isotropic, i.e. \( \gamma_0 \) and \( M \) are constants and \( \sigma = 0 \), then (1.1) is the mean curvature flow equation. The function \( \sigma \) in (1.1) is a driving force. For a snow crystal growth it is supersaturation of water molecules on \( \Gamma_t \). It may depend on the position and the time. In general model like the Stefan model it is coupled with diffusion equations outside crystal surface \( \Gamma_t \). If \( \sigma \) is given, the model (1.1) is called an interface controlled model (or local model).
To see the structure of (1.1) it is convenient to recall notion the Frank diagram [Gu]

$$\text{Frank}_\gamma = \{ p \mid \gamma(p) \leq 1 \}. \quad (1.4)$$

If Frank$_\gamma$ is convex, then (1.1) is at least degenerate parabolic under suitable regularity of $\gamma$, say $C^2$. If Frank$_\gamma$ is convex but loses $C^1$ regularity, then (1.1) becomes a very singular diffusion equation and is nontrivial to handle. A typical example is the case when Frank$_\gamma$ is a convex polytope. In this case $\gamma_0$ is called a crystalline energy density and (1.1) is called a crystalline flow. Formally, the polar set of Frank$_\gamma$ called a Wulff shape of $\gamma$ of the form

$$W_\gamma = \bigcap_{|\vec{m}|=1} \{ x \mid x \cdot \vec{m} \leq \gamma(\vec{m}) \} \quad (1.5)$$

plays a role of a sphere in the sense that

$$\kappa_\gamma = -(n - 1) \quad \text{on} \quad \partial W_\gamma \quad (1.6)$$

where $\vec{n}$ is taken outward. If Frank$_\gamma$ has a corner, then $W_\gamma$ has a flat portion (a facet) with normal corresponding to the corner direction. To understand (1.6) in a reasonable way, one should interpret that the curvature $\kappa_\gamma$ on the facet of $\partial W_\gamma$ is not zero but some positive quantity despite the fact that the surface is flat. This suggests that $\kappa_\gamma$ is not an infinitesimal quantity. It should be defined in a nonlocal way. This nonlocal character causes several difficulties. For an evolving curve (i.e. $n = 2$) various well-posedness results are established for the initial value problem for (1.1) when $\sigma$ is a spatially constant [GG98], [GG01]. However, for $n \geq 3$ or non-constant $\sigma$ even well-posedness is not well-established. The main reason for $n \geq 3$ is that $\kappa_\gamma$ may not be constant on a facet [BNP] (even if $\sigma = 0$) if one interprets $\kappa_\gamma$ in a reasonable way. Similarly, for non-constant $\sigma$ the quantity $\kappa_\gamma + \sigma$ may not be constant on a facet [GG98a].

For $n \geq 3$ the unique solvability result is established for $V = \gamma \kappa_\gamma$ for convex initial data [BCCN] by a variational approach. When $\Gamma_t(n = 2)$ is the graph of a function of one space variable, i.e. a graph-like function, the unique solvability result is established in [GG98a], when the equation is written in a divergence form even if $\sigma$ may not be a spatially constant. Recently, a viscosity approach enables us to assert well-posedness for more general equations for graph-like functions [GGR] when $n = 2$. This formulation allows “facet bending” or “facet breaking”. An explicit solution allowing facet bending is constructed in various settings, e.g. [GR08], [GG0R11]. For a general background of these problems the reader is referred to reviews articles [G00], [G04], [GG10] and [B].

In this paper we consider (1.1) in a very simple setting. We consider a planar motion (i.e. $n = 2$) and postulate that $\gamma_0$ is crystalline and $\sigma$ is a given positive constant. We start with a convex crystal surrounded by $\Gamma_0$ and show that facets are instantaneously formed. Such a kind of result is already proved for a different setting in [GG98] and recently studied for a case when Frank$_\gamma$ has a curved part by P. Mucha and P. Rybka but for graphs. We call this phenomenon the instant
formation of facet. We next study whether or not a crystal becomes fully faceted after some short time. We only discuss a simple situation when Frank $\gamma$ is a regular polygon centered at the origin. If $M$ has the same symmetry as $\gamma_0$, a growing convex crystal starting from nearly the “critical size” (i.e. $\kappa_\gamma + \sigma = 0$) becomes fully faceted in a finite time and it is similar (homothetic) to $W_\gamma$. In this paper we prove these statements by approximating by a crystalline flow which is a system of ordinary differential equations [T], [AG]. The approximation is justified by [GG01]. Note that even solvability is nontrivial for (1.1) for general (convex) initial data $\Gamma_0$ and it is established in [GG01].

The merit of crystalline approximation is that one can prove these statements as we intuitively observed. A fully faceted crystal grows further and its large time asymptotic is once influenced by the mobility. In fact, it is known that $\Gamma_t/t \to \sigma W_M$ (Hausdorff distance sense) as $t \to \infty$ [IPS]. So a fully faceted crystal may be rounded again. The whole time growth behavior starting from very small convex shape is numerically calculated by [KG].

It is often believed that growth phenomena is due to mobility and that anisotropy of curvature is negligible. This is true for a scaled down profile of larger time asymptotics. However, if the curvature $\kappa_\gamma$ has no nonlocal nature, there is no facet provided that $M$ is Lipschitz (continuous) and Frank $\gamma$ is $C^2$ and strictly convex by the strong maximum principle as observed in [KG]. Unless interfacial energy is degenerate or singular, it is impossible to explain formation of facets when $M$ is Lipschitz.

To explain snow crystal growth one has to couple (1.1) with a diffusion equation for $\sigma$ to form the Stefan type problem. One of reasonable ways to model snow crystal growth is to consider a quasi-static approximation of one-phase Stefan type problem with Gibbs-Thomson effect and kinetic cooling. Its explicit form is

$$\Delta \sigma = 0 \quad \text{in} \quad \Omega_t \subset \mathbb{R}^3, \quad \text{(1.7)}$$

$$V = \partial \sigma / \partial \vec{n} \quad \text{on} \quad \Gamma_t = \partial \Omega_t, \quad \text{(1.8)}$$

$$V = M(\vec{n})(\kappa_\gamma + \sigma) \quad \text{on} \quad \Gamma_t, \quad \text{(1.9)}$$

where $\Omega_t$ is a region outside crystal. Of course one should assign the value $\sigma$ at $|x| = \infty$ and initial surface $\Gamma_0$. (We take all physical constants just one for simplicity.) Recently, J. Barrett, H. Garcke and R. Nürnberg [BGN1], [BGN2], [BGN3] invented a nice numerical scheme to calculate for singular $\gamma$ and reproduce snow crystals both $n = 2$ and $n = 3$. They take realistic values for mobility due to experiments while basic physics (1.7)–(1.9) including interfacial energy follows physics [L]. In [BGN3] it appears that they successfully reproduce Nakaya’s diagram [N] on snow crystal shapes depending on temperature and supersaturation. In particular, they reproduce a hexagonal prism like shape when the crystal is very small. Mathematical analysis is not well-developed for this system. However, it is known that the problem is locally solvable in a class of admissible evolving crystals [GR02]. In some cases there even exist self-similar solutions [GR05] at least for small crystal. However, facet may break if $\sigma$ is coupled so that $\sigma$ is not a constant [GR05].

In [Y] evolution of snowflakes is calculated by (1.7)–(1.9); see also [YK]. However, the term $\kappa_\gamma$
is omitted. According to [BGN3], if there is no $\kappa_\gamma$, no hexagonal pattern is produced. It seems that the numerical treatment in [Y] and [YK] includes some “regularizing effect” corresponding to $\kappa_\gamma$ to reproduce snowflakes. Roughly speaking, anisotropy of mobility plays a role to determine rough shape of crystals (see also [YGR]) while anisotropy of interface energy plays a role to determine detailed shape.

Our results correspond to the case when the crystal is sufficiently small. Although for a snow crystal growth $\sigma$ is of course not a constant and also coupled, full faceted nature seems to be very similar. In fact, if the crystal is very small compared with gradient of $\sigma$, flatness (of a facet) is preserved; see e.g. [GR05]. In our analysis, when $\gamma_0$ is crystalline with $M > 0$ and constant $\sigma > 0$, the mobility $M$ plays a little role if one is interested in formation of facets. Even for general mobility full faceted nature itself does not seem to depend mobility. Only singular interfacial energy plays a role. However, mobility in the direction of facet seems to be important to determine the “shape” of fully faceted crystal $\Gamma_t$. We do not touch these problems in this paper. However, if we discuss the shape of small slowly growing crystals, this point seems to be very important because there are several nice experiments [FK], [M] which are believed to find equilibrium shape i.e. $\kappa_\gamma + \sigma = 0$ but one should be careful about the role of mobility if $M$ is not proportional to $\gamma$.

This paper is organized as follows. In section 2 we state our main result on instant formation of facet after reviewing definition and a few properties of solutions. In section 3 we state our main result on formation of a fully faceted shape. In section 4 we prove our main results by using a crystalline algorithm. Our selection of references is not at all exhaustive.

2 Instant formation of facet

We first recall well-posedness results in [GG01] for (1.1) with $n = 2$ when Frank-$\gamma$ has singularities. Our formulation is based on adjustment of a level-set method developed by [ES], [CGG]; see also [G06]. Instead of considering (1.1), we consider

$$u_t/|\nabla u| = M(\vec{n}) \left( - \text{div} (\nabla_p \gamma(\vec{n})) + \sigma \right) \quad \text{with} \quad \vec{n} = -\nabla u/|\nabla u| \quad (2.1)$$

which is formally equivalent to (1.1) on $\Gamma_t = \{ x \in \mathbb{R}^2 | u(x, t) = 0 \}$. We consider (2.1) not only on $\Gamma_t$ but also for all $\mathbb{R}^2$. As in [G06] we say that an open set $D \subset \mathbb{R}^2 \times [0, \infty)$ is an open evolution of (1.1) with initial data $D_0$ if there is a solution $u \in C(\mathbb{R}^2 \times [0, \infty))$ of (2.1) such that $D = \{(x, t) | u(x, t) > 0 \}$ and $D_0 = \{ x | u(x, 0) > 0 \}$ such that $u$ equals a negative constant outside a big ball (depending on $t$). A closed evolution $E \subset \mathbb{R}^2 \times [0, \infty)$ of (1.1) with initial data $E_0$ is defined in a parallel way by replacing $>$ by $\geq$. The set $\Gamma = E \setminus D$ is regarded as an interface evolution which is a generalized solution of (1.1) starting with initial curve $\Gamma_0 = E_0 \setminus D_0$ with $E_0 = \bar{D}_0$. Here by a solution of (2.1) we mean a certain viscosity like solution [GG01], which is a generalized notion of solution based on maximum principle [G06]. By definition the orientation $\vec{n}$ is taken outward from $D$. Our formulation restricts that $D(t)$, $E(t)$ the cross-section of $D$ and $E$ at
Let $t$, i.e. $D(t) = \{ x \in \mathbb{R}^2 \mid (x,t) \in D \}$ is bounded. We warn the reader that $E$ may be strictly larger than $\tilde{D}$ for $E_0 = \tilde{D}_0$ even for smooth $\gamma$. This phenomenon is called fattening [ES], [G06]. Thus we say that $E$ is regular if $E = \tilde{D}$ for $E_0 = \tilde{D}_0$. This implicitly assumes that there is no spike for $E_0$.

We consider a class of singular interfacial energy including a crystalline energy. Let $I$ be defined by

$$I = \{ \gamma : \mathbb{R}^2 \to (0, \infty) \mid \gamma \text{ is convex, positively homogeneous of degree 1 and } \text{Frank}\gamma \text{ is } C^2 \text{ except finitely many points. Moreover,}$$

$$\text{the curvature of } \partial (\text{Frank}\gamma) \text{ is bounded except singularities} \}.$$  

Here is a typical well-posedness result proved in [GG01], where more general curvature flow equations are discussed.

**Lemma 2.1** (Unique existence, [GG01, Corollary 8.2, Theorem 6.4]). Let $M$ be a nonnegative continuous function defined on $S^1 = \{ p \in \mathbb{R}^2 \mid |p| = 1 \}$ and $\gamma \in I$. Assume that $\sigma \in \mathbb{R}$ is a constant. For a given bounded open set $D_0$ (resp. closed set $E_0$) there is a unique open evolution $D$ (resp. closed evolution $E$) with initial data $D_0$ (resp. $R_0$) for (1.1).

It turns out such evolutions have a nice stability result [GG99]. So one can approximate the singular problem by a problem with smoother interfacial energy. Here is a typical result proved in [GG01].

**Lemma 2.2** (Approximation, [GG01, Corollary 8.3]). Assume that a sequence of continuous functions $M_\varepsilon : S^1 \to [0, \infty)$ converges to $M$ uniformly as $\varepsilon \to 0$ and that $\gamma_\varepsilon \in I$ converges to $\gamma \in I$ uniformly on $S^1$ as $\varepsilon \to 0$. Moreover, $\sigma_\varepsilon \in \mathbb{R} \to \sigma \in \mathbb{R}$. Let $E_\varepsilon^0$ and $E$ be bounded closed sets in $\mathbb{R}^2$. Let $E^\varepsilon$ be a closed evolution of

$$V = M_\varepsilon(\vec{n})(\kappa_{\gamma_\varepsilon} + \sigma_\varepsilon) \quad (2.2)$$

with initial data $E_0$ and $E$ be a closed evolution of (1.1) with initial data $E_0$. Assume that

$$d_H(E^\varepsilon_0, E_0) \to 0 \quad \text{as} \quad \varepsilon \to 0,$$

where $d_H$ is the Hausdorff distance in $\mathbb{R}^2$. Assume that $E$ is regular. Then

(i) $d_H''(E^\varepsilon, E) \to 0$ as $\varepsilon \to 0$, where $d_H''$ denotes the Hausdorff distance in $\mathbb{R}^2 \times [0, T]$ for a fixed $T > 0$.

(ii) Assume that $t \mapsto E(t)$ is continuous as a set-valued function for $t \geq 0$. Assume that $E$ is strongly regular in $[0, T]$ in the sense that $E(t) = \overline{D(t)}$ for all $t \in [0, T]$, where $D$ is the open evolution of (1.1) with initial data $D_0$ such that $E_0 = \overline{D_0}$. Then

$$\lim_{\varepsilon \to 0} \sup_{0 \leq t \leq T} d_H(E^\varepsilon(t), E(t)) = 0.$$
Approximation by smoother energy is first established in [FG] for a graph-like function for a special equations of divergence type. It is extended for general equations by [GG99]. Note that our approximation result (Lemma 2.2) also allows the approximation of the problem with smooth $\gamma$ by singular $\gamma_{\varepsilon}$ like crystalline. Such a kind of approximations is discussed in a special setting – graph-like solutions by [FG], [GK] and convex curves [Gir].

We now consider a convex initial data. We would like to show that the convexity is preserved and the corresponding closed evolution is regular.

**Theorem 2.3.** Assume the same hypothesis of Lemma 2.1 concerning $M$, $\gamma$ and $\sigma$. Let $E_0$ be the closure of a bounded, open and convex set $D_0$. Let $E$ be the closed evolution of (1.1) with initial data $E_0$.

(i) (Convexity preserving) The cross-section $E(t) \subset \mathbb{R}^2$ is convex for all $t \geq 0$.

(ii) (Non-fattening) The closed evolution $E$ is regular. Moreover, $E$ is strongly regular in $[0,T]$ for all $T < T_*$, i.e. $E(t) = \overline{D(t)}$ for $0 \leq t < T_*$, where $D$ is the open evolution of (1.1) with initial data $D_0$ and $T_*$ is the extinction time, i.e. $T_* = \sup \{ t \mid \text{int } E(t) \neq \emptyset \} \leq \infty$.

**Proof.** For smooth energy $\gamma$ we have convexity preserving property proved by [GGIS]; see [G06, Remark 3.5.5]. For a level-set equation (2.1) we have concavity preserving property for an auxiliary function $u(x,t)$ for (2.1) for smooth $\gamma$ [G06, Remark 3.5.2]. Note that in our definition an auxiliary function is taken so that it equals a negative constant at the space infinity. However, this restriction is not essential. In fact, we may allow spatially uniformly continuous functions. Thus at least for convex set $E_0$ there is a solution $u \in C(\mathbb{R}^2 \times [0,\infty))$ of (2.1) in $\mathbb{R}^2 \times (0,\infty)$ such that $x \mapsto u(x,t)$ is concave and uniformly continuous with the property:

$$E = \{(x,t) \mid u(x,t) \geq 0\}, \quad E(t) = \{ x \mid u(x,t) \geq 0 \}.$$

By convergence to a singular problem [G06, Theorem 8.1] such $u$ converges to the problem with singular interfacial energy if it is approximated by smooth interfacial energy. Thus for singular $\gamma$ the concavity preserving property $u$ for (2.1) is inherited. This in particular implies that convexity is preserved and also yields non-fattening property since the level-set flow is a level set of a concave function.

We are now in position to state our main result on the instant formation of facet.

**Theorem 2.4** (Instant formation of facet). Assume that Frank $\gamma$ is a convex polygon, i.e. $\gamma \in \mathcal{I}$ is crystalline. Assume that $M : S^1 \to (0,\infty)$ is continuous and $\sigma \in \mathbb{R}$. Let $E_0$ be the closure of a bounded open and convex set $D_0$. Let $E$ be the closed evolution of (1.1) with initial data $E_0$. Let $\{\Gamma_t\}$ be the interface evolution defined by $\Gamma_t = E(t) \setminus D(t)$. Let $\mathcal{N}$ be the singular set of $\gamma$ i.e. $\gamma \in C^2(S^1 \setminus \mathcal{N})$ and $\nabla \gamma$ has jumps exactly on $\mathcal{N}$. Then, for each $\vec{n} \in \mathcal{N}$ there is a facet (a flat portion) of $\Gamma_t$ (the boundary of a convex open set) with orientation $\vec{n}$ for all $t \in (0,T_*)$, where $T_*$ is the extinction time. In other words, a facet is instantaneously created and stays.
We shall postpone the proof in Section 4. The basic idea is to approximate by crystalline algorithm. This is possible by a general approximation result (Lemma 2.2) and consistency result in [GG00]. It seems to be possible to extend (Theorem 2.4) to a general \( \gamma \in \mathcal{I} \) not necessarily crystalline but we do not pursue this problem.

Our Theorem 2.4 implicitly asserts that the solution becomes admissible even if initially it is a non-essentially admissible crystal. A missing direction in \( \mathcal{N} \) is actually formed. Such a problem is studied in [GGH].

### 3 Formation of fully faceted small crystals

We consider the equation (1.1) when \( \sigma \) is a positive constant. It is easy to see that the rescaled Wulff shape \( C = (1/\sigma)W_\gamma \) a stationary closed evolution of (1.1). By the comparison principle [GG01] if the initial data int \( E_0 \) includes \( C \), the closed evolution \( E \) of (1.1) with initial data always contains \( C \) and never disappears for all \( t > 0 \). If \( E_0 \subset \text{int} \), then the corresponding solution \( E \) disappears in finite time if \( \inf M > 0 \). Thus the set \( C \) is called a critical shape. We are interested in shapes of crystals \( E(t) \) when \( E_0 \) contains in \( C \) but close to \( C \). It turns out that if we assume that Frank \( \gamma \) is a convex polygon so that its Wulff shape \( W_\gamma \) is a dual polygon, then \( E(t) \) becomes a convex polygon with the same set of orientations as that of \( W_\gamma \) after some time. We call this polygon a fully faceted shape with respect to \( \gamma \). To avoid extra difficulty we state a typical result.

**Theorem 3.1 (Fully faceted)**. Assume that Frank \( \gamma \) is a regular polygon centered at the origin. Assume that \( M : S^1 \to (0, \infty) \) is continuous and \( \sigma > 0 \). Let \( E_0 \) be the closure of a bounded open and convex set \( D_0 \) containing the crystal shape \( C \). Let \( E \) be the interface evolution of (1.1) with initial data \( E_0 \).

1. If \( E_0 \) is sufficiently close to \( E_0 \), there \( E(t) \) becomes fully faceted with respect to \( \gamma \) in finite time.

2. If \( E_0 \) and \( M \) has the same symmetry as \( \gamma \), then the full faceted shape is similar to \( W_\gamma \) i.e.
   \[ E(t) = c(t)W_\gamma. \]

3. If \( E_0 \) has the same symmetry as \( \gamma \) and \( M \) is proportional to \( \gamma \), then \( E(t) = c(t)W_\gamma \) for all \( t > t_0 \) with some \( t_0 > 0 \).

**Remark 3.2.**

1. Unless \( M \) is proportional to \( \gamma \), the large time asymptotics may be different from \( W_\gamma \) even in case (b). Actually, it is essentially known that \( E(t)/t \to W_M \) so \( t \to \infty \), where \( W_M \) is the Wulff shape of \( M \). This asymptotic behavior is proved in [IPS] for smooth \( \gamma \) but it can be easily extended to the singular case as noted in [KG].

2. There are several numerical simulations for \( E \) by changing anisotropy of \( \gamma \) and \( M \) in [KG]. For a short time a fully faceted shape with respect \( \gamma \) is obtained. In a large time the rough
shape is $tW_M$ but facets with orientation $\vec{n} \in \mathcal{N}$ stay for all time even if $W_M$ and $W_\gamma$ has different orientations of their edges.

(iii) So far the effect of the mobility seems to be little for $E(t)$ which is close to $C$. However, if $M/\gamma$ depends on $\vec{n} \in \mathcal{N}$, then the fully faceted shape is not similar $W_\gamma$ (nor $W_M$). We conjecture that $\sigma E(t)$ converges to $cW_\gamma$ with $\gamma \kappa/\gamma = M\kappa/\gamma$ as $\sigma \to 0$ with some constant $c > 0$. Such $\gamma$ is very related to the existence problem for self-similar shrinking solutions for $V = M\kappa/\gamma$. In fact, there is a unique self-similar solution whose cross section is similar to $W_\gamma$ for some $\gamma$ provided that $\gamma$ and $M$ is smooth and $\gamma(\vec{n}) = \gamma(-\vec{n})$, $M(\vec{n}) = M(-\vec{n})$ and that Frank-$\gamma$ is strictly convex; see [Ga], [DG], [DGM] and a review paper [G00] and a book [G06]. A similar result is proved for crystalline flow by [St1], [St2]. So it is likely that the value of $M(\vec{n})/\gamma(-\vec{n})$ on $\mathcal{N}$ plays an important role to determine the fully faceted shape. For example in three dimension the Wulff shape $W_\gamma$ is a hexagonal prolonged prism while we often find thin or thick hexagonal prism of snowflakes. This is caused by a difference of $M/\gamma$ on basal and prism surface.

(iv) Even if $\sigma$ is not constant, admissible facets are preserved provided that the crystal is sufficiently small (so that $\kappa_\gamma$ is large) with respect to the gradient of $\sigma$. On the facet the driving force turns to be equal to its average over the facet in this case. In fact, a comparison principle holds for such small crystals [BGN]. Moreover, even one considers a coupled system (1.7)–(1.9), there exists a special solution which is self-similar and fully faceted for a certain time when $M$ and $\gamma$ is chosen so that $M/\gamma$ is constant as in the case of (c). This is actually proved for special $\gamma$ and $M$ in [GR05].

4 Approximation by crystalline flow

We shall prove Theorems 2.4 and 3.1 by approximating by crystalline flows. In other words, we use a crystalline algorithm. We first recall an essentially admissible evolving crystal which is a special evolving polygon preserved by a crystalline curvature flow equation. Let Frank-$\gamma$ be a convex $m$-polygon. Let $q_i (i = 1, 2, \ldots, m)$ be its vertices. Then the singular set $\mathcal{N}(\subset S^1)$ is of the form

$$\mathcal{N} = \{ q_i/|q_i| \mid i = 1, 2, \ldots, m \}.$$ 

We say that a simple oriented polygonal curve $S$ in $\mathbb{R}^2$ is an essentially admissible crystal if the (outward) unit normal vector $\mathbf{n}$ and $\hat{\mathbf{n}}$ of any adjacent segments (facets) of $S$ satisfies

$$\frac{(1 - \lambda)\mathbf{n} + \lambda\hat{\mathbf{n}}}{|(1 - \lambda)\mathbf{n} + \lambda\hat{\mathbf{n}}|} \not\in \mathcal{N}$$

(4.1)

for any $\lambda \in (0, 1)$. In other words, there is no singular direction between orientations $\mathbf{n}$ and $\hat{\mathbf{n}}$ of two adjacent segments. If we further impose that all orientations of facets of $S$ belongs to $\mathcal{N}$, then $S$
is called an admissible crystal which is a conventional admissibility proposed by [T], [AG]; see also [GGu]. We say that a family of polygon \(\{S_t\}_{t \in J}\) is an essentially admissible evolving crystal if \(S_t\) is an essentially admissible crystal for all \(t \in J\) and each corner moves continuously differentially in time as well as each facet keeps its orientation. The notion of essentially admissibility is found in [HGGD]. An admissible evolving crystal is defined in a similar way.

We consider an essentially admissible crystal of closed polygonal curves with finite length for simplicity. By definition \(S_t\) is of the form

\[ S_t = \bigcup_{j=1}^{r} S_j(t), \]

where \(S_j(t)\) is a maximal, nontrivial, closed segment and its unit outward normal vector in \(n_j\). Here we number facets clockwise. We say that \(\{S_t\}_{t \in J}\) is a \(\gamma\)-regular flow of (1.1) if

\[ V_j = M(n_j) \left( \frac{\chi_j \Delta(n_j)}{L_j(t)} + \sigma \right) \quad \text{on} \quad S_j(t), \quad t \in J \]  

for \(j = 1, 2, \ldots, r\), where \(V_j\) denotes the normal velocity of \(S_j(t)\) in the direction of \(n_j\). The quantity \(\chi_j \Delta(n_j)/L_j(t)\) is a nonlocal weighted curvature \(\kappa_j(n_j)\) for \(n_j \in N\), where \(L_j(t)\) denotes the length of \(S_j(t)\). The quantity \(\Delta(m_i)\) is defined by

\[ \Delta(m_i) = \hat{\gamma}'(\theta_i + 0) - \hat{\gamma}'(\theta_i - 0) \quad \text{if} \quad m_i \in N, \]

\[ \Delta(m_i) = 0 \quad \text{if} \quad m_i \notin N, \]

where \(m_i = (\cos \theta_i, \sin \theta_i)\) and \(\hat{\gamma}(\theta) = \gamma(\cos \theta, \sin \theta)\). The quantity \(\chi_j\) is a transition number. It takes \(+1\) (resp. \(-1\)) if \(S_t\) is convex (resp. concave) in the direction of \(n_j\); we use the convention that \(\chi_j = -1\) for all \(j = 1, \ldots, r\) if \(S_t\) is convex. We note that \(\Delta(m_i)\) has a geometric meaning. It is the length of facet of the Wulff shape \(W_\gamma\) with outward normal \(m_i\). We have assumed that \(\sigma \in \mathbb{R}\) is a constant.

Since \(\{S_t\}_{t \in J}\) is an essentially admissible evolving crystal, by elementary geometry one obtains a transport equation

\[ \dot{L}_j(t) = \frac{dL_j(t)}{dt} = \left( \cot \psi_j + \cot \psi_{j+1} \right) V_j - \frac{1}{\sin \psi_j} V_{j-1} - \frac{1}{\sin \psi_{j+1}} V_{j+1} \]  

for \(j = 1, \ldots, r\); index \(j\) is considered modulo \(r\). Here \(\psi_j = \theta_j - \theta_{j-1}\) (modulo \(2\pi\)) with \(n_j = (\cos \theta_j \sin \theta_j)\). Thus the equation (4.2) forms a system of ordinary differential equations (ODE) with (4.3) for \(L_j\)'s. A fundamental theory of ODE yields the (local-in-time) unique solvability of (4.2)–(4.3) for a given initial data \(S(0)\) for \(J = [0, t_0]\), where \(J\) is the maximal existence time interval. We shall restrict ourselves for convex \(S(0)\). Arguing in a similar way as in [GG00] and [I], one observes that only facet with \(n_j \notin N\) may disappear for \(\gamma\)-regular flow at \(t = t_0\) unless the enclosed set of \(S_{t_0 - 0}\) has an interior. One can extend the solution after \(t_0\) by solving (4.2)–(4.3) if the enclosed set of \(S_{t_0 - 0}\) has no interior. Thus one is able to continue the ‘solution’ until the time \(T_0\).
when the enclosed area is zero. Such a solution is called a *crystalline flow* of (1.1) and $T_0$ is called an extinction time.

One should be careful that the consistency of a crystalline flow with an interface evolution (a level-set flow). This topic is well-discussed for admissible evolving crystals in [GG00]. It is easy to adjust their argument for essentially admissible evolving crystals. We need the corner preserving condition [GG00, (3.2)]. It is easy to see that the corners of

$$A_i = H_i \cap H_{i+1}, \quad B_i = H_i \cup H_{i+1}$$

with $H_{i+j} = \{ x \in \mathbb{R}^2 \mid x \cdot m_{i+j} \leq \sigma M(m_{i+j}) \}$ stays a corners for $V = M(\vec{m})\sigma$ if and only if

$$A_i \subset \{ x \in \mathbb{R}^2 \mid x \cdot m \leq \sigma M(m) \} \subset B_i$$

(4.4)

for all $m = (\cos \theta, \sin \theta)$ such that $\theta_{i+1} \leq \theta \leq \theta_i$, where $m_{i+j} = (\cos \theta_{i+j}, \sin \theta_{i+j})$. We state the consistency only for a convex closed evolution, which develops no fattening as observed in Theorem 2.3.

**Lemma 4.1 (Consistency).** Assume the same hypotheses of Theorem 2.4 concerning $\gamma, M, \sigma$. Assume that $E_0$ is a convex closed polygon such that $S_0 = \partial E_0 (= \bigcup_{j=1}^r S_j(0))$ is essentially admissible (with respect to $\gamma$). Let $E$ be the closed evolution of (1.1) with initial data $E_0$. Then $S_t = \partial E(t)$ is a crystalline flow in $J = [0, T_\ast)$ with initial data $S_0$ provided that the corner preserving property (4.4) with $i = j$ holds for $M$ with $m_j = n_j$ for all $j = 1, \ldots, r$.

The corner preserving condition (4.4) uniquely interpolates the values of $M(m)$ from the value of $M$ at $n_j (j = 1, \ldots, r)$. The way of interpolation is given in [GG00, (3.3)]. Geometrically speaking, if $\sigma > 0$, one considers an $r$-polygon $W$ whose vertices consist of $M(n_j)n_j$ and consider its polar set $F$ i.e.,

$$F = \left\{ p \in \mathbb{R}^2 \mid \sup_{x \in W} p \cdot x \leq 1 \right\}.$$  

The interpolated $\tilde{M}$ should be defined by the Minkowski functional of $F$ i.e.,

$$\tilde{M}(p) = \sup \{ \lambda \mid p \in \lambda F \}.$$  

Notice that if the set $\{n_j\}_{j=1}^{r(\varepsilon)}$ converges to $S^1$ in the sense of Hausdorff distance as $\varepsilon \to 0$, $\tilde{M} = \tilde{M}^{\varepsilon}$ converges to $M$ uniformly on $S^1$. Thus, combining Lemma 2.2 and Theorem 2.3 with consistency (Lemma 4.1), we are able to conclude the convergence of crystalline algorithm.

**Lemma 4.2 (Convergence of crystalline algorithm).** Assume the same hypotheses of Theorem 2.4 concerning $\gamma, M, \sigma$. Let $E_0$ be the closure of bounded, convex open set $D_0 \neq \emptyset$. Let $E$ be the closed evolution of (1.1) with initial data $E_0$ and let $\{\Gamma_t \}_{t \geq 0}$ be the corresponding level-set flow with initial data $\Gamma_0 = E_0 \setminus D_0$ with extinction time $T_\ast \in (0, \infty]$. Let $E_0^\varepsilon$ be a convex polygon such that its
The left hand side is bounded from below as $\varepsilon \to 0$. However, this is impossible since $L_{i}^{\varepsilon}(t) \to 0$ uniformly in $[t_{0}, t_{1}]$. We have thus proved that $L_{i}(t) > 0$ for a dense subset of $(0, T)$.
As for the proof of crystalline flow [I], [GG00] combining (4.2) and (4.3) for approximation, one is able to prove that facets of \( \Gamma_t \) with orientation in \( N \) has a positive length for a short time if it has initially positive length. We do not give a detailed proof. This implies \( L_l(t) > 0 \) for all \( t \in (0, T] \) so the proof is now complete.

In the rest of this section we are going to prove formation of a fully faceted pattern stated in Theorem 3.1. To motivate the idea we consider a crystalline flow when Frank \( \gamma \) is a regular polygon centered at the origin.

1. **Monotone motion.** Our first observation is the monotonicity property that \( V_j(t) \geq 0 \) for all time and \( j = 1, \ldots, r \) provided that \( V_j(0) > 0 \) with \( j = 1, \ldots, r \) for a \( \gamma \)-regular flow \( \{S_t\}_{t \in J}, J = [0, t_0) \) of (1.1). This easily follows from comparison between flow starting from \( S_h \) and \( S_0 \) for small \( h > 0 \). A necessary comparison principle has been established in [GGu] (see also [T]) for general crystalline \( \gamma \). Indeed, if \( S_h \) encloses \( S_0 \), then the comparison principle implies that \( S_{t+h} \) encloses \( S_t \) for all \( t \) such that \( t + h \in J \). This implies \( V_j(t) \geq 0 \).

Note that this monotonicity property is inherited for a crystalline flow.

2. **Comparison with self-similar solutions and estimate for admissible facet.** Let \( S_t = \partial E(t) \) be a crystalline flow of (1.1) (with \( \sigma > 0 \)) which is growing for all time in the sense that its outward normal velocity is always nonnegative. By the comparison principle [GGu] \( S_t \) is enclosed by a crystalline flow \( S_t^* \) of

\[
V = a (\kappa_\gamma + \sigma) \quad \text{with} \quad a = \sup_{S^*} M
\]

if the initial data \( S_0^* \) enclosing \( S_0 \). As well-known, the equation (4.5) admits a self-similar crystalline flow of the form \( S_t^* = z(t) \partial W_\gamma \) when Frank \( \gamma \) is a regular polygon centered at the origin [Gu, 12G]. The function \( z(t) \) solves

\[
\dot{z}(t) = ab^{-1} (-1/z(t) + \sigma)
\]

where \( b = \gamma(n_i) \) for \( n_i \in N \) which is independent of \( i = 1, \ldots, m \) because Frank \( \gamma \) is a regular polygon centered at the origin. It is convenient to recall support functions. Let \( \{d_j(t)\}_{j=1}^r \) be a support function of \( E(t) \) in the direction of \( n_j \). Let \( \{\lambda_i(t)\}_{i=1}^m \) be the support function of \( z(t)W_\gamma \) in the direction of \( n_i \). Since Frank \( \gamma \) is a regular polygon centered at the origin we easily observe that \( \lambda_i(t) = \lambda(t) \) is independent of \( i = 1, 2, \ldots, m \) and \( \lambda(t) = z(t)b \). Thus (4.6) for \( \lambda \) is of the form

\[
\dot{\lambda}(t) = a (-b/\lambda(t) + \sigma).
\]

By the comparison principle if \( S_0 \) is enclosed by \( S_0^* \) i.e., \( d_i(0) \leq \lambda(0) \) for all \( i = 1, \ldots, m \), then

\[
d_i(t) \leq \lambda(t)
\]
for \( i \) such that \( n_i \in \mathcal{N} \). In other words, the support function in the singular direction (often called admissible direction) is always dominated from above by \( \lambda(t) \). The corresponding facet is called an admissible facet.

3. **Estimate for velocity of non-admissible facets.** As we already observed non-admissible facets of \( S_t \), i.e. \( n_j \notin \mathcal{N} \) may disappear in finite time. However, it is rather clear by (4.2)

\[
\dot{d}_j(t) = M(n_j) \sigma \geq m \sigma, \quad m = \inf_{S^i} M
\]

since \( V_j = \dot{d}_j \) provided that the corresponding facet \( S_j(t) \) exists. This yields the estimate

\[
d_j(t) \geq m \sigma t + d_j(0).
\] (4.9)

4. **Disappearing of non-admissible facets.** We recall an elementary observation on support functions.

**Lemma 4.3.** Let \( H_l(l = 1, 2) \) be a half space of the form

\[
H_l = \left\{ x \in \mathbb{R}^2 \mid x \cdot n_l \leq 1 \right\}
\]

with \( n_l = (\cos \theta_l, \sin \theta_l) \), \( \theta_1 > \theta_2 > \theta_1 - \pi \). The half space

\[
K_{\theta} = \left\{ x \in \mathbb{R}^2 \mid x \cdot n_{\theta} \leq d_{\theta} \right\}, \quad n_{\theta} = (\cos \theta, \sin \theta)
\]

contains \( H_1 \cap H_2 \) if and only if \( d_{\theta} \geq c_{\theta} \) with

\[
c_{\theta} = \cos (\theta - (\theta_1 + \theta_2)/2) / \cos ((\theta_1 - \theta_2)/2)
\]

Moreover, \( \inf \{ c_{\theta} \mid \theta_1 \leq \theta \leq \theta_2 \} =: \bar{c} > 0 \).

Note that \( d_{\theta} < c_{\theta} \) is equivalent to saying that \( H_1 \cap H_2 \cap K_{\theta} \) has a facet with orientation \( n_{\theta} \). By this observation one concludes that if \( n_j = (\cos \theta, \sin \theta) \) is between two admissible (singular) direction say \( n_1, n_2 \in \mathcal{N} \) then any non-admissible facet corresponding to \( n_j \) disappears when

\[
d_j(t) > \bar{c} \lambda(t)
\] (4.10)

with \( \bar{c} \) defined by Lemma 4.3. Assume that \( S_0 \) strictly encloses a critical Wulff shape \( C = (1/\sigma)W_\gamma \), in other words, \( d_i(0) > b/\sigma \) with \( n_i \in \mathcal{N} \). By geometry for non-admissible facets we have

\[
d_j(0) \geq c_{\theta} b / \sigma \geq \bar{c} b / \sigma
\]

with \( n_j = (\cos \theta, \sin \theta) \). By (4.8) \( d_j(t) \) is estimated from below by (4.9) to set

\[
d_j(t) \geq m \sigma t + \bar{c} b / \sigma.
\]
For \( \lambda(0) = \lambda_0 = \delta + b/\sigma \) the solution \( \lambda = \lambda^\delta(t) \) of (4.7) is monotone increasing and strictly convex for \( \delta > 0 \) and \( \lambda^\delta \downarrow b/\sigma \) locally uniform in \([0, \infty)\) as \( \delta \downarrow 0 \). Thus, for sufficiently small \( \delta > 0 \) one observes that

\[
\bar{c}\lambda^\delta(t) < m\sigma t + \bar{c}b/\sigma
\]

on some interval \((t^\delta_1, t^\delta_2) \subset [0, \infty)\); \( t^\delta_2 \) can be \(+\infty\). If \( d_i(0) \) (\( > b/\sigma \)) is taken close to \( b/\sigma \), say \( d_i(0) < \lambda_0 \), then by the criterion (4.8) we have (4.10) which implies that \( n_j \)-facet disappears in the time interval \((t^\delta_1, t^\delta_2)\). Thus all non-admissible facet must disappear in finite time.

**Proof of Theorem 3.1.** (i) If \( E_0 \) (\( \supset C \)) is close to \( C \) so that \( S^*_0 \) with \( \lambda_0 = \delta + b/\sigma \) encloses essentially admissible crystal \( E_0^\varepsilon \) approximating \( E_0 \) for small \( \varepsilon \), say \( 0 < \varepsilon < \varepsilon_0 \), then \( d^\varepsilon_i(t) \leq \lambda(t) \). By the above observation for a crystalline flow we conclude that

\[
d^\varepsilon_j(t) > \bar{c}\lambda(t) \quad \text{in} \quad (t^\delta_1, t^\delta_2),
\]

where the interval is independent of \( \varepsilon \). This implies that in time interval \((t^\delta_1, t^\delta_2)\), \( E^\varepsilon(t) \) is a fully faceted convex polygon with admissible facets with orientations \( n_1, \ldots, n_m \). Moreover, since \( V_j \geq 0 \), the length of each facet with orientation \( n_i \in \mathcal{N} \) (\( i = 1, \ldots, m \)) is bounded away from zero independent of \( \varepsilon \in (0, \varepsilon_0) \). By Lemma 2.2. (iii) we have \( d_H(E^\varepsilon(t), E(t)) \to 0 \) as \( \varepsilon \to 0 \). We thus observe that \( E(t) \) is a fully faceted convex polygon with admissible facets \( m_i \in \mathcal{N} \) for \( t \in (t^\delta_1, t^\delta_2) \).

(ii) If \( E_0 \) and \( M \) have the same symmetry as \( W_\gamma \), then \( E(t) \) has the same symmetry as \( W_\gamma \). In \((t^\delta_1, t^\delta_2)\), \( E(t) \) is fully faceted with all orientations in \( \mathcal{N} \) so if it has the same symmetry as \( W_\gamma \), then it must be similar (homothetic) to \( W_\gamma \).

(iii) If \( M \) is proportional to \( W_\gamma \), the equation becomes

\[
V = \text{const}\gamma (\kappa_\gamma + \sigma)
\]

and there is a self-similar solution for this equation (cf. [G06], [GGu], [Gu]). So once \( E(t) \) becomes homothetic to \( W_\gamma \) in \((t^\delta_1, t^\delta_2)\), then it stays homothetic to \( W_\gamma \) for all time. Note that without proportionality of \( M \) against \( \gamma \), there might happen the corner may rounded after \( t^\delta_2 \).

\( \square \)

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