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

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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 $\mathbf{R}^n$ $(n \geq 2)$ 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 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 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 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

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

where $\gamma(p) = |p|\gamma_0\left(p/|p|\right)$ is the 1-homogeneous extension of γ_0 to $\mathbf{R}^n$ and div_Γ 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 $\kappa_\gamma = -\mathrm{div}_\Gamma \vec{n}$ 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 [K], [H], [KK]. It seems that there is no reasonable way to calculate mobility M. The anisotropy in 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 notion the Frank diagram [Gu]

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

If Frankγ is convex, then (1.1) is at least degenerate parabolic under suitable regularity of γ, say C^2. If Frankγ 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 Frankγ 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 Frankγ called a Wulff shape of γ of the form

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

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 Frankγ 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 [GG98], [GG01].

However, for $n \geq 3$ or non-constant σ even well-posedness is not well-established. The main reason for $n \geq 3$ is that κ_γ may not be constant on a facet [BNP] (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 [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 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 [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], [GGoR11]. 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 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 [GG98] and recently studied for a case when Frankγ 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 Frankγ 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. $\kappa_\gamma + \sigma = 0$) 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 [T], [AG]. The approximation is justified by [GG01]. Note that even solvability is nontrivial for (1.1) for general (convex) initial data Γ_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 κ_γ has no nonlocal nature, there is no facet provided that M is Lipschitz (continuous) and Frankγ 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 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 [BGN1], [BGN2], [BGN3] invented a nice numerical scheme to calculate for singular γ 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 σ is coupled so that σ is not a constant [GR05].

In [Y] evolution of snowflakes is calculated by (1.7)–(1.9); see also [YK]. However, the term κ_γ

is omitted. According to [BGN3], if there is no κ_γ, no hexagonal pattern is produced. It seems that the numerical treatment in [Y] and [YK] 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 [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 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. [GR05]. 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 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 [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 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 [GG01] for (1.1) with $n = 2$ when Frankγ 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

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

which is formally equivalent to (1.1) on $\Gamma_t = \{\, x \in \mathbf{R}^2 |\ u(x,t) = 0\}$. We consider (2.1) not only on Γ_t but also for all $\mathbf{R}^2$. As in [G06] 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 $u \in C\,(\mathbf{R}^2 \times [0,\infty))$ of (2.1) such that $D = \{(x,t) |\ u(x,t) > 0\}$ 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 $\geq$. The set $\Gamma = E \backslash D$ is regarded as 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 [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

t, i.e. $D(t) = \left\{ x \in \mathbf{R}^2 \;\middle|\; (x,t) \in D \right\}$ is bounded. 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 [ES], [G06]. 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

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

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 $S^1 = \left\{ p \in \mathbf{R}^2 \;\middle|\; |p| = 1 \right\}$ 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 [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 $\gamma_\varepsilon \in \mathcal{I}$ 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 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 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 $t \geq 0$. 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

$$\lim_{\varepsilon \to 0} \sup_{0 \leq t \leq T} d_H\left(E^\varepsilon(t), E(t)\right) = 0.$$

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 γ by singular γ_ε 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, 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 $t \geq 0$.

(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 γ 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 γ [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 $u \in C(\mathbf{R}^2 \times [0, \infty))$ 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:

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

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 γ 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 Frankγ 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 $\mathcal{N}$ be the singular set of γ i.e. $\gamma \in C^2(S^1 \backslash \mathcal{N})$ 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 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 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 σ 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 $E_0 \subset$ 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 contains in C but close to C. It turns out that if we assume that Frankγ 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 extra difficulty we state a typical result.

Theorem 3.1 (Fully faceted)**.** Assume that Frankγ 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.

(a) If E_0 is sufficiently close to E_0, there $E(t)$ becomes fully faceted with respect to γ in finite time.

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

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

Remark 3.2. (i) Unless M is proportional to γ, the large time asymptotics may be different from W_γ 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 γ but it can be easily extended to the singular case as noted in [KG].

(ii) There are several numerical simulations for E by changing anisotropy of γ and M in [KG]. 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_γ with $\tilde{\gamma}\kappa_{\tilde{\gamma}} = M\kappa_{\tilde{\gamma}}$ 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 Frankγ 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_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 are preserved 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. 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 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 [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 Frankγ 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

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

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

$$\frac{(1-\lambda)\mathbf{n} + \lambda\hat{\mathbf{n}}}{|(1-\lambda)\mathbf{n} + \lambda\hat{\mathbf{n}}|} \notin \mathcal{N} \tag{4.1}$$

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

$$S_t = \bigcup_{j=1} S_j(t),$$

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

$$V_j = M(\mathbf{n}_j)\left(\frac{\chi_j \Delta(\mathbf{n}_j)}{L_j(t)} + \sigma\right) \quad \text{on} \quad S_j(t),\ t \in J \tag{4.2}$$

for $j = 1, 2, \ldots, r$, where V_j denotes the normal velocity of $S_j(t)$ in the direction of $\mathbf{n}_j$. The quantity $\chi_j \Delta(\mathbf{n}_j)/L_j(t)$ is a nonlocal weighted curvature $\kappa_\gamma(\mathbf{n}_j)$ for $\mathbf{n}_j \in \mathcal{N}$, where $L_j(t)$ denotes the length of $S_j(t)$. The quantity $\Delta(\mathbf{m}_i)$ is defined by

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

where $\mathbf{m}_i = (\cos\theta_i, \sin\theta_i)$ 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 $\Delta(\mathbf{m}_i)$ has a geometric meaning. It is the length of facet of the Wulff shape W_γ with outward normal $\mathbf{m}_i$. 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

$$\dot{L}_j(t) = \frac{\mathrm{d}L_j(t)}{\mathrm{dt}} = (\cot\psi_j + \cot\psi_{j+1})V_j - \frac{1}{\sin\psi_j}V_{j-1} - \frac{1}{\sin\psi_{j+1}}V_{j+1} \tag{4.3}$$

for $j = 1, \ldots, r$; index j is considered modulo r. Here $\psi_j = \theta_j - \theta_{j-1}$ (modulo 2π) with $\mathbf{n}_j = (\cos\theta_j \sin\theta_j)$. Thus the equation (4.2) forms a system of ordinary differentiation 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 $\mathbf{n}_j \notin \mathcal{N}$ may disappear for γ-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

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

with $H_{i+j} = \left\{ x \in \mathbf{R}^2 \,\middle|\, x \cdot \mathbf{m}_{i+j} \le \sigma M\left(\mathbf{m}_{i+j}\right) \right\}$ stays a corners for $V = M(\vec{n})\sigma$ if and only if

$$A_i \subset \left\{ x \in \mathbf{R}^2 \,\middle|\, x \cdot \mathbf{m} \le \sigma M(\mathbf{m}) \right\} \subset B_i \tag{4.4}$$

for all $\mathbf{m} = (\cos\theta, \sin\theta)$ such that $\theta_{i+1} \le \theta \le \theta_i$, where $\mathbf{m}_{i+j} = (\cos\theta_{i+j}, \sin\theta_{i+j})$. 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 γ, M, σ. Assume that E_0 is a convex closed polygon 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 crystalline flow in $J = [0, T_*)$ with initial data S_0 provided that the corner preserving property (4.4) with $i = j$ holds for M with $\mathbf{m}_j = \mathbf{n}_j$ for all $j = 1, \ldots, r$.

The corner preserving condition (4.4) uniquely interpolates the values of $M(\mathbf{m})$ from the value of M at $\mathbf{n}_j (j = 1, \ldots, r)$. 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 $M(\mathbf{n}_j)\mathbf{n}_j$ and consider its polar set F i.e.,

$$F = \left\{ p \in \mathbf{R}^2 \,\middle|\, \sup_{x \in W} p \cdot x \le 1 \right\}.$$

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

$$\tilde{M}(p) = \sup \left\{ \lambda \,\middle|\, p \in \lambda F \right\}.$$

Notice that if the set $\{\mathbf{n}_j\}_{j=1}^{r(\varepsilon)}$ 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 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 $\{\Gamma_t\}_{t \ge 0}$ 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

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

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

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

(We call $h(\mathbf{m})$ the support function of E_0 in the direction of $\mathbf{m}$). We approximate E_0 by E_0^ε by

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

where $\mathcal{M}_\varepsilon = \left\{(\cos\theta_i, \sin\theta_i) \;\middle|\; \theta_{i+1} \le \theta_i \text{ with } |\theta_{i+1} - \theta_i| \le \varepsilon,\ i = 1, 2, \dots N(\varepsilon) \right\}$. 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.

Proof of Theorem 2.4. We use crystalline approximation given in Lemma 4.2. Since $E^\varepsilon(t)$ and $E(t)$ are convex sets we may represent these sets by a support function for example

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

with a support function $d_j^\varepsilon(t)$. 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

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

We shall prove that the length of a facet with the orientation $\mathbf{n}_l \in \mathcal{N}$ of Γ_t is positive in a dense subset of $(0, T)$. Let $L_l(t)$ be the length of the facet with normal $\mathbf{n}_l$ allowing that $L_l(t) = 0$, i.e. the facet is degenerated to a point. We do not assume that $L_l(0) > 0$. By the convergence of convex set and Lemma 4.2 we conclude that $L_l^\varepsilon(t) \to L_l(t)$ and $d_l^\varepsilon(t) \to d_l(t)$ uniformly on $[0, T]$, where $d_l(t)$ is the support function corresponding to the facet of Γ_t with normal $\mathbf{n}_l \in \mathcal{N}$. Assume that $L_l(t) = 0$ for $[t_0, t_1] \subset (0, T)$. Since $\dot{d}_l^\varepsilon(t)$ is the normal velocity $V_l = V_l^\varepsilon$, integrating (4.2) over $[t_0, t_1]$ yields

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

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 $L_l(t) > 0$ 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 Γ_t with orientation in $\mathcal{N}$ 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 Frankγ 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 γ-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 γ. 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

$$V = a\,(\kappa_\gamma + \sigma) \quad \text{with} \quad a = \sup_{S^1} M \tag{4.5}$$

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 Frankγ is a regular polygon centered at the origin [Gu, 12G]. The function $z(t)$ solves

$$\dot{z}(t) = ab^{-1}\,(-1/z(t) + \sigma) \tag{4.6}$$

where $b = \gamma(\mathbf{n}_i)$ for $\mathbf{n}_i \in \mathcal{N}$ which is independent of $i = 1, \ldots, m$ because Frankγ 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 $\mathbf{n}_j$. Let $\{\lambda_i(t)\}_{i=1}^m$ be the support function of $z(t)W_\gamma$ in the direction of $\mathbf{n}_i$. Since Frankγ 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 λ is of the form

$$\dot{\lambda}(t) = a\,(-b/\lambda(t) + \sigma)\,. \tag{4.7}$$

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

$$d_i(t) \leq \lambda(t) \tag{4.8}$$

for i such that $\mathbf{n}_i \in \mathcal{N}$. 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. $\mathbf{n}_j \notin \mathcal{N}$ may disappear in finite time. However, it is rather clear by (4.2)

$$\dot{d}_j(t) = M(\mathbf{n}_j)\sigma \geq m\sigma,\ m = \inf_{S^1} M$$

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

$$d_j(t) \geq m\sigma t + d_j(0). \tag{4.9}$$

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

$$H_l = \left\{\ x \in \mathbf{R}^2 \ \middle|\ x \cdot \mathbf{n}_l \leq 1\ \right\}$$

with $\mathbf{n}_l = (\cos\theta_l, \sin\theta_l)$, $\theta_1 > \theta_2 > \theta_1 - \pi$. The half space

$$K_\theta = \left\{\ x \in \mathbf{R}^2 \ \middle|\ x \cdot \mathbf{n}_\theta \leq d_\theta\ \right\},\ \mathbf{n}_\theta = (\cos\theta, \sin\theta)$$

contains $H_1 \cap H_2$ if and only if $d_\theta \geq c_\theta$ with

$$c_\theta = \cos\left(\theta - (\theta_1 + \theta_2)/2\right) \Big/ \cos\left((\theta_1 - \theta_2)/2\right)$$

Moreover, $\inf\left\{c_\theta \ \middle|\ \theta_1 \leq \theta \leq \theta_2\right\} =: \bar{c} > 0$.

Note that $d_\theta < c_\theta$ is equivalent to saying that $H_1 \cap H_2 \cap K_\theta$ has a facet with orientation $\mathbf{n}_\theta$. By this observation one concludes that if $\mathbf{n}_j = (\cos\theta, \sin\theta)$ is between two admissible (singular) direction say $\mathbf{n}_1, \mathbf{n}_2 \in \mathcal{N}$ then any non-admissible facet corresponding to $\mathbf{n}_j$ disappears when

$$d_j(t) > \bar{c}\lambda(t) \tag{4.10}$$

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 $\mathbf{n}_i \in \mathcal{N}$. By geometry for non-admissible facets we have

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

with $\mathbf{n}_j = (\cos\theta, \sin\theta)$. 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 $\left(t_1^\delta, t_2^\delta\right) \subset [0, \infty)$; t_2^δ can be $+\infty$. If $d_i(0)$ $(> b/\sigma)$ is taken close to b/σ, say $d_i(0) < \lambda_0$, then by the criterion (4.8) we have (4.10) which implies that $\mathbf{n}_j$-facet disappears in the time interval $\left(t_1^\delta, t_2^\delta\right)$. 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^ε approximating E_0 for small ε, say $0 < \varepsilon < \varepsilon_0$, then $d_i^\varepsilon(t) \leq \lambda(t)$. By the above observation for a crystalline flow we conclude that

$$d_j^\varepsilon(t) > \bar{c}\lambda(t) \quad \text{in} \quad \left(t_1^\delta, t_2^\delta\right),$$

where the interval is independent of ε. This implies that in time interval $\left(t_1^\delta, t_2^\delta\right)$, $E^\varepsilon(t)$ is a fully faceted convex polygon with admissible facets with orientations $\mathbf{n}_1, \ldots, \mathbf{n}_m$. Moreover, since $V_j \geq 0$, the length of each facet with orientation $\mathbf{n}_i \in \mathcal{N}$ $(i = 1, \ldots, m)$ is bounded away from zero independent of $\varepsilon \in (0, \varepsilon_0)$. By Lemma 2.2. (iii) we have $d_H\left(E^\varepsilon(t), E(t)\right) \to 0$ as $\varepsilon \to 0$. We thus observe that $E(t)$ is a fully faceted convex polygon with admissible facets $\mathbf{m}_i \in \mathcal{N}$ for $t \in \left(t_1^\delta, t_2^\delta\right)$.

(ii) If E_0 and M have the same symmetry as W_γ, then $E(t)$ has the same symmetry as W_γ. In $\left(t_1^\delta, t_2^\delta\right)$, $E(t)$ is fully faceted with all orientations in $\mathcal{N}$ so if it has the same symmetry as W_γ, then it must be similar (homothetic) to W_γ.

(iii) If M is proportional to W_γ, the equation becomes

$$V = \text{const}\gamma\left(\kappa_\gamma + \sigma\right)$$

and there is a self-similar solution for this equation (cf. [G06], [GGu], [Gu]). So once $E(t)$ becomes homothetic to W_γ in $\left(t_1^\delta, t_2^\delta\right)$, then it stays homothetic to W_γ for all time. Note that without proportionality of M against γ, there might happen the corner may rounded after t_2^δ.

□

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