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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
E-mail: 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
E-mail: labgiga@ms.u-tokyo.ac.jp

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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 [38]. 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 $\{\Gamma_t\}_{t\geqslant 0}$ (physically a crystal surface) in $\mathbf{R}^n$ $(n \geqslant 2)$ 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 Γ_t in the direction of unit normal $\vec{n}$ of Γ_t. The function M is called a *mobility*. It is a positive function defined on the unit sphere. In many models it is considered as a given function. The quantity $1/M$ is called a *kinetic coefficient* [38]. The quantity κ_γ is a *weighted mean curvature* or *anisotropic mean curvature*. It is the first variation of the interfacial energy I of the hypersurface Γ:

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

where γ_0 is a given positive function depending on the normal (orientation) called the *interfacial energy density* and $\mathrm{d}\mathcal{H}^{n-1}$ denotes the area element. We may write

$$\kappa_\gamma = -\frac{\delta I}{\delta \Gamma}$$

in a symbolic way. Its explicit form is formally as

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

where $\gamma(p) = |p|\gamma_0(p/|p|)$ is the 1-homogeneous extension of γ_0 to $\mathbf{R}^n$ and $\operatorname{div}_\Gamma$ is the surface divergence and $\nabla_p\gamma$ is the gradient of γ. If γ_0 is identically equal to 1 so that γ_0 is isotropic, the interfacial energy I is nothing but the surface area of Γ. In this case $\gamma(p) = |p|$ and $\kappa_\gamma = -\operatorname{div}_\Gamma \vec{n}$ which is $(n-1)$-times mean curvature. The function γ_0 is determined by a crystal lattice structure. At least in very low temperature it is theoretically computable [46], [39], [45]. It seems that there is no reasonable way to calculate mobility M. The anisotropy γ_0 is called interfacial anisotropy while the anisotropy in M is called kinetic anisotropy. If both γ_0 and M are isotropic, i.e. γ_0 and M are constants and $\sigma = 0$, then (1.1) is the mean curvature flow equation. The function σ in (1.1) is a driving force. For a snow crystal growth it is supersaturation of water molecules on Γ_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 Γ_t. If σ 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 the notion of the Frank diagram [38]

$$\operatorname{Frank}\gamma = \{\, p \mid \gamma(p) \leqslant 1\}. \tag{1.4}$$

If $\operatorname{Frank}\gamma$ is convex, then (1.1) is at least degenerate parabolic under suitable regularity of γ, say C^2. If $\operatorname{Frank}\gamma$ 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 $\operatorname{Frank}\gamma$ is a convex polytope. In this case γ_0 is called a crystalline energy density and (1.1) is called a crystalline flow. Formally, the polar set of $\operatorname{Frank}\gamma$ called a Wulff shape of γ of the form

$$W_\gamma = \bigcap_{|\vec{m}|=1} \left\{\, x \mid x\cdot\vec{m} \leqslant \gamma(\vec{m})\right\} \tag{1.5}$$

plays a role of a sphere in the sense that

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

where $\vec{n}$ is taken outward. If $\operatorname{Frank}\gamma$ has a corner, then W_γ 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 κ_γ on the facet of ∂W_γ is not zero but some positive quantity despite the fact that the surface is flat. This suggests that κ_γ 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 σ is a spatially constant [18], [22].

However, for $n \geqslant 3$ or non-constant σ even well-posedness is not well-established. The main reason for $n \geqslant 3$ is that κ_γ may not be constant on a facet [8] (even if $\sigma = 0$) if one interprets κ_γ in a reasonable way. Similarly, for non-constant σ the quantity $\kappa_\gamma + \sigma$ may not be constant on a facet [19].

For $n \geqslant 3$ the unique solvability result is established for $V = \gamma\kappa_\gamma$ for convex initial data [6] 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 [19], when the equation is written in a divergence form even if σ may not be a spatially constant. Recently, a viscosity approach enables us to assert well-posedness for more general equations for graph-like functions [25] when $n = 2$. This formulation allows "facet bending" or "facet breaking". An explicit solution allowing facet bending is constructed in various settings, e.g. [34], [29]. For a general background of these problems the reader is referred to reviews articles [26], [27], [23] and [5].

In this paper we consider (1.1) in a very simple setting. We consider a planar motion (i.e., $n = 2$) and postulate that γ_0 is crystalline and σ is a given positive constant. We start with a convex crystal surrounded by Γ_0 and show that facets are instantaneously formed. Such a kind of result is already proved for a different setting in [18] and recently studied for a case when Frank γ has a curved part by P. Mucha [50] and P. Mucha and P. Rybka [51], [52] but for graphs. We call this phenomenon the instant formation of a facet. We next study whether or not a crystal becomes fully faceted after some short time. We only discuss a simple situation when Frank γ is a regular polygon centered at the origin. If M has the same symmetry as γ_0, a growing convex crystal starting from nearly the "critical size" (i.e. the curve satisfying $\kappa_\gamma + \sigma = 0$) becomes fully faceted in a finite time and it is similar (homothetic) to W_γ. In this paper we prove these statements by approximating by a crystalline flow which is a system of ordinary differential equations [58], [1]. The approximation is justified by [22]. Note that even solvability is nontrivial for (1.1) for general (convex) initial data Γ_0 and it is established in [22]. 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 $t \to \infty$ [41]. So a fully faceted crystal may be rounded again. The whole time growth behavior starting from very small convex shape is numerically calculated by [44].

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 Frank γ is C^2 and strictly convex so that the curvature κ_γ has no nonlocal nature, there is no facet provided that M is Lipschitz (continuous) by the strong maximum principle as observed in [44]. Unless the 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 σ 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

$$\Delta\sigma = 0 \qquad \text{in} \quad \Omega_t \subset \mathbf{R}^3, \tag{1.7}$$

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

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

where Ω_t is a region outside crystal. Of course one should assign the value σ at $|x| = \infty$ and initial surface Γ_0. (We take all physical constants just one for simplicity.) Recently, J. Barrett, H. Garcke and R. Nürnberg [2], [3], [4] invented a nice numerical scheme to calculate for singular γ and reproduce snow crystals both for $n = 2$ and $n = 3$. They take realistic values for mobility due to experiments while basic physics (1.7)–(1.9) including interfacial energy is taken as discussed in physical literature [47]. In [4] it appears that they successfully reproduce Nakaya's diagram [53] on snow crystal shapes depending on temperature and supersaturation. In particular, they reproduce a hexagonal prism like shape when the crystal is very small. There is another approach based on cell automaton which also produce nice pictures of snow flakes in computation [37]; however, it is not clear in what way physical parameters like σ_∞ is involved.

Mathematical analysis is not well-developed for (1.7)–(1.9) (called also one-phase Hele-Shaw type problem), even if Frank γ is smooth and strictly convex. If the problem has two-phases, it is known that the initial value problem is locally solvable and equilibrium shape is stable [14] when γ is isotropic. The anisotropic version has been established in [10]. For the one-phase problem the solvability is proved in [49] for isotropic case. If the equation (1.7) is replaced by the heat equation, the system is called the Stefan type problem and there is a large literature for two-phase problems; the reader is referred to [55] and papers cited there. However, except [43] one-phase problem is less studied.

If the interfacial energy is singular so that its Wulff shape is a cylinder, it is known that the initial value problem is locally solvable provided that one restricts the class of a solution as a cylindrical evolution [32]. In some cases there even exist self-similar solutions [33]. However, a facet may break if σ is coupled so that σ is not a constant [33]. It is restrictive to consider a class of cylindrical evolution. A sufficient condition is given so that a cylindrical evolution is still a "reasonable solution" and this is actually fulfilled for small self-similar solution [33].

In [60] evolution of snowflakes is calculated by (1.7)–(1.9); see also [62]. However, the term κ_γ is omitted. According to [4], if there is no κ_γ, no hexagonal pattern is produced. It seems that the numerical treatment in [60] and [62] includes some "regularizing effect" corresponding to κ_γ to reproduce snowflakes. Roughly speaking, anisotropy of mobility plays a role to determine rough shape of crystals (see also [61]) 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 σ 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 σ, flatness (of a facet) is preserved; see e.g. [33]. In our analysis, when γ_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 on 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 Γ_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 [16], [48] 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 γ.

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 [22] for (1.1) with $n = 2$ when Frank γ has singularities. Our formulation is based on adjustment of a level-set method developed by [14], [9]; see also [28]. Instead of considering (1.1), we consider

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

which is formally equivalent to (1.1) on $\Gamma_t = \left\{ x \in \mathbf{R}^2 \mid u(x,t) = 0 \right\}$. We consider (2.1) not only on Γ_t but also for all $\mathbf{R}^2 \times [0, +\infty)$. As in [28] we say that an open set $D \subset \mathbf{R}^2 \times [0, \infty)$ is an *open evolution* of (1.1) with initial data D_0 if there is a solution $u \in C\left(\mathbf{R}^2 \times [0, \infty)\right)$ of (2.1) such that $D = \{(x,t) \mid u(x,t) > 0\}$ and $D_0 = \{ x \mid u(x,0) > 0\}$ such that u equals a negative constant outside a big ball (depending on t). A *closed evolution* $E \subset \mathbf{R}^2 \times [0, \infty)$ of (1.1) with initial data E_0 is defined in a parallel way by replacing $>$ by $\geqslant$. The set $\Gamma = E \backslash D$ is called an *interface evolution* which is a generalized solution of (1.1) starting with initial curve $\Gamma_0 = E_0 \backslash D_0$ with $E_0 = \bar{D}_0$. Here by a solution of (2.1) we mean a certain viscosity like solution [22], which is a generalized notion of solution based on the maximum principle [28]. By definition the orientation $\vec{n}$ is taken outward from D. Our formulation restricts that $D(t)$ (resp. $E(t)$) the cross-section of D (resp. E) at t, i.e. $D(t) = \left\{ x \in \mathbf{R}^2 \mid (x,t) \in D \right\}$ is bounded (resp. $E(t) = \left\{ x \in \mathbf{R}^2 \mid (x,t) \in E \right\}$). Moreover, for a given $T > 0$ there is a big ball B, such that $D(t) \subset E(t) \subset B$ for all $t \in (0, T]$. We warn the reader that E may be strictly larger than $\bar{D}$ for $E_0 = \bar{D}_0$ even for smooth γ. This phenomenon is called fattening [14], [28]. Thus we say that E is *regular* if $E = \bar{D}$ for $E_0 = \bar{D}_0$. This implicitly assumes that there is no spike for E_0.

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

$$\begin{aligned}\mathcal{I} = \Big\{ \gamma : \mathbf{R}^2 \to (0,\infty) \mid\ & \gamma \text{ is convex, positively homogeneous of degree 1} \\ & \text{and Frank } \gamma \text{ is } C^2 \text{ except finitely many points. Moreover,} \\ & \text{the curvature of } \partial\,(\text{Frank } \gamma) \text{ is bounded except singularities} \Big\}.\end{aligned}$$

Here is a typical well-posedness result proved in [22], 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 $S^1 = \left\{ p \in \mathbf{R}^2 \,\middle|\, |p| = 1 \right\}$ and $\gamma \in \mathcal{I}$. Assume that $\sigma \in \mathbf{R}$ 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 [20]. So one can approximate the singular problem by a problem with smoother interfacial energy. Here is a typical result proved in [22].

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 $\gamma_\varepsilon \in \mathcal{I}$ converges to $\gamma \in \mathcal{I}$ uniformly on S^1 as $\varepsilon \to 0$. Moreover, $\sigma_\varepsilon \in \mathbf{R} \to \sigma \in \mathbf{R}$. Let E_0^ε and E_0 be bounded closed sets in $\mathbf{R}^2$. Let E^ε be a closed evolution of

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

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

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

where d_H is the Hausdorff distance in $\mathbf{R}^2$. 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 $\mathbf{R}^2 \times [0, T]$ for a fixed $T > 0$.

(ii) Assume that $t \mapsto E(t)$ is continuous as a set-valued function for $t \geqslant 0$. 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

$$\lim_{\varepsilon \to 0} \sup_{0 \leqslant t \leqslant T} d_H\big(E^\varepsilon(t), E(t)\big) = 0.$$

Approximation by smoother energy is first established in [15] for a graph-like function for a special equations of divergence type. It is extended for general equations by [20]. Note that our approximation result (Lemma 2.2) also allows the approximation of the problem with smooth γ by singular γ_ε like crystalline. Such a kind of approximations is discussed in a special setting – graph-like solutions by [15], [36] and convex curves [35].

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, γ and σ. 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 $E(t) \subset \mathbf{R}^2$ is convex for all $t \geqslant 0$.

(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 $0 \leqslant t < T_*$, where D is the open evolution of (1.1) with initial data D_0 and T_* is the *extinction time*, i.e. $T_* = \sup\{\, t \mid \text{int } E(t) \neq \emptyset\} \leqslant \infty$.

Proof. For smooth energy γ we have convexity preserving property proved by [30]; see [28, 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 γ [28, 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 $u \in C\left(\mathbf{R}^2 \times [0, \infty)\right)$ of (2.1) in $\mathbf{R}^2 \times (0, \infty)$ such that $x \mapsto u(x, t)$ is concave and uniformly continuous with the property:

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

By convergence to a singular problem [22, Theorem 8.1] such u converges to the problem with singular interfacial energy if it is approximated by smooth interfacial energy. Thus for singular γ the concavity preserving property u for (2.1) is inherited. This in particular implies that the convexity of $E(t)$ 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 γ is a convex polygon, i.e. $\gamma \in \mathcal{I}$ is crystalline. Assume that $M : S^1 \to (0, \infty)$ is continuous and $\sigma \in \mathbf{R}$. 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 $\Gamma_t = E(t) \backslash D(t)$. Let $\mathcal{N} \subset S^1$ be the singular set of γ, i.e. $\gamma_0 = \gamma|_{S^1} \in C^2(S^1 \backslash \mathcal{N})$ and $\nabla\gamma|_{S^1}$ has jumps exactly on $\mathcal{N}$. Then, for each $\vec{n} \in \mathcal{N}$ there is a facet (a flat portion) of Γ_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 to 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 [21]. 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 "essentially admissible" even if initially it is a non-essentially admissible crystal. For essentially admissibility, see Section 4. A missing direction in $\mathcal{N}$ is actually formed. Such a problem is studied in [24] and [54] for a polygonal evolution.

3. Formation of fully faceted small crystals

We consider the equation (1.1) when σ is a positive constant. It is easy to see that the rescaled Wulff shape $C = (1/\sigma)W_\gamma$ is a stationary closed evolution of (1.1). By the comparison principle [22] if the initial data int E_0 includes C, the closed evolution E of (1.1) with initial data always includes C and never disappears for all $t > 0$. If $E_0 \subset$ int C, 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 includes in C but close to C. It turns out that if we assume that Frank γ is a convex polygon so that its Wulff shape W_γ is a dual polygon, then $E(t)$ becomes a convex polygon with the same set of orientations as that of W_γ after some time. We call this polygon a *fully faceted* shape with respect to γ. To avoid pathological situation we impose a kind of monotonicity of M in a singular direction $\vec{n} \in \mathcal{N}$ of γ.

We extend M to $\mathbf{R}^2$ so that it is 1-homogeneous, i.e.,

$$M(p) = |p| M\,(p/|p|)\,, \quad p \neq 0.$$

The Frank diagram is defined like (1.4), i.e.,

$$\text{Frank}\, M = \left\{p \in \mathbf{R}^2 \mid M(p) \leqslant 1\right\}.$$

Let $C(\mathbf{m}_1, \mathbf{m}_2)$ be a closed (proper) cone in $\mathbf{R}^2$ spanned by two unit vectors $\mathbf{m}_1,\ \mathbf{m}_2$. Let f_i be the height function of $W_i = \text{Frank}\, M \cap C(\vec{n}_{i-1}, \vec{n}_{i+1})$ in a direction $\vec{n}_i \in \mathcal{N}$ as in [22]. Here $\vec{n}_{i-1}$ and $\vec{n}_{i+1}$ are adjacent directions of $\vec{n}_i$ in Frank M. In other words,

$$f_i(x) = \sup\left\{y \mid x\vec{n}_i^{\perp} + y\vec{n}_i \in W_i\right\},$$
$$x \in \operatorname{dom} f_i = \left\{x \mid x\vec{n}_i^{\perp} + y\vec{n}_i \in W_i \quad \text{for some} \quad y \in \mathbf{R}\right\}.$$

Here $\vec{n}_i^{\perp}$ is an unit vector orthogonal to $\vec{n}_i$. (To fix idea we take $\vec{n}_i^{\perp}$ so that $\vec{n}_i^{\perp} \cdot \vec{n}_{i+1} > 0$.)

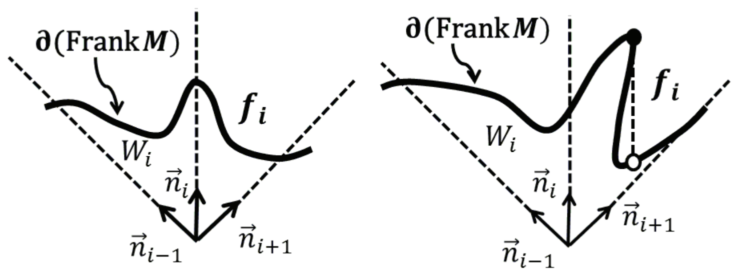

FIG. 1. Height functions of W_i

DEFINITION 3.1 (Monotonicity of M) We say that M is monotone with respect to $\mathcal{N}$ if for each $\vec{n}_i \in \mathcal{N}$ there is a constant $\alpha_i \in (0, \pi/2)$ such that

$$f_i(x+h) - f_i(x) \geqslant -(\tan\alpha_i)h, \quad h > 0,\ x > 0,\ x+h \in \operatorname{dom} f_i,$$
$$f_i(x-h) - f_i(x) \geqslant -(\tan\alpha_i)h, \quad h > 0,\ x < 0,\ x-h \in \operatorname{dom} f_i,$$

where f_i is the height function of W_i in the direction of $\vec{n}_i$.

The left in Figure 1 is an example that M is monotone in the direction of $\vec{n}_i$ while the right in Figure 1 is an example that M is not monotone.

We give a typical result for a fully faceted phenomena.

THEOREM 3.2 (Fully faceted phenomena) Assume that Frank γ is a regular k-polygon centered at the origin. Assume that $M : S^1 \to (0,\infty)$ is continuous and $\sigma > 0$. Assume furthermore that M is monotone with respect to $\mathcal{N}$, where $\mathcal{N}$ is the singular set of γ. Let E_0 be the closure of a bounded open and convex set D_0 containing the critical shape $C = (1/\sigma)W_\gamma$. Let E be the interface evolution of (1.1) with initial data E_0.

(a) If E_0 is sufficiently close to C, there $E(t)$ becomes fully faceted with respect to γ in finite time $t = t_0$ with some $t_0 > 0$.
(b) Assume that E_0 is sufficiently close to C so that E has the property in (a). If E_0 and M has the same symmetry as γ i.e., $\mathbf{Z}_k$-symmetry in the sense that E_0 is invariant under rotation of angle $2\pi/k$, then the full faceted shape is similar to W_γ on some time interval i.e. $E(t) = c(t)W_\gamma$ for $t \in (t_0, t_1)$ with some $t_0, t_1 > 0$ with some positive constant $c(t)$.
(c) Assume that E_0 is sufficiently close to C so that E has the property in (a). If E_0 has the same symmetry as γ and if M is proportional to γ, then $E(t) = c(t)W_\gamma$ for all $t > t_0$ with some $t_0 > 0$ with some positive constant $c(t)$.

REMARK 3.3 (i) Unless M is proportional to γ, the large time asymptotics may be different from W_γ up to dilation even in case (b). Actually, it is essentially known that $E(t)/t \to W_M$ (Hausdorff distance sense) so $t \to \infty$, where W_M is the Wulff shape of M. This asymptotic behavior is proved in [41] for smooth γ but it can be easily extended to the singular case as noted in [44].
(ii) There are several numerical simulations for E by changing anisotropy of γ and M in [44]. In their examples for a short time a fully faceted shape with respect γ 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_γ 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/γ depends on $\vec{n} \in \mathcal{N}$, then the fully faceted shape is not similar W_γ (nor W_M). We conjecture that $\sigma E(t)$ converges to $cW_{\tilde{\gamma}}$ with $\tilde{\gamma}\kappa_{\tilde{\gamma}} = M\kappa_\gamma$ as $\sigma \to 0$ with some constant $c > 0$. Such $\tilde{\gamma}$ 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 $W_{\tilde{\gamma}}$ for some $\tilde{\gamma}$ provided that γ and M is smooth and $\gamma(\vec{n}) = \gamma(-\vec{n})$, $M(\vec{n}) = M(-\vec{n})$ and that Frank γ is strictly convex; see [17], [11], [12] and a review paper [26] and a book [28]. A similar result is proved for crystalline flow by [56], [57]. 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_γ is a hexagonal prolonged prism while we often find thin or thick hexagonal prism of snowflakes. This is caused by a difference of M/γ on basal and prism surface.

(iv) Even if σ is not constant, admissible facets stay admissible provided that the crystal is sufficiently small (so that κ_γ is large) with respect to the gradient of σ. On the facet the driving force turns to be equal to its average over the facet in this case [19], [33]. In fact, a comparison principle holds for such small crystals [7]. 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 γ is chosen so that M/γ is constant as in the case of (c). This is actually proved for special γ and M in [33].

(v) The monotonicity of M with respect to γ is not very restrictive. Typical examples include $M \equiv 1$ (for $k > 4$) and $M \equiv \gamma$. Examples in numerical simulation [44], [4] also fulfill this monotonicity.

4. Approximation by crystalline flow

We shall prove Theorems 2.4 and 3.2 by approximating by (generalized) crystalline flows. We first recall flows with no curvature term to explain corner preserving conditions.

4.1 *Corner preservation*

We consider the Hamilton-Jacobi equation

$$V = M(\vec{n})\sigma \tag{4.1}$$

where $M > 0$ is continuous and σ is a positive constant. In other words, we drop the curvature term in (1.1). We consider the closure of convex polygonal domain K_0 with facets whose orientations consist of $\mathcal{M} = \{\mathbf{m}_j\}_{j=1}^r \subset S^1$ ($r \geqslant 3$). The numbering is taken clockwise. We consider a flow of (4.1) starting from $S_0 = \partial K_0$. We are interested in the problem whether or not the solution stays a convex polygon with the same orientation of facets. For this purpose we recall an elementary geometric fact.

LEMMA 4.1 Let $H(\mathbf{m}, h)$ be the half space with orientation $\mathbf{m} \in S^1$ and the support parameter $h > 0$, i.e.,

$$H(\mathbf{m}, h) = \left\{x \in \mathbf{R}^2 \mid x \cdot \mathbf{m} \leqslant h\right\}.$$

Let $\mathbf{m}_1, \mathbf{m}_2 \in S^1$ ($\mathbf{m}_1 \neq \mathbf{m}_2$) satisfy $\mathbf{m}_1 \cdot \mathbf{m}_2 > 0$. Let $\mathbf{n} \in S^1$ be a point on the (shorter) arc $\widehat{\mathbf{m}_1\mathbf{m}_2}$. Let $h_1,\ h_2$ be positive parameters. Then

$$H(\mathbf{m}_1, h_1) \cap H(\mathbf{m}_2, h_2) \subset H(\mathbf{n}, h)$$

if and only if

$$h \geqslant \frac{1}{\sin\varphi}\left(h_1 \sin\varphi_2 + h_2 \sin\varphi_1\right). \tag{4.2}$$

Here φ is the angle of (vectors) $\mathbf{m}_1$ and $\mathbf{m}_2$ and φ_ℓ is the angle of $\mathbf{m}_\ell$ and $\mathbf{n}$ so that $\varphi_1 + \varphi_2 = \varphi$. The equality in (4.2) holds if and only if $\partial H(\mathbf{n}, h) \cap H(\mathbf{m}_1, h_1) \cap H(\mathbf{m}_2, h_2)$ is a singleton.

We now consider the initial value problem for (4.1) with initial data $S_0 = \partial K_0$. We may assume that K_0 includes the origin as an interior point so that it is of the form

$$K_0 = \bigcap_{j=1}^{r} H\left(\mathbf{m}_j, h_j^0\right). \tag{4.3}$$

The problem is whether or not

$$K_t = \bigcap_{j=1}^{r} H\left(\mathbf{m}_j, h_j(t)\right), \quad t > 0 \tag{4.4}$$

$$h_j(t) = h_j^0 + M(\mathbf{m}_j)\sigma t$$

is the solution (the closed evolutions) of (4.1) starting from K_0 in level-set sense or viscosity sense (e.g. [28]). For example, if $M \equiv 1$, then the corner of solutions is immediately rounded. The next property easily follows from Lemma 4.1 and definition of solution.

LEMMA 4.2 (Corner preservation) Assume that for all $j \in \{1, \ldots, r\}$ M satisfies

$$M(\mathbf{m}) = \frac{1}{\sin\varphi_{jj+1}}\left\{M(\mathbf{m}_j)\sin\varphi_{j+1} + M(\mathbf{m}_{j+1})\sin\varphi_j\right\}, \tag{4.5}$$

where $\mathbf{m}$ is on the (shorter) arc between $\mathbf{m}_j$ and $\mathbf{m}_{j+1}$ and φ_{jj+1} is the angle of $\mathbf{m}_j$ and $\mathbf{m}_{j+1}$ and φ_k is the angle of $\mathbf{m}_k$ and $\mathbf{m}$ with convention that $\mathbf{m}_{r+1} = \mathbf{m}_1$. Then K_t given by (4.4) is the solution of (4.1) (with $\sigma > 0$) starting with K_0 given by (4.3).

REMARK 4.3 Actually, it is enough to assume $\geqslant$ in (4.5). The condition (4.5) is a necessary and sufficient condition so that the solution stays a polygon with orientations contained in $\mathcal{M}$ if K_0, which is not necessarily convex, has $\mathcal{M}$ as the set of orientations. We also note that some corner may disappear so Lemma 4.2 gives a condition that no new corners or round parts are created. The same condition (4.5) at each corner is given for example in [21, (3.2)] or [38] in a different way of description.

We give a geometric interpretation. We extend M to $\mathbf{R}^2$ so that it is 1-homogeneous, i.e.,

$$M(p) = |p| M\left(p/|p|\right), \quad p \neq 0.$$

The Frank diagram is defined like (1.4).

LEMMA 4.4 Assume that the polygonal domain whose vertices consist of points in $\mathcal{M}$ contains the origin. The condition (4.5) holds for all $j \in \{1, \ldots, r\}$ if and only if Frank M is a polygon (not necessarily convex) whose vertices consist of $\left(1/M\left(\mathbf{m}_j\right)\right)\mathbf{m}_j$, $j \in \{1, \ldots, r\}$ (allowing that the angle of a vertex equals π).

The proof is elementary so is left to the readers. If (4.5) is fulfilled for all $j \in \{1, \ldots, r\}$, then the orientation of the Wulff shape W_M corresponding to direction of vertices of the convex hull of Frank M. In the solution K_t determined (4.4) for sufficiently large t the orientation which does not appear in W_M stays bounded or disappear. The large time behavior in Remark 3.3 (i) can be directly proved in this setting.

4.2 *Crystalline flow for essentially admissible crystals*

We consider (1.1) for a polygonal flow. We first recall an essentially admissible evolving crystal which is a special evolving polygon preserved by a crystalline curvature flow equation. Let Frank γ be a convex k-polygon. Let q_i $(i = 1, 2, \ldots, k)$ be its vertices. Then the singular set $\mathcal{N}(\subset S^1)$ is of the form

$$\mathcal{N} = \left\{ q_i/|q_i| \;\middle|\; i = 1, 2, \ldots, k \right\}.$$

We say that a simple oriented polygonal curve S in $\mathbf{R}^2$ 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

$$\frac{(1-\lambda)\mathbf{n} + \lambda\hat{\mathbf{n}}}{|(1-\lambda)\mathbf{n} + \lambda\hat{\mathbf{n}}|} \notin \mathcal{N} \tag{4.6}$$

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 [58], [1]; see also [31]. We say that a family of polygons $\{S_t\}_{t\in J}$ 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 with $J = [0, T)$. The notion of essentially admissibility is found in [40], where σ is assumed to be zero. 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 is $\mathbf{n}_j$. Here we number facets clockwise. We say that $\{S_t\}_{t\in J}$ is a γ*-regular flow* [21] of (1.1) if

$$V_j = M\left(\mathbf{n}_j\right)\left(\frac{\chi_j \Delta\left(\mathbf{n}_j\right)}{L_j(t)} + \sigma\right) \quad \text{on} \quad S_j(t),\ t \in J \tag{4.7}$$

for $j = 1, 2, \ldots, r$, where V_j denotes the normal velocity of $S_j(t)$ in the direction of $\mathbf{n}_j$. For the derivation, see e.g. [21]. The quantity $\chi_j \Delta\left(\mathbf{n}_j\right)/L_j(t)$ is a nonlocal weighted curvature $\kappa_\gamma\left(\mathbf{n}_j\right)$ for

$\mathbf{n}_j \in \mathcal{N}$, where $L_j(t)$ denotes the length of $S_j(t)$. The quantity $\Delta\left(\mathbf{m}_j\right)$ is defined by

$$\begin{aligned} \Delta\left(\mathbf{m}_j\right) &= \tilde{\gamma}'\left(\theta_j + 0\right) - \tilde{\gamma}'\left(\theta_j - 0\right) && \text{if} \quad \mathbf{m}_j \in \mathcal{N}, \\ \Delta\left(\mathbf{m}_j\right) &= 0 && \text{if} \quad \mathbf{m}_j \notin \mathcal{N}, \end{aligned}$$

where $\mathbf{m}_j = \left(\cos\theta_j, \sin\theta_j\right)$ and $\tilde{\gamma}(\theta) = \gamma(\cos\theta, \sin\theta)$. The quantity χ_j is a transition number. It takes $+1$ (resp. -1) if S_t is convex (resp. concave) in the direction of $\mathbf{n}_j$; we use the convention that $\chi_j = -1$ for all $j = 1, \ldots, r$ if S_t is convex. We note that $\Delta(\mathbf{n}_i)$ has a geometric meaning. It is the length of facet of the Wulff shape W_γ with outward normal $\mathbf{n}_i \in \mathcal{N}$. We have assumed that $\sigma \in \mathbf{R}$ is a constant.

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

$$\dot{L}_j(t) = \frac{\mathrm{d}L_j(t)}{\mathrm{dt}} = \left(\cot\psi_j + \cot\psi_{j+1}\right) V_j - \frac{1}{\sin\psi_j} V_{j-1} - \frac{1}{\sin\psi_{j+1}} V_{j+1} \tag{4.8}$$

for $j = 1, \ldots, r$; index j is considered modulo r. Here $\psi_j = \theta_j - \theta_{j-1}$ (modulo 2π) with $\mathbf{n}_j = \left(\cos\theta_j \sin\theta_j\right)$. Thus the equation (4.7) forms a system of ordinary differentiation equations (ODE) with (4.8) for L_j's. A fundamental theory of ODE yields the (local-in-time) unique solvability of (4.7)–(4.8) 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 [21] and [42], one observes that only facet with $\mathbf{n}_j \notin \mathcal{N}$ may disappear for γ-regular flow at $t = t_0$ if the enclosed set of S_{t_0-0} has no interior. One can extend the solution after t_0 by solving (4.7)–(4.8) if the enclosed set of S_{t_0-0} has no interior. In the case when $\sigma = 0$ we just repeat this procedure 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. Such a flow is well-studied in [59] for $\sigma = 0$.

One should be careful to see the consistency of a crystalline flow with an interface evolution (also called a level-set flow). This topic is well-discussed for admissible evolving crystals in [21]. It is easy to adjust their argument for essentially admissible evolving crystals when $\sigma = 0$ under corner preservation condition. However, if $\sigma > 0$ some facets with non-admissible direction, i.e. $\mathbf{m}_j \notin \mathcal{N}$ need to be created to be a level-set flow when "admissible facet" becomes large. Because of the presence of M a new facet may be created. We prepare some notion of convexification.

DEFINITION 4.5 (Convexification associated with $\mathcal{Z}$) Let $C(\mathbf{m}_1, \mathbf{m}_2)$ be a closed (proper) cone spanned by two unit vectors $\mathbf{m}_1$, $\mathbf{m}_2$. Let F be a closed set. Define

$$F_{C(\mathbf{m}_1,\mathbf{m}_2)} = \mathrm{co}\left(F \cap C(\mathbf{m}_1, \mathbf{m}_2)\right),$$

where co denotes the convexification. For $\mathcal{Z} = \left\{\mathbf{s}_j\right\}_{j=1}^{\ell} \subset S^1$ let

$$\mathrm{co}\,(F; \mathcal{Z}) = \bigcup_{j=1}^{\ell} F_{C(\mathbf{s}_j,\mathbf{s}_{j+1})}$$

and call $\mathrm{co}\,(F; \mathcal{Z})$ the *convexification of F associated with $\mathcal{Z}$*. Here $\mathbf{s}_j$ is numbered clockwise with convention that $\mathbf{s}_{\ell+1} = \mathbf{s}_1$. Here the angle of $\mathbf{s}_j$ and $\mathbf{s}_{j+1}$ is assumed to be less than π (so that $\ell \geqslant 3$ and the polygon whose vertices consist of all points of $\mathcal{Z}$ encloses the origin).

DEFINITION 4.6 Let M be a continuous 1-homogeneous function in $\mathbf{R}^2$ such that $M|_{S^1} > 0$. For a given $\mathcal{Z} \subset S^1$ let $M_{\mathcal{Z}}$ be the 1-homogeneous function defined by

$$\text{Frank}\,(M_{\mathcal{Z}}) = \text{co}\,(\text{Frank}\,M; \mathcal{Z})$$

We call $M_{\mathcal{Z}}$ the *hull* of M associated with $\mathcal{Z}$.

Assume that M fulfills the corner preserving condition (4.5) with respect to a given set $\mathcal{M} = \{\mathbf{m}_j\}_{j=1}^r$. Then by Lemma 4.4 Frank M is a polygon whose vertices consist of $1/M(\mathbf{m}_j)\mathbf{m}_j$, $j = 1, \dots, r$. In this case, evidently $M_{\mathcal{M}} = M$. For $\mathcal{N} \subset \mathcal{M}$ consider $M_{\mathcal{N}}$, the hull of M associated with $\mathcal{N}$, i.e., Frank $(M_{\mathcal{N}}) = \text{co}\,(\text{Frank}\,M, \mathcal{N})$. Let $\mathcal{M}_{\mathcal{N}}$ be the set of all vertex directions of Frank $(M_{\mathcal{N}})$. By definition $\mathcal{M}_{\mathcal{N}} \subset \mathcal{M}$.

We give a generic condition which is especially preserved under evolution. In particular, we are interested in sufficient conditions so that no new facet is created. For this purpose we need to modify Frank M depending upon the length of an *admissible facet*, i.e., a facet with the orientation in the singular set $\mathcal{N} \subset S^1$. Assume that $\sigma > 0$. For a given $L_i \in [0, \infty]$ we set

$$\Sigma_i = \left\{\lambda \mathbf{n}_i \mid 0 \leqslant \lambda \leqslant 1/\left[M(\mathbf{n}_i)\,(1 - \Delta(\mathbf{n}_i)/L_i\sigma)_+\right]\right\}, \quad \mathbf{n}_i \in \mathcal{N}$$

with interpretation that

$$\begin{aligned} \Sigma_i = &\quad \{\lambda \mathbf{n}_i \mid 0 \leqslant \lambda\} \quad \text{when} \quad L_i\sigma \leqslant \Delta(\mathbf{n}_i), \\ \Sigma_i = &\quad \{\lambda \mathbf{n}_i \mid 0 \leqslant \lambda \leqslant 1/M(\mathbf{n}_i)\} \quad \text{when} \quad L_i = \infty. \end{aligned}$$

We further denote the totality of these rays by $\Sigma(L)$, i.e.,

$$\Sigma(L) = \bigcup_{i=1}^{k} \Sigma_i$$

for $L = (L_1, \dots, L_k)$.

DEFINITION 4.7 (Property G) Let $\mathcal{M}$ be a finite set of S^1 containing $\mathcal{N}$. Assume that M satisfies (4.5) with respect to $\mathcal{M}$. Assume that $\mathcal{K} \subset S^1$ satisfies $\mathcal{N} \subset \mathcal{K} \subset \mathcal{M}$. Assume that $\sigma > 0$. For a given L we say that $\mathcal{K}$ has the property G_L if all $\mathbf{m}/M(\mathbf{m})$ ($\mathbf{m} \in \mathcal{M}\backslash\mathcal{K}$) belongs to the interior of the convexification of Frank $M \cup \Sigma(L)$ associated with $\mathcal{K}$, i.e. co (Frank $M \cup \Sigma(L), \mathcal{K}$). In the case $L = (\infty, \dots \infty)$ by definition Frank M = Frank $M \cup \Sigma(L)$ and we simply write G_L by G_∞. Let K be the closure of a convex polygonal region in $\mathbf{R}^2$. Let $\mathcal{K}$ be the set of all orientations of facets of K (satisfying $\mathcal{N} \subset \mathcal{K} \subset \mathcal{M}$). Let L_i denote the length of admissible facet of K whose orientation is $\mathbf{n}_i \in \mathcal{N}$ ($1 \leqslant i \leqslant k$). We say that K has the property G if $\mathcal{K}$ has the property G_L with $L = (L_1, \dots, L_k)$.

Evidently, the property G_∞ implies G_L so if $\mathcal{K}$ has the property G_∞, then K has the property G independent of the length of an admissible facet.

To understand property G we consider the case when $\mathcal{N}$ is empty. We move a convex set K_0 by (4.1) with $\sigma > 0$. More precisely, we consider the closed evolution of (4.1) starting from K_0. Assume that ∂K_0 is a convex polygon and the set of all orientations of facets of K_0 satisfies G_∞. It is easy to see that the property G is preserved although the set of orientations may decrease. No new facet is created.

In the case when $\mathcal{N}$ is non-empty the closed evolution of (1.1) is more complicated when $\sigma > 0$. Since G is an open property, during a short time, the property G is preserved. However, if the length of an admissible facet becomes large, there might be chance that some non-admissible facets with direction in $\mathcal{M}\backslash\mathcal{K}$ near the admissible direction, i.e. the direction $\mathbf{n}_i \in \mathcal{N}$ may be created so that it is consistent with the level-set flow. A general principle is that in a growing crystal a slow facet remains while a fast facet may disappear. The speed depends on the length for an admissible facet and this may break the property G. This kind of phenomena never occurs in the case $\sigma = 0$.

We consider γ-regular flow of (1.1) starting from $S_0 = \partial K_0$ and assume that the set $\mathcal{K}$ of orientations of K_0 agrees with $\mathcal{M}$. We consider the case $\sigma > 0$. Evidently, K_0 has the property G. There is a chance that some non-admissible facets may disappear at some time t_0 but we extend γ-regular flow with initial data S_{t_0-0} (enclosing K_{t_0-0}) as far as the property G is preserved. However, there might be chance that this *extended* γ-regular flow may lose the property G at some time t_1 so we need to modify by inserting some non-admissible facets.

DEFINITION 4.8 (Modified γ-regular flow) Let $\mathcal{M}$ be a finite set of S^1 containing $\mathcal{N}$. Assume that M satisfies (4.5) with respect to $\mathcal{M}$. Let $\{S_t\}_{t\in[0,t_1)}$ be an extended γ-regular flow of (1.1) (with $\sigma > 0$) with initial data $S_0 = \partial K_0$ and S_0 is a convex polygon such that the set of its orientation agrees with $\mathcal{K}$ ($\mathcal{N} \subset \mathcal{K} \subset \mathcal{M}$). Assume that K_t enclosed by S_t has the property G for $t \in [0, t_1)$ but loses the property G at $t = t_1$. If there is a non-admissible direction $\mathbf{m}_j \in \mathcal{M}\backslash\mathcal{K}_{t_1}$ such that $\mathbf{m}_j/M(\mathbf{m}_j)$ is on the set

$$\partial\left(\mathrm{co}\left(\mathrm{Frank}\, M \cup \Sigma(L_{t_1})\right), \mathcal{K}_{t_1}\right),$$

then we insert all these non-admissible facets with such orientations for $t > t_1$ and solve (4.7) with adding these facets. Here $\mathcal{K}_t$ denotes the set of orientations of K_t and $L_t = (L_{1,t}, \ldots, L_{k,t})$ is the set of lengths of admissible facets of K_t. Note that some inserted facets may instantaneously disappear but the resulting solution for $t > t_1$ close to t_1 has the property G. We call this new solution *modified* γ-regular flow.

We say that an extended γ-regular flow of (1.1) starting from $S_0 = \partial K_0$ is a *(generalized) crystalline flow* of (1.1) when $\sigma \leqslant 0$ provided that the set of orientation of K_0 equals $\mathcal{M}$. In the case $\sigma > 0$ we call modified γ-regular flow of (1.1) starting from $S_0 = \partial K_0$ (with $\mathcal{K} = \mathcal{M}$) a *(generalized) crystalline flow* of (1.1). For $\sigma > 0$ a generalized crystalline flow preserves the property G except times of inserting non-admissible facets.

We are ready to state the consistency with the closed evolution, which develops no fattening as observed in Theorem 2.1.

LEMMA 4.9 (Consistency) Assume the same hypotheses of Theorem 2.4 concerning γ, M, σ. Assume that E_0 is a convex closed polygonal region such that $S_0 = \partial E_0 \left(= \cup_{j=1}^r S_j(0)\right)$ is essentially admissible (with respect to γ). Let E be the closed evolution of (1.1) with initial data E_0. Then $S_t = \partial E(t)$ is a (generalized) crystalline flow in $J = [0, T_*)$ with initial data S_0 provided that the corner preservation property (4.5) holds for all $j = 1, \ldots, r$. Here T_* is the extinction time $\leqslant \infty$.

The proof is similar to [21] but of course more involved. We take $\mathcal{M}$ consisting of all orientations of facets of the initial convex polygon S_0.

The criterion to insert non-admissible facet for $\sigma > 0$ is based on the fact whether property G holds. As far as G holds, there need no creation of non-admissible facets. If an admissible faced becomes large, then its growing speed is larger and may lose the property G, so it may not prohibit creation of suitable non-admissible facets. Here is a condition for no creation of non-admissible facets. We invoke the monotonicity condition for M given in Definition 4.6.

LEMMA 4.10 (No creation of non-admissible facets) Let $\mathcal{M}$ be a finite set of S^1 containing $\mathcal{N}$ and assume that M satisfies (4.5) with respect to $\mathcal{M}$. Assume that M is monotone with respect to $\mathcal{N}$ and with parameter $\alpha = (\alpha_1, \ldots, \alpha_k)$. Assume that $\mathcal{K}$ ($\mathcal{N} \subset \mathcal{K} \subset \mathcal{M}$) has the property G_0 with $\sigma > 0$.

(i) There exists a constant $L_i^* > \Delta(\mathbf{n}_i)/\sigma$ such that if $L_i \leqslant L_i^*$ ($i = 1, \ldots, k$) then $\mathcal{K}$ has the property G_L with $L = (L_1, \ldots, L_k)$. The constant L_i^*'s can be taken so that it only depends on α (independent of $\mathcal{K}$).

(ii) Let K be a convex closed polygonal region where the set of its orientations equals $\mathcal{K}$. Then there is $\delta' > 0$ depending only on α such that if $K \subset C_{\delta'} = (1 + \delta')C,\ C = (1/\sigma)W_\gamma$, then K has the property G.

The second statement is a simple collorary of the first statement because smaller δ we choose, L_i's becomes closer to $\Delta(\mathbf{n}_i)/\sigma$. The first statement is easily proved by elementary geometry.

Our generalized crystalline flow approximates the solution of (1.1) as we see below.

The corner preserving condition (4.5) uniquely interpolates the values of $M(\mathbf{m})$ from the value of M at $\mathbf{m}_j$ ($j = 1, \ldots, r$). The way of interpolation is given in [21, (3.3)]. Geometrically speaking, if $\sigma > 0$, one considers an r-polygon F whose vertices consist of $\mathbf{m}_j/M(\mathbf{m}_j)$. The interpolated $\tilde{M}$ is defined such that Frank $\tilde{M}$ agrees with F.

Notice that if the set $\{\mathbf{m}_j\}_{j=1}^{r(\varepsilon)}$ 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 4.9), we are able to conclude the convergence of crystalline algorithm.

LEMMA 4.11 (Convergence of crystalline algorithm) Assume the same hypotheses of Theorem 2.4 concerning γ, M, σ. 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 $\{\Gamma_t\}_{t \geqslant 0}$ be the corresponding level-set flow with initial data $\Gamma_0 = E_0 \backslash D_0$ with extinction time $T_* \in (0, \infty]$. Let E_0^ε be a convex polygon such that its boundary $S_0^\varepsilon = \cup_{j=1}^{r(\varepsilon)} S_j^\varepsilon(0)$ is an essentially admissible crystal (with respect to γ). Let S_t^ε be the crystalline flow with initial data S_0^ε. Then

$$\sup_{0 \leqslant t \leqslant T} d_H\left(S_t^\varepsilon, \Gamma_t\right) \to 0$$

for all $T \in (0, T_*)$ provided that $d_H\left(S_0^\varepsilon, \Gamma_0\right) \to 0$ as $\varepsilon \downarrow 0$.

There are several ways to approximate Γ_0 by an essentially admissible crystal S_0^ε. We here give a typical way. A convex set $E_0 = \overline{D_0}$ is written by using a suitable support function $h(\mathbf{m})$ (convex in $\mathbf{R}^2$) so that

$$E_0 = \left\{ x \in \mathbf{R}^2 \mid x \cdot \mathbf{m} \leqslant h(\mathbf{m}) \text{ for all } \mathbf{m} \in S^1 \right\}.$$

We approximate E_0 by E_0^ε by

$$E_0^\varepsilon = \left\{ x \in \mathbf{R}^2 \mid x \cdot \mathbf{m} \leqslant h(\mathbf{m}) \text{for all } \mathbf{m} \in \mathcal{N} \cup \mathcal{M}_\varepsilon \right\}.$$

where $\mathcal{M}_\varepsilon = \{(\cos\theta_i, \sin\theta_i) \mid \theta_{i+1} \leqslant \theta_i \text{ with } |\theta_{i+1} - \theta_i| \leqslant \varepsilon,\ i = 1, 2, \ldots N(\varepsilon)\}$. It is not difficult to see that $E_0^\varepsilon \to E_0$ in the Hausdorff distance sense. Evidently, ∂E_0^ε is an essentially admissible crystal by modifying h slightly if necessary.

Because of this approximability, approximation by crystalline flow is often called a crystalline algorithm [36], [35] since crystalline flow is obtained by solving ODEs. The convergence rate is proved for heat equation and curve shortening equation of graph-like function for smooth solution in [36] and for convex curve [35]. Note that convergence result is also proved in [15] for graphs. However, in both cases there is no driving force σ.

4.3 *Formation of admissible facets*

We use above approximation to conclude instant formation of an admissible facets.

Proof of Theorem 2.4. We use crystalline approximation given in Lemma 4.11. Since $E^\varepsilon(t)$ and $E(t)$ are convex sets we may represent these sets by

$$E^\varepsilon(t) = \bigcap_{j=1}^{r(\varepsilon)} \left\{ x \in \mathbf{R}^2 \mid x \cdot \mathbf{n}_j \leqslant d_j^\varepsilon(t) \right\}$$

with $d_j^\varepsilon(t)$'s, we say d_j^ε is he support function at $\mathbf{n}_j$. For the case $\sigma > 0$ we have to allow that $d_j^\varepsilon(t)$ may have jump for non-admissible facet since some non-admissible facets may be created. By definition of T_* for $T \in (0, T_*)$ there is a small open disk B such that $B \subset E(t)$ and $B \subset E^\varepsilon(t)$ for $t \in [0, T]$ and for small $\varepsilon > 0$. We may assume that the center of B is the origin. This implies

$$\inf_{0<\varepsilon<\varepsilon_0} \inf_{t\in[0,T]} d_j^\varepsilon(t) > 0 \quad \text{for} \quad j = 1, \ldots, r.$$

We shall prove that the length of a facet with the orientation $\mathbf{n}_\ell \in \mathcal{N}$ of Γ_t is positive in a dense subset of $(0, T)$. Let $L_\ell(t)$ be the length of the facet with normal $\mathbf{n}_\ell$ allowing that $L_\ell(t) = 0$, i.e., the facet is degenerated to a point. We do not assume that $L_\ell(0) > 0$. By the convergence of convex set and Lemma 4.11 we conclude that $L_l^\varepsilon(t) \to L_\ell(t)$ and $d_l^\varepsilon(t) \to d_\ell(t)$ uniformly on $[0, T]$, where $d_\ell(t)$ is the support function at $\mathbf{n}_\ell \in \mathcal{N}$ corresponding to the facet of Γ_t. Assume that $L_\ell(t) = 0$ for $[t_0, t_1] \subset (0, T)$. Since $\dot{d}_l^\varepsilon(t)$ is the normal velocity $V_\ell = V_\ell^\varepsilon$, integrating (4.7) over $[t_0, t_1]$ yields

$$d_l^\varepsilon(t_1) - d_l^\varepsilon(t_0) = M(\mathbf{n}_\ell) \int_{t_0}^{t_1} \left(\frac{-\Delta(\mathbf{n}_\ell)}{L_\ell^\varepsilon(t)} + \sigma \right) \mathrm{d}t, \ \mathbf{n}_\ell \in \mathcal{N}.$$

The left hand side is bounded from below as $\varepsilon \to 0$. However, this is impossible since $L_l^\varepsilon(t) \to 0$ uniformly in $[t_0, t_1]$. We have thus proved that $L_\ell(t) > 0$ for a dense subset of $(0, T)$. Since $\mathcal{N}$ is finite, there is a dense set J_0 of $(0, T)$ such that $L_\ell(t) > 0$ for all $t \in J_0$ and $\mathbf{n}_\ell \in \mathcal{N}$.

As for the proof of crystalline flow [42], [21] combining (4.7) and (4.8) for approximation, one is able to prove that facets of Γ_t with orientation in $\mathcal{N}$ has a positive length for a short time if it has initially of positive length. If admissible facets surrounded by parts of non-admissible direction, these parts move by (4.1) so it does not affect admissible facets especially when admissible facets are short. We do not give a detailed proof. This implies $L_\ell(t) > 0$ for all $t \in (0, T]$ so the proof is now complete. □

4.4 *Fully faceted pattern*

We shall prove formation of a fully faceted pattern stated in Theorem 3.2. The basic idea is to show a similar statement for crystalline flows and a general flow by approximation by a crystalline flow. Of course, one should be careful to check that the time duration of fully faceted pattern is take uniform with respect to approximation.

We shall always assume that

$$\text{Frank } \gamma \text{ is a regular } k\text{-polygon centered at the origin,} \tag{4.9}$$

to simplify the situation. Our strategy to prove formation of a fully faceted pattern consists of (i) upper bound for growth of admissible facets by a self-similar solution and (ii) lower bound for growth of non-admissible facets. Two bounds imply disappearance of non-admissible facets in some time interval by Lemma 4.1.

Let C be the critical shape, i.e., $C = (1/\sigma)W_\gamma$. We consider

$$V = a(\kappa_\gamma + \sigma) \tag{4.10}$$

with $a = \sup_{S^1} M$. As well-known, the equation (4.10) admits a self-similar crystalline flow of the form $S_t^* = z(t)\partial C$ under (4.9) [38, 12G]. The function $z(t)$ solves

$$\dot{z}(t) = ab^{-1}(-1/z(t) + \sigma) \tag{4.11}$$

where $b = \gamma(\mathbf{n}_i)$. If initial data is taken as a boundary of $C_\delta = (1 + \delta)C$ with $\delta > 0$,the corresponding growing self-similar solution S_t^* encloses convex set K_t^* of the form

$$K_t^* = \bigcap_{i=1}^{k} H\left(\mathbf{n}_i, \lambda(t)\right), \ \lambda(t) = z(t)b, \ z(0) = (1 + \delta)/\sigma, \ \mathbf{n}_i \in \mathcal{N}.$$

PROPOSITION 4.12 (Upper bound) Assume (4.9) and $\sigma > 0$. Let Γ_t^* be the crystalline flow of (1.1) of the form

$$\Gamma_t^* = \partial G_t^*, \quad G_t^* = \bigcap_{i=1}^{k} H\left(\mathbf{n}_i, d_i^*(t)\right), \quad t \in [0, T]$$

starting from $\Gamma_0^* = \partial C_\delta$. Then $G_t^* \subset K_t^*$ or equivalently

$$d_i^*(t) \leqslant \lambda(t)$$

where $\lambda(t) = z(t)b$ is given by (4.11) with $z(0) = (1 + \delta)/\sigma$.

Proof. We first note that the (outward) normal velocity of each facet of Γ_t^* is always non-negative. Indeed, $G_0^* = C_\delta \subset G_h^*$ for small $h > 0$ because speed of Γ_0^* is positive everywhere. By a comparison principle [31] $G_t^* \subset G_{t+h}^*$ for all $t > 0$ which yields that the normal velocity of Γ_t^* is non-negative.

We have observed that $\kappa_\gamma + \sigma \geqslant 0$ on each facet of Γ_t^*. Thus we conclude that Γ_t^* is a “subsolution” of (4.10). By a comparison principle [31] we see that $G_t^* \subset K_t^*$. □

PROPOSITION 4.13 (Upper bound for admissible facets) Assume (4.9) and $\sigma > 0$. Let $\mathcal{M} \subset S^1$ so that $\mathcal{N} \subset \mathcal{M}$ where $\mathcal{N}$ is the set of admissible directions. Let K_0 be a closed convex polygonal region satisfying the property G. Assume that $C \subset K_0 \subset C_\delta$. Let ∂K_t be the (generalized) crystalline flow starting from ∂K_0. Then $K_t \subset K_t^*$. In particular,

$$h_i(t) \leqslant \lambda(t) \quad \text{for} \quad \mathbf{n}_i \in \mathcal{N}, \quad t \in [0, T]$$

where $\lambda(t)$ is the same as Proposition 4.12 provided that K_t is expressed as (4.4) for $t \in [0, T]$.

Proof. This follows from comparison principle of a level-set flow [22]. One should interpret (generalized) crystalline flow as a level-set flow of (1.1) by interpolating M outside $\mathcal{M}$ so that (4.5) holds by Lemma 4.9. The comparison principle yields $K_t \subset G_t^*$ so that Proposition 4.12 yields the desired result. □

PROPOSITION 4.14 (Lower bound for non-admissible facets) Assume the same hypothesis of Proposition 4.13. Then

$$h_j(t) \geqslant m\sigma t + h_j(0) \quad \text{for} \quad \mathbf{m}_j \in \mathcal{M}\backslash\mathcal{N}, \quad t \in [0, T]$$

with $m = \inf_{S^1} M$ provided that a non-admissible facet of orientation $\mathbf{m}_j$ exists in $[0, T]$.

Proof. For non-admissible facet we know

$$\dot{h}_j(t) = M(\mathbf{m}_j)\sigma \geqslant m\sigma$$

which yields the desired result. □

Proof of Theorem 3.2. We first prove (a) for a generalized crystalline flow. We take δ' as in Lemma 4.10. For a given $T > 0$ we take $\delta > 0$ sufficiently small, say $\delta < \delta_0$ so that

$$\lambda^\delta(t) \leqslant \frac{(1+\delta')}{\sigma} b \quad \text{in} \quad [0, T]$$

with $\lambda^\delta(t) = z(t)b$, where z be a solution of (4.11) with $z(0) = (1+\delta)/\sigma$. (This is possible since λ^δ converges to a constant b/σ uniformly on $[0, T]$ as $\delta \to 0$.) If $K_0 \subset C_\delta$, then the solution K_t is contained in K_t^* by Proposition 4.13. Thus $K_t \subset C_{\delta'}$ for $t \in [0, T]$. By Lemma 4.10 K_t has the property G for all $t \in [0, T]$ which means that no new facets are created so we may assume that K_t is expressed as (4.4) as in Proposition 4.13 on the time interval $[0, T]$.

We take T large, say $m\sigma T > \bar{c}(1+\delta')b/\sigma$, where $\bar{c} = 1/\cos(\varphi/2)$, $\varphi = 2\pi/k$. Evidently, λ^δ is a convex, monotone increasing function and converges to a constant b/σ uniformly on $[0, T]$ as $\delta \to 0$. By this behavior of λ^δ there is always an interval $\left[t_1^\delta, t_2^\delta\right) \subset (0, \infty)$ such that

$$\bar{c}\lambda^\delta(t) \leqslant m\sigma t + b/\sigma \quad \text{on} \quad \left[t_1^\delta, t_2^\delta\right) \quad \text{with} \quad t_1^\delta < T \tag{4.12}$$

with sufficiently small δ, say $\delta < \delta_1$ $(< \delta_0)$. (By the choice of δ_0 and T the inequality $t_1^\delta < T$ is guaranteed.)

We shall prove that a non-admissible facet with orientation $\mathbf{m}_j$ must disappear before $t = t_1^\delta$ if $\delta < \delta_1$. Assume that $\mathbf{m}_j$-facet exists up to $t \leqslant T$. There is $\mathbf{n}_i$, $\mathbf{n}_{i+1} \in \mathcal{N}$ such that $\mathbf{m}_j$ is between $\mathbf{n}_i$ and $\mathbf{n}_{i+1}$ on S^1. By Lemma 4.1

$$h_j(t) < \frac{1}{\sin\varphi}\left(h_i(t)\sin\varphi_1 + h_{i+1}(t)\sin\varphi_2\right)$$

where $\varphi = 2\pi/k$, $\varphi_1 + \varphi_2 = \varphi$, $\varphi_1 > 0$, $\varphi_2 > 0$. By Proposition 4.13 we have $h_i(t) \leqslant \lambda^\delta(t)$ so that

$$h_j(t) < \bar{c}\lambda^\delta(t);$$

here $\bar{c} = \sup\{(\sin\varphi_1 + \sin\varphi_2)/\sin\varphi \mid \varphi_1 + \varphi_2 = \varphi,\ \varphi_1 > 0,\ \varphi_2 > 0\} = 1/\cos(\varphi/2)$. By geometry we have

$$h_j(0) \geqslant b/\sigma.$$

Proposition 4.14 now implies

$$h_j(t) \geqslant m\sigma t + b/\sigma$$

to get

$$\bar{c}\lambda^\delta(t) > m\sigma t + b/\sigma$$

which evidently contradicts (4.12). Thus all non-admissible facets disappear at some $t \leqslant t_1^\delta$ and is not created until time T.

Since we know that crystalline flow approximates a general level-set flow by Lemma 4.11, we get the same conclusion as above for general convex initial data by noting that all constants are independent of approximations. One should note that the constant appearing in the monotonicity of M can be taken uniformly in the approximation of M. This implies that t_1^δ is taken independent of approximations. Thus the proof of (a) is now complete.

If we have symmetry, the symmetry is preserved by uniqueness of solution. This implies (b) since $\mathbf{Z}_k$-symmetric admissible polygon must be a regular k-polygon. In the case (c) since k-regular polygon always satisfies G, there occurs no facet creation of non-admissible facets thus the solution stays as a k-regular polygon. □

REMARK 4.15 In this section we consider a crystalline flow to (1.1) for admissible evolving convex crystals. Such a problem is studied when $\sigma = 0$ in [59], where it is shown that all non-admissible facets disappear before the flow shrinks to a point. In the case $\sigma = 0$, there is no need to insert non-admissible facets during evolutions so the problem is substantially different.

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