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Interface motion of a negative crystal and its analysis

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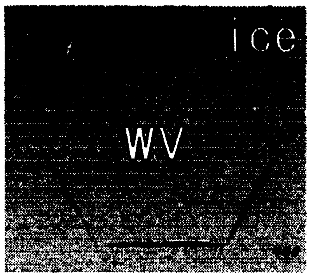
1 Introduction

When a block of ice crystal is illuminated by strong beams, the ice crystal starts to melt inside of the crystal as well as the surface and each water region forms a snowflake-like-pattern which has six petals, called "Tyndall figure" (see Figure 1 (a)). This figure has a vapor bubble in water region and when this figure is refrozen, the vapor bubble remains in the ice as a hexagonal disk (see Figure 1 (b)). This hexagonal disk is a kind of negative crystals and the interior region is filled with water vapor saturated at that temperature. McConnel([7]) found these disks in the ice of Davos lake. Nakaya called this hexagonal disk "Kuuzou(空像)" in Japanese and investigated its properties [8].



(a) (b)

Figure 1: (a) Tyndall figures (seen from 45° to the c-axis) and (b) a negative crystal (by U. Nakaya).

In [6], we proposed a simple two dimensional model to understand the process of formation of negative crystals after the water region in a Tyndall figure is completely refrozen. This model equation is obtained by a gradient flow of total surface energy under an area-preserving constraint:

$$V_i = \overline{H} - H_i.$$

Here V_i is the outward normal velocity on the i-th facet S_i of vapor region $\Omega(t)$ (enclosed region by a polygon), H_i is the crystalline curvature of S_i and $\overline{H}$ is the average of

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all crystalline curvatures. This equation is called area-preserving crystalline curvature flow. Crystalline curvature flow is a singular weighted curvature flow with non-smooth surface energy γ and J. Taylor[9] and Angenent and Gurtin [1] proposed the framework of crystalline motions. In this framework, the interfaces are restricted in the class of polygonal curves (two dimensional case) which satisfy an admissibility condition based on the equilibrium shape of the crystal. This equilibrium shape is called the *Wulff shape* and plays important roles for not only the definition of the crystalline curvature and admissibility condition, but also the asymptotic behavior of the solution polygons. The detailed formulations will be mentioned in next section.

When an initial shape $\Omega(0)$ is convex, the solution polygon $\Omega(t)$ keeps its convexity. S. Yazaki ([10],[11, Part I]) show that no edges disappear globally in time and the solution polygon converges to the rescaled Wulff shape whose area is equal to that of $\Omega(0)$ in the Hausdorff metric. In this note, we consider non-convex case. In this case, there appear some singularities: edge-disappearing and self-touching of the boundary. Thus, the admissibility of solution polygons may break down in finite time. We show the sufficient conditions on the Wulff shape and an initial polygon to keep admissibility of the solution polygons. We also show that under this sufficient conditions non-convex solution polygons eventually become convex.

2 Area-preserving crystalline curvature flow

Crystalline energy and the Wulff shape. Let $\gamma = \gamma(\boldsymbol{n})$ be a positive continuous function defined on S^1 and describe interfacial energy density for the direction $\boldsymbol{n}$. In this note, we consider the case where the Wulff shape of γ, $\mathcal{W}_\gamma = \{x \in \mathbb{R}^2 | x \cdot \boldsymbol{n} \leq \gamma(\boldsymbol{n}) \text{ for all } \boldsymbol{n} \in S^1\}$, is a convex polygon. Such γ is called *crystalline energy.* If $\mathcal{W}_\gamma$ is a J-sided convex polygon ($J \geq 3$), then $\mathcal{W}_\gamma$ is expressed as

$$\mathcal{W}_\gamma = \bigcap_{i=1}^{J} \{\boldsymbol{x} \in \mathbb{R}^2;\ \boldsymbol{x} \cdot \boldsymbol{\nu}_i \leq \gamma(\boldsymbol{\nu}_i)\},$$

where $\boldsymbol{\nu}_i = \boldsymbol{n}(\phi_i)$ and ϕ_i is the exterior normal angle of the i-th edge with $\phi_i \in (\phi_{i-1}, \phi_{i-1} + \pi)$ for all i ($\phi_0 = \phi_J$, $\phi_{J+1} = \phi_1$). We define a set of normal vectors of $\mathcal{W}_\gamma$ by $\mathcal{N}_\gamma = \{\boldsymbol{\nu}_1, \boldsymbol{\nu}_2, \dots, \boldsymbol{\nu}_J\}$.

Polygons and polygonal curves. Let Ω be N-sided polygon in the plane $\mathbb{R}^2$, $\mathcal{P}$ its boundary, that is, $\mathcal{P} = \partial\Omega$ and label the position vector of vertices $\boldsymbol{p}_i$ ($i = 1, 2, \dots, N$) in an anticlockwise order: $\mathcal{P} = \bigcup_{i=1}^{N} \mathcal{S}_i$, where $\mathcal{S}_i = \{(1-t)\boldsymbol{p}_i + t\boldsymbol{p}_{i+1};\ t \in [0,1]\}$ is the i-th edge ($\boldsymbol{p}_0 = \boldsymbol{p}_N$, $\boldsymbol{p}_{N+1} = \boldsymbol{p}_1$). The length of $\mathcal{S}_i$ is $d_i = |\boldsymbol{p}_{i+1} - \boldsymbol{p}_i|$, and then the i-th unit tangent vector is $\boldsymbol{t}_i = (\boldsymbol{p}_{i+1} - \boldsymbol{p}_i)/d_i$ and the i-th unit outward normal vector is $\boldsymbol{n}_i = -\boldsymbol{t}_i^\perp$, where $(a,b)^\perp = (-b, a)$. We define a set of normal vectors of $\mathcal{P}$ by $\mathcal{N} = \{\boldsymbol{n}_1, \boldsymbol{n}_2, \dots, \boldsymbol{n}_N\}$. Let θ_i be the exterior normal angle of $\mathcal{S}_i$. Then $\boldsymbol{n}_i = \boldsymbol{n}(\theta_i)$ and $\boldsymbol{t}_i = \boldsymbol{t}(\theta_i)$ hold ($\theta_0 = \theta_N$, $\theta_{N+1} = \theta_1$), where $\boldsymbol{t}(\theta) = (-\sin\theta, \cos\theta)$.

We define the i-th hight function $h_i = \boldsymbol{p}_i \cdot \boldsymbol{n}_i = \boldsymbol{p}_{i+1} \cdot \boldsymbol{n}_i$ ($h_0 = h_N$, $h_{N+1} = h_1$). By using $\{h_{i-1}, h_i, h_{i+1}\}$ and $\{\boldsymbol{n}_{i-1}, \boldsymbol{n}_i, \boldsymbol{n}_{i+1}\}$, the length of i-th edge d_i is described as follows:

$$d_i = \frac{\chi_{i-1,i}(h_{i-1} - (\boldsymbol{n}_{i-1} \cdot \boldsymbol{n}_i)h_i)}{\sqrt{1 - (\boldsymbol{n}_{i-1} \cdot \boldsymbol{n}_i)^2}} + \frac{\chi_{i,i+1}(h_{i+1} - (\boldsymbol{n}_i \cdot \boldsymbol{n}_{i+1})h_i)}{\sqrt{1 - (\boldsymbol{n}_i \cdot \boldsymbol{n}_{i+1})^2}}, \quad i = 1, 2, \ldots, N,$$

where $\chi_{i,j} = \operatorname{sgn}(\boldsymbol{n}_i \wedge \boldsymbol{n}_j)$ and $\boldsymbol{a}_1 \wedge \boldsymbol{a}_2 = \det(\boldsymbol{a}_1, \boldsymbol{a}_2)$ is the determinant of the 2×2 matrix with column vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$. Since $\boldsymbol{n}_i \cdot \boldsymbol{n}_j = \cos(\theta_i - \theta_j)$, we have another expression:

$$d_i = -(\cot \vartheta_i + \cot \vartheta_{i+1})h_i + h_{i-1} \operatorname{cosec} \vartheta_i + h_{i+1} \operatorname{cosec} \vartheta_{i+1}, \quad i = 1, 2, \ldots, N, \tag{1}$$

where $\vartheta_i = \theta_i - \theta_{i-1}$. Note that $0 < |\vartheta_i| < \pi$ holds for all i. Furthermore, the i-th vertex $\boldsymbol{p}_i$ ($i = 1, 2, \ldots, N$) is described as follows:

$$\boldsymbol{p}_i = h_i \boldsymbol{n}_i + \frac{h_{i-1} - (\boldsymbol{n}_{i-1} \cdot \boldsymbol{n}_i)h_i}{\boldsymbol{n}_{i-1} \cdot \boldsymbol{t}_i} \boldsymbol{t}_i. \quad i = 1, 2, \ldots, N. \tag{2}$$

Admissibility and crystalline curvature. We call Ω and $\mathcal{P}$ N-*admissible* (associated with $\mathcal{W}_\gamma$) if and only if $\mathcal{N} = \mathcal{N}_\gamma$ holds and any adjacent two normal vectors in the set $\mathcal{N}$ are also adjacent in the set $\mathcal{N}_\gamma$, i.e., for any i, there exists j such that $\{\boldsymbol{\nu}_j, \boldsymbol{\nu}_{j+1}\} = \{\boldsymbol{n}_i, \boldsymbol{n}_{i+1}\}$ holds.

Let $\mathcal{P}$ be an N-admissible polygonal curve. For each edge $\mathcal{S}_i$ a *crystalline curvature* is defined by

$$H(\mathcal{S}_i) = \chi_i \frac{l_\gamma(\boldsymbol{n}_i)}{d_i}, \quad i = 1, 2, \ldots, N,$$

where $\chi_i = (\chi_{i-1,i} + \chi_{i,i+1})/2$ is the transition number and it takes $+1$ (resp. -1) if $\mathcal{P}$ is convex (resp. concave) around $\mathcal{S}_i$ in the direction of $-\boldsymbol{n}_i$, otherwise $\chi_i = 0$; and $l_\gamma(\boldsymbol{n}_i)$ is the length of the j-th edge of $\mathcal{W}_\gamma$ if $\boldsymbol{n}_i = \boldsymbol{\nu}_j$. If Ω is an N-admissible convex polygon, then $\boldsymbol{n}_i = \boldsymbol{\nu}_i$ and $\chi_i = 1$ for all $i = 1, 2, \ldots, N = J$; and moreover, if $\Omega = \mathcal{W}_\gamma$, then the crystalline curvature is 1. In this note, we call a edge which zero transition number "inflection edge."

We note that the total interfacial crystalline energy on $\mathcal{P}$ is

$$\mathcal{E}_\gamma = \sum_{i=1}^{N} \gamma(\boldsymbol{n}_i) d_i, \tag{3}$$

and the crystalline curvature $H(\mathcal{S}_i)$ is characterized as the first variation of $\mathcal{E}_\gamma$ on $\mathcal{P}$ at $\mathcal{S}_i$ with a suitable norm. Here and hereafter, we denote $H(\mathcal{S}_i)$ by H_i for short.

Area-preserving crystalline curvature flow. The normal velocity on $\mathcal{S}_i$ in the direction $\boldsymbol{n}_i$ is $V_i = \dot{h}_i$. Here and hereafter, we denote that the derivative of a function $u = u(t)$ with respect to time t by $\dot{u}$. The area-preserving crystalline curvature flow is the gradient flow of $\mathcal{E}_\gamma$ along $\mathcal{P}$ which encloses a fixed area, and it is described as follows:

$$V_i = \overline{H} - H_i, \quad i = 1, 2, \ldots, N, \tag{4}$$

where

$$\overline{H} = \frac{\sum_{i=1}^{N} H_i d_i}{\mathcal{L}}$$

is the average of the crystalline curvature, and $\mathcal{L} = \sum_{k=1}^{N} d_k$ is the total length of the curve $\mathcal{P}$. From (1), we have

$$\dot{d}_i = -(\cot\vartheta_i + \cot\vartheta_{i+1})V_i + V_{i-1}\operatorname{cosec}\vartheta_i + V_{i+1}\operatorname{cosec}\vartheta_{i+1}, \quad i = 1, 2, \ldots, N. \tag{5}$$

Furthermore, by (2) we have

$$\dot{\boldsymbol{p}}_i = V_i \boldsymbol{n}_i + \frac{V_{i-1} - (\boldsymbol{n}_{i-1} \cdot \boldsymbol{n}_i)V_i}{\boldsymbol{n}_{i-1} \cdot \boldsymbol{t}_i}\boldsymbol{t}_i, \quad i = 1, 2, \ldots, N. \tag{6}$$

Note that (4), (5) and (6) are equivalent each other. It is easy to check that the enclosed area $\mathcal{A}(t) = \sum_{i=1}^{N} h_i d_i/2$ is preserving in time: $\dot{\mathcal{A}}(t) = \sum_{i=1}^{N} V_i d_i = 0$.

3 Problem

Applying the area-preserving crystalline curvature flow to understand the motion of the boundary of negative crystals, we will introduce the concept of negative polygons. For usual crystal case, enclosed region describes the crystal and then normal vector $\boldsymbol{n}$ is direction from the crystal to its outside region. However, for negative crystal case, the outside region describes the crystal. Thus, we need to consider $\gamma(-\boldsymbol{n})$ as the interfacial energy density. Therefore, from now on, we use the figure:

$$\bigcap_{i=1}^{J} \left\{ \boldsymbol{x} \in \mathbb{R}^2;\ \boldsymbol{x} \cdot (-\boldsymbol{\nu}_i) \leq \gamma(\boldsymbol{\nu}_i) \right\},$$

as the Wulff shape.

Our problem is stated as follows:

Problem. For a given admissible polygon Ω_0, find a family of admissible polygons $\{\Omega(t)\}_{0 \leq t < T}$ satisfying (4) with $\Omega(0) = \Omega_0$. Since (5) are the system of ordinary differential equations, the maximal existence time is positive: $T > 0$.

4 Results

Known results for convex polygons. What might happen to $\Omega(t)$ as t tends to $T \leq \infty$? For this question, we have the following two results. The first result is the case where motion is isotropic.

Theorem 1 Let the interfacial energy be isotropic $\gamma \equiv 1$. Assume the initial polygon Ω_0 is an N-sided admissible convex polygon. Then the solution admissible polygon $\Omega(t)$ exists globally in time keeping the area enclosed by the polygon constant $\mathcal{A}$, and $\Omega(t)$ converges to the shape of the boundary of the Wulff shape $\partial\mathcal{W}_{\gamma_*}$ in the Hausdorff metric as t tends to infinity, where $\gamma_*(\boldsymbol{n}_i) \equiv \sqrt{2\mathcal{A}/\sum_{k=1}^{N} l_1(\boldsymbol{n}_k)}$ is constant. In particular, if Ω_0 is centrally symmetric with respect to the origin, then we have an exponential rate of convergence.

This theorem is proved by Yazaki [10] by using the isoperimetric inequality and the theory of dynamical systems. We note that $\partial\mathcal{W}_{\gamma_*}$ is the circumscribed polygon of a circle with radius γ_*, and then this result is a semidiscrete version of Gage [3].

The second result is the case where motion is anisotropic and polygon is admissible.

Theorem 2 Let the crystalline energy be $\gamma > 0$. Assume the initial polygon Ω_0 is an N-sided admissible convex polygon. Then the solution admissible polygon $\Omega(t)$ exists globally in time keeping the area enclosed by the polygon constant $\mathcal{A}$, and $\Omega(t)$ converges to the shape of the boundary of the Wulff shape $\partial\mathcal{W}_{\gamma_*}$ in the Hausdorff metric as t tends to infinity, where $\gamma_*(\boldsymbol{n}_i) = \gamma(\boldsymbol{n}_i)/W$, $W = \sqrt{|\mathcal{W}_\gamma|/\mathcal{A}}$ for all $i = 1, 2, \ldots, N$ and $|\mathcal{W}_\gamma| = \sum_{k=1}^{N} \gamma(\boldsymbol{n}_k) l_\gamma(\boldsymbol{n}_k)/2$ is enclosed area of $\mathcal{W}_\gamma$.

This theorem is proved in Yazaki [11, Part I] by using the anisoperimetric inequality or Brünn and Minkowski's inequality and the theory of dynamical systems which is the similar technique as in Yazaki [10].

Our results for non-convex polygons.

In the previous case, the solution polygon keeps its convexity and admissibility, that is, the length of each edge is positive globally in time and the self-touching of $\mathcal{P}(t)$ never occur. However, if Ω_0 is non-convex, edge-disappearing singularity and the self-touching singularity may occur in finite time. Indeed, we can easily construct the example of the self-touching of $\mathcal{P}(t)$ and $\Omega(t)$ becomes non-admissible after the singularity. Thus, the admissibility of solution polygons may break down in finite time. To track the motion globally in time in the class of admissible polygons, we prepare the following three assumptions:

(A0) $\mathcal{W}_\gamma$ is symmetric with respect to the origin.

(A1) Ω_0 is an N-admissible non-convex polygon in the plane $\mathbb{R}^2$.

(A2) transition numbers of Ω_0 are all nonnegative: $\chi_i \geq 0$ ($\forall i$).

From (A0), the number of edges of $\mathcal{W}_\gamma$ is even, and $\gamma(\boldsymbol{n}(\phi_i + \pi)) = \gamma(\boldsymbol{n}(\phi_i))$ holds for all i. Under the assumption (A1) and (A2), crystalline curvatures of Ω_0 are also all nonnegative and there exists at least one edge which crystalline curvature is zero. These polygons are said to be "almost convex".

Theorem 3 Assume the assumptions (A0), (A1) and (A2). Then, there exists $T_1 > 0$ such that the solution polygon is an N-sided admissible polygon for $0 \le t < T_1$ and there exists at least one inflection edge whose length tends to zero as $t \to T_1$. Moreover, $\Omega(t)$ converges to an admissible polygon Ω^* in the Hausdroff topology as $t \to T_1$ and area of Ω^* is equal to area of $\Omega(0)$.

In fact, two consecutive inflection edges disappear at $t = T_1$ locally on $\mathcal{P}$ since number of consecutive inflection edges is even for almost convex polygons.

This theorem means that we can restart the motion with the initial polygon Ω^* and obtain the solution in the class of admissible polygons beyond the singularity.

Again by Theorem 3, the number of edges is monotone non-increasing in time and we have a finite sequence of edge-disappearing time : $0 < T_1 < T_2 < \cdots < T_m < +\infty$.

Then, we obtain the following convexity result.

Theorem 4 Assume that the same assumption as in Theorem 3. Then, the solution polygon becomes convex at $t = T_m$.

After the convexity phenomena occurs, we can apply Theorem 1 and 2. Therefore, the solution polygon exists globally in time in the class of admissible polygons and the solution polygon finally converges to the rescaled Wulff shape.

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