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Existence of self-similar evolution of crystals grown from supersaturated vapor

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Abstract

We study a cylindrical crystalline flow in three dimensions coupled to a diffusion field. This system arises in modeling crystals grown from supersaturated vapor. We show existence of self-similar solutions to the system under a special choice of interfacial energy and kinetic coefficients.

1 Introduction

In [GR1] we considered a model of crystals grown from supersaturated vapor. We established there existence of solutions to the evolution equations. Here we want to construct a special kind of maximal solutions, namely a self-similar motion.

Our work was motivated by experiments. Namely, Gonda and Gomi [GoG] have grown in their laboratory specimens of elongated prisms of ice crystals similar to that formed in the atmosphere and found mostly in Antarctica. Theoretical foundation for our work has been laid down by Seeger, [Se], who studied planar polygonal crystals. Later his approach was extended to three dimensions by Kuroda *et al.* [KIO]. These papers, however, do not include Gibbs-Thomson relation on the free boundary. We think that including this effect is important, especially for small crystals.

In [GR1] and here we make a simplifying assumption that the evolving crystal is a cylinder $\Omega(t)$ not a hexagonal prism. Such an approach is in fact quite frequent in the physics literature, see [Ne], [YSF]. The description of the evolving interface is then relatively easy. Namely, it requires specifying the radius R and the height $2L$.

We recall now the equations of motion which we studied in [GR1]. The first one for supersaturation σ outside crystal $\Omega(t)$ is

$$\Delta\sigma = 0 \quad \text{in } \mathbb{R}^3 \setminus \Omega(t). \quad (1.1)$$

It means that the mass is transported by diffusion and this transport is much faster than the motion of free boundary $\partial\Omega(t)$, hence the term σ_t on the right-hand-side of (1.1) is

dropped. It is also physically reasonable to assume that σ has a specific value at infinity, *i.e.*

$$\lim_{|x| \rightarrow \infty} \sigma(x) = \sigma^\infty. \quad (1.2)$$

The velocity of the growing crystal is determined by the normal derivative of σ at the surface,

$$\frac{\partial \sigma}{\partial \mathbf{n}} = V \quad \text{on} \quad \partial \Omega(t), \quad (1.3)$$

where \mathbf{n} is the outer normal. This equation expresses the mass conservation. Here \mathbf{n} is the outer normal to Ω and V is assumed to be constant on each facet $S_i \subset \partial \Omega(t)$, $i = T, B, \Lambda$, *i.e.* top, bottom and the lateral surface. The notation we use is explained in Section 2.

The hypothesis that V is spatially constant on each S_i 's relates to stability properties of facets or facet non-breaking properties. It is not always natural especially when $\Omega(t)$ is large, see [GiGi], [BNP1], [BNP2]. We do not touch this issue in the present paper.

We also need an equation for the motion of the free boundary, it is

$$- \int_{S_i} \sigma d\mathcal{H}^2 = (\kappa_i - \beta_i V_i) |S_i| \quad i = T, B, \Lambda, \quad (1.4)$$

where β_i 's are the kinetic coefficients and for simplicity of notation $|S_i|$ stands for $\mathcal{H}^2(S_i)$, *i.e.* the two-dimensional Hausdorff measure of S_i . Here κ_i denotes for crystalline curvature of S_i .

Condition (1.4) is in fact the Gibbs-Thomson relation. Due to lack of smoothness of $\partial \Omega$ the pointwise curvature makes no sense. Instead we use crystalline curvatures κ_i of facets S_i , see [GR1]. The notion of crystalline curvature was first introduced by J.Taylor [Ta] and independently by Angenent and Gurtin [AG]. We stress that the Gibbs-Thomson relation in a similar form to (1.4) has been derived by Gurtin, ([G, Chapter 8], see also [GM]) for polygonal interfaces.

These equations have to be augmented with an initial condition on Ω , *i.e.*

$$\Omega(0) = \Omega_0. \quad (1.5)$$

In [GR1] we showed that this system (1.1–1.5) for (L, R, σ) is well posed and we have local in time existence of solutions for any admissible initial data. However, in that paper we did not study any subtle properties of the dynamics.

Here we are interested in establishing existence of special maximal solutions (we allow for finite extinction times). Namely, we want to establish existence of self-similar solutions, *i.e.* such that

$$\Omega(t) = a(t)\Omega(0) \quad (1.6)$$

holds for a scale factor $a(t)$. By showing their existence we hope to gain new insight into the dynamics of (1.1–1.5).

At this point we mention that the existence of self-similar solutions to the anisotropic curvature flow of the form $\beta V = \kappa_\gamma$ is well-studied in the plane, where κ_γ is a weighted curvature with respect to the interfacial energy γ . In fact there exists a self-similar shrinking solution for smooth strictly convex γ : [Ga], [GaL], [DG], [DGM]. It is extended to a planar crystalline flow by [St1], [St2] and to a crystalline flow in \mathbb{R}^3 by [PP]. Note that if $\beta\gamma =$

const, it is clear that the Wulff shape of γ always shrinks self-similarly. The reader is referred to a review article [Gi] and a nice book [CZ] on this topic. If there is a driving force term, *i.e.* we deal with equation $\beta V = \kappa_\gamma + C$ with some constant $C > 0$, then there is a self-similar expanding solution, provided that $\beta\gamma = \text{const}$ as shown in [So, §12]. It can be easily extended for crystalline case. The main difference between these problems and our problem lies in the fact that our system may be understood as a crystalline flow **coupled** to a diffusion field. However, it turns out that the relation $\beta\gamma = \text{const}$. is a necessary condition for existence of self-similar solutions, too.

Close to our work is the study of isotropic Stefan problem undertaken in [HV]. However, the essential difference is that they do not assume the Gibbs-Thomson at the free boundary.

Our main goal is to establish existence of (expanding or shrinking) self-similar solutions to (1.1–1.5). However, we will see that this is not always possible. Our result is sensitive to a choice of 2 sets of parameters: (a) the Wulff shape of interfacial energy density γ ; (b) the kinetic coefficients β_i 's. Geometrically speaking the crystalline curvature κ_i depends on our selection of surface energy density γ , hence on the Wulff shape W_γ . We note that W_γ is a cylinder with constant crystalline curvature equal to -2 , see §2 for more details. We can now give a rough indication of this dependence. We mentioned that the evolution of Ω is in fact a system of ODE's for L and R . However, when we try to reduce this system to a single equation for the scale factor a in (1.6) it turns out that this is possible only for special values of the aspect ratio

$$\frac{L}{R} = \rho_0,$$

which must be equal to the quotient of the kinetic coefficients $\beta_\Lambda/\beta_T = \rho_0$, see Proposition 4.2. More precisely, ρ_0 is a positive zero of a function which is not given in an explicit way. Our main thrust is then on studying this function and proving that it has at least one positive root, this is done in §4.

Our work requires some preparations, they are done in §2, where we also explain the notation. What is more important we present the structure of the solutions of (1.1–1.5) and their behavior under scaling, which is an important ingredient of our argument.

We also show in §3 that the only steady state of (1.1–1.5) is a properly scaled Wulff shape, with the scale factor depending upon σ^∞ . We also explain how the signs of speeds V_i depend on σ^∞ and curvatures κ_i , $i = T, B, \Lambda$.

2 Preliminaries

In this section we set up the problem. We present here our assumptions and known results. We also recall the structure of solutions and exhibit a scaling law.

2.1 The set up

Our evolving crystal $\Omega(t)$ is assumed to be, as it is done in the physics literature, see [Ne], [YSF], a straight cylinder,

$$\Omega(t) = \{(x, x_2, x_3) \in \mathbb{R}^3, x_1^2 + x_2^2 \leq R^2(t), |x_3| \leq L(t)\}.$$

In other words, we only have to know $R(t)$ and $L(t)$ to describe its evolution. We shall call by *facets* the following subsets of $\partial\Omega(t)$

$$\begin{aligned} S_\Lambda &= \{x \in \partial\Omega(t) : x_1^2 + x_2^2 = R^2\} \\ S_T &= \{x \in \partial\Omega(t) : x_3 = L\} \\ S_B &= \{x \in \partial\Omega(t) : x_3 = -L\} \end{aligned}$$

and we shall call them the lateral side, top and bottom. We also define the set of indices $I = \{\Lambda, T, B\}$. We shall specify the initial data $\Omega(0) = \Omega_0$. We denote by V_i the speed of facet S_i , $i \in I$, in the direction of \mathbf{n} , the outer normal to $\partial\Omega(t)$.

We explicitly assume that σ enjoys the symmetry of $\Omega(t)$, *i.e.* σ is axisymmetric and symmetric with respect to the plane $x_3 = 0$:

$$\sigma = \bar{\sigma}(\sqrt{x_1^2 + x_2^2}, |x_3|).$$

We want to consider a surface energy density function γ which is consistent with our $\Omega(t)$. We recall that γ is to be Lipschitz continuous, convex and 1-homogeneous. To be specific we take

$$\gamma(x_1, x_2, x_3) = r\gamma_\Lambda + |x_3|\gamma_{TB}, \quad \gamma_\Lambda, \gamma_{TB} > 0, \quad (2.1)$$

where $r^2 = x_1^2 + x_2^2$ and $\gamma_\Lambda, \gamma_{TB}$ are positive constants. Hence, its Frank diagram F_γ defined as

$$F_\gamma = \{p \in \mathbb{R}^3 : \gamma(p) \leq 1\}$$

consists of two straight cones with common base, which is the disk $\{(x_1, x_2, 0), x_1^2 + x_2^2 \leq 1/\gamma_\Lambda\}$, the same height and the vertices at

$$(0, 0, \pm 1/\gamma_{TB}).$$

Now, the Wulff shape of γ is defined by

$$W_\gamma = \{x \in \mathbb{R}^3 : \forall \mathbf{n} \in \mathbb{R}^3, |\mathbf{n}| = 1, \quad x \cdot \mathbf{n} \leq \gamma(\mathbf{n})\}.$$

In our setting W_γ is a cylinder of radius R equal to γ_Λ and half-height L equal to γ_{TB} . Hence, all cylinders like $\Omega(t)$ above are *admissible*, in the sense that normal \mathbf{n} to the top facet of $\Omega(t)$ (respectively: bottom, lateral surface of $\Omega(t)$) is the normal to top facet of W_γ (respectively: bottom, lateral surface of W_γ).

We now explain how the ‘‘mean crystalline curvatures’’ κ_i of facet S_i may be defined, in this respect we follow [GR1]. Let us set the surface energy E by formula,

$$E(S) = \int_S \gamma(\mathbf{n}(x)) d\mathcal{H}^2(x).$$

Then we define

$$\kappa_i = - \lim_{h \rightarrow 0} \frac{\Delta E}{\Delta V},$$

where h is the amount of motion of S_i in the direction of the outer normal to $S(t)$; ΔE is the resulting change of surface energy, and ΔV is the change of volume. We now recall the calculation of κ_i performed in [GR1]. Namely, for γ given by (2.1) we obtain

$$\kappa_T = -\frac{2\gamma(\mathbf{n}_\Lambda)}{R} \equiv \kappa_B, \quad \kappa_\Lambda = -\frac{\gamma(\mathbf{n}_T)}{L} - \frac{1}{R}\gamma(\mathbf{n}_\Lambda).$$

In [GR1] we pointed to a relation between κ_i and the surface divergence of a selection of Cahn-Hoffmann vector ξ . Here we will not pursue this topic.

We have established existence of solutions (L, R, σ) to system (1.1)–(1.4).

Proposition 2.1 (see [GR1, Theorem 1]) *There exists (R, L, σ) a unique local-in-time weak solution to*

$$\Delta\sigma = 0 \quad \text{in } \mathbb{R}^3 \setminus \Omega(t), \quad \lim_{|x| \rightarrow +\infty} \sigma(x) = \sigma^\infty \quad (2.2)$$

$$\frac{\partial\sigma}{\partial\mathbf{n}} = V \quad \text{on } \partial\Omega(t) \quad (2.3)$$

$$-\int_{S_i} \sigma = (\kappa_i - \beta_i V_i) |S_i| \quad (2.4)$$

augmented with an initial condition $\Omega(0) = \Omega_0$, where Ω_0 is an admissible cylinder. Moreover,

$$R, L \in C^{1,1}([0, T]) \\ \nabla\sigma \in C^{0,1}([0, T]; L^2(\mathbb{R}^3 \setminus \Omega(t))).$$

□

From now on, for the sake of simplicity we shall denote the unique solution to (2.2)–(2.4) by (Ω, σ) instead of (R, L, σ) .

Constructing the desired solutions requires a detailed knowledge of the structure of σ . This is presented below.

2.2 The structure of σ and the scalings

In order to present the useful structure of σ we have to introduce some additional objects. Namely, we need f_i which is a unique solution to

$$-\Delta f_i = 0 \quad \text{in } \mathbb{R}^3 \setminus \Omega \quad (2.5)$$

$$\frac{\partial f_i}{\partial\nu} = \delta_{ij} \quad \text{on } S_j, \quad j \in I \quad (2.6)$$

such that $\nabla f_i \in L^2(\mathbb{R}^3 \setminus \Omega)$ and $\lim_{x \rightarrow \infty} f_i(x) = 0$, (see [GR1]), where Ω is a straight cylinder in \mathbb{R}^3 given at the beginning of Section 2.1 (with time fixed). Here, δ_{ij} is the Kronecker delta and ν denotes the inner normal to $\partial\Omega$. For functions f, g such that $\nabla f, \nabla g \in L^2(\mathbb{R}^3 \setminus \Omega)$ we also define the following quantities

$$(f, g) := \int_{\mathbb{R}^3 \setminus \Omega} \nabla f(x) \cdot \nabla g(x) dx, \quad \|f\|^2 := (f, f).$$

Let us mention that the equation (2.5)–(2.6) takes the following weak form

$$\int_{\mathbb{R}^3 \setminus \Omega} \nabla f_i(x) \cdot \nabla h(x) dx = \int_{S_i} h(x) d\mathcal{H}^2(x) \quad (2.7)$$

for all h such that $\nabla h \in L^2(\mathbb{R}^3 \setminus \Omega)$.

We showed in [GR1] that (2.2)–(2.4) can be reduced to the following system of ODE's

$$(\mathcal{A} + \mathcal{D})\mathbf{V} = \mathbf{B}, \quad (2.8)$$

where

$$\begin{aligned} \mathbf{V} &= (V_\Lambda, V_T, V_B), \quad \mathbf{B} = (|S_\Lambda|(\sigma^\infty + \kappa_\Lambda), |S_T|(\sigma^\infty + \kappa_T), |S_B|(\sigma^\infty + \kappa_B)) \\ \mathcal{A} &= \{(f_i, f_j)\}_{i,j=\Lambda,T,B}, \quad \mathcal{D} = \text{diag}\{\beta_\Lambda|S_\Lambda|, \beta_T|S_T|, \beta_B|S_B|\}. \end{aligned}$$

In order to explain that (2.8) is indeed an ODE we recall that

$$V_\Lambda = \frac{dR}{dt}, \quad V_T = V_B = \frac{dL}{dt}.$$

In fact, (2.8) is a system of two equations for (R, L) , but for the sake of compatibility with [GR1] we wrote it as if it were a system of three unknowns (R, L_1, L_2) for which $L_1 = L_2$.

Moreover, σ is given by

$$\sigma(t) = - \sum_{i \in I} V_i f_j + \sigma^\infty. \quad (2.9)$$

The purpose of the present section is to clarify the behavior of our system under scaling of domains. Suppose we define a new variable y by formula

$$y = ax$$

where $a > 0$, thus Ω is transformed to $a\Omega = \tilde{\Omega}$, S_i goes to $aS_i = \tilde{S}_i$. If h is defined on Ω , then we transform it to $\tilde{h} : \tilde{\Omega} \rightarrow \mathbb{R}$, by setting

$$\tilde{h}(y) = h\left(\frac{y}{a}\right)$$

we also define

$$f_i^a(y) = af_i\left(\frac{y}{a}\right), \quad i = T, B, \Lambda. \quad (2.10)$$

The Proposition below clarifies the role of definition of f_i^a .

Proposition 2.2. Let us suppose that f_i satisfies (2.7), then

$$\int_{\mathbb{R}^3 \setminus a\Omega} \nabla_y f_i^a(y) \nabla_y \tilde{h}(y) dy = \int_{aS_i} \tilde{h}(y) d\mathcal{H}^2(y)$$

for all h with $\nabla h \in L^2(\mathbb{R}^3 \setminus \Omega)$.

Proof. Let us note $\nabla_y \tilde{h}(y) = \nabla_x h\left(\frac{y}{a}\right) \frac{Dx}{Dy} = \frac{1}{a} \nabla_x h(x)$. Then indeed

$$\begin{aligned} \int_{\mathbb{R}^3 \setminus \tilde{\Omega}} \nabla_y f_i^a(y) \nabla_y \tilde{h}(y) dy &= \int_{\mathbb{R}^3 \setminus \Omega} \frac{a^3}{a} \nabla_x f_i(x) \nabla_x h(x) dx = a^2 \int_{S_i} h(x) d\mathcal{H}^2(x) \\ &= \int_{\tilde{S}_i} \tilde{h}(y) d\mathcal{H}^2(y) \end{aligned}$$

□

3 Critical size crystals

First, we want to determine stationary states of (2.2)–(2.4). They will certainly depend upon σ^∞ . Indeed, we have the following result.

Proposition 3.1 Let us assume that $\sigma^\infty > 0$ is given and γ is defined by (2.1). Then $(\Omega(t), \sigma(t))$ is a stationary solution to (2.2)–(2.4) if and only if

$$\Omega(0) = aW_\gamma \quad \text{and} \quad \sigma(t) = \sigma^\infty,$$

where $a = 2/\sigma^\infty$.

Proof. Let us suppose first that $\Omega(0) = aW_\gamma$, $a = 2/\sigma^\infty$ and $\sigma(t) = \sigma^\infty$. With this definition of the scale a , we see that the right-hand-side of equation (2.8) vanishes,

$$(\mathcal{A} + \mathcal{D})\mathbf{V} = 0.$$

Hence $\mathbf{V} = 0$, because the matrix $\mathcal{A} + \mathcal{D}$ is nonsingular. Moreover, by (2.9) $\sigma(t) \equiv \sigma^\infty$. Thus $(2/\sigma^\infty W_\gamma, \sigma^\infty)$ furnishes a solution to (2.2)–(2.4).

Conversely, if $(\Omega(t), \sigma(t))$ is a stationary solution, then $V_i \equiv 0$, $i \in I$ and (2.9) implies that $\sigma(t) = \sigma^\infty$. In addition, the left-hand-side of equation (2.8) vanishes, implying that $\mathbf{B} = 0$. Thus, $\Omega(t)$ is of a constant crystalline curvature:

$$\kappa_T = \kappa_B = \kappa_\Lambda = -\sigma^\infty,$$

i.e. $\Omega(t)$ is a scaled Wulff crystal. Equivalently, we reached,

$$\frac{\gamma_{TB}}{L} = \frac{\gamma_\Lambda}{R} = \frac{\sigma^\infty}{2}$$

and the dimensions R, L are determined by σ^∞ . □

We may now say that if σ^∞ is given, then $\frac{2}{\sigma^\infty}W_\gamma$ is of *critical size*. We expect that $\Omega(0)$ (not necessarily a scaled Wulff shape) containing $\frac{2}{\sigma^\infty}W_\gamma$ will have the tendency to grow, while those Ω contained in $\frac{2}{\sigma^\infty}W_\gamma$ will shrink. We express it below.

Proposition 3.2 Let us suppose $\sigma^\infty > 0$ and a solution $(\Omega(t), \sigma(t))$ to (2.2)–(2.4) is given. We also assume that $V_\Lambda(t) \cdot V_T(t) > 0$.

(a) If the crystalline curvatures of $\Omega(t)$ satisfy $\sigma^\infty + \kappa_i > 0$, $i \in I$, then $V_i(t) > 0$, for all $i \in I$.

(b) If the crystalline curvatures of $\Omega(t)$ satisfy $\sigma^\infty + \kappa_i < 0$, $i \in I$, then $V_i(t) < 0$, for all $i \in I$.

Remark. The condition $V_i \cdot V_j > 0$ looks strange, but we may not exclude the possibility that it is violated. However, in the case of self-similar motion constructed in next section it is automatically satisfied.

Proof of the Proposition. We shall prove (a) since (b) is handled in a similar way.

Let us recall that the matrix $\mathcal{A} + \mathcal{D}$ in (2.8) is positive definite. Thus,

$$0 < \lambda_0 |V|^2 \leq ((\mathcal{A} + \mathcal{D})\mathbf{V}, \mathbf{V}) = \sum_{i \in I} (\sigma^\infty + \kappa_i) |S_i| V_i.$$

Since $\sigma^\infty + \kappa_i > 0$ and all terms on the right-hand-side are of the same sign, we conclude that

$$V_i > 0 \quad \text{for} \quad i \in \{\Lambda, T, B\}. \quad \square$$

4 Existence of self-similar solutions

We are interested in special solutions to the evolution equations that are simple yet important. We shall say that a solution $(\Omega(t), \sigma(t))$ is *self-similar* if at all time instances the region $\Omega(t)$ satisfies

$$\Omega(t) = a(t)\Omega(0), \quad a(t) \neq 1 \quad (4.1)$$

for a real valued function $a : \mathbb{R}_+ \rightarrow \mathbb{R}_+$. We require that it is non-constant for otherwise we would obtain a stationary solution.

We shall examine consequences of (4.1). We have to express (4.1) in terms of R , L and the speeds of facets. Later we shall see that self-similar evolution exists only for **some** choices of the Wulff shapes W_γ and kinetic coefficients β_i , $i = \Lambda, T, B$.

We note that in the case of evolving cylinder the self-similar evolution is equivalent to constancy of the aspect ratio

$$\frac{L(t)}{R(t)} \equiv \rho. \quad (4.2)$$

Subsequently we shall find an equivalent characterization of (4.2) in terms of the speeds

$$\dot{L}(t) = V_T(t) \equiv V_B(t), \quad \dot{R} = V_\Lambda.$$

Proposition 4.1 *Let us suppose that $(\Omega(t), \sigma(t))$ is a self-similar solution to (2.2)–(2.4). Then (4.2) is equivalent to*

$$\frac{V_T(t)}{V_\Lambda(t)} \equiv \rho, \text{ for all } t \in [0, T_{\max}) \quad \text{and} \quad \frac{L(0)}{R(0)} = \rho. \quad (4.3)$$

Proof. \Rightarrow We notice that $\Omega(t) = a(t)\Omega(0)$ is equivalent to

$$z_i(t) = a(t)z_i(0), \quad i \in \{\Lambda, T, B\}, \quad (4.4)$$

where $(z_\Lambda, z_T, z_B) = (R, L, L)$. After differentiation of this identity we see

$$V_i(t) = \dot{a}(t)z_i(0) \quad i \in \{\Lambda, T, B\}.$$

This implies that

$$\frac{V_T(t)}{V_\Lambda(t)} = \frac{\dot{a}L(0)}{\dot{a}R(0)} = \rho.$$

Possibility of $\dot{a} \equiv 0$ has been already excluded in the definition.

\Leftarrow Obviously, we have

$$z_i(t) = z_i(0) + \int_0^t V_i(s) ds.$$

Conditions (4.3) imply

$$\begin{aligned} \frac{L(t)}{R(t)} &= \frac{L(0) + \int_0^t V_T(s) ds}{R(0) + \int_0^t V_\Lambda(s) ds} = \frac{\rho R(0) + \int_0^t \rho V_\Lambda(s) ds}{R(0) + \int_0^t V_\Lambda(s) ds} \\ &= \rho. \end{aligned} \quad \square$$

In particular it follows from Proposition 4.1 that

$$\frac{V_T(0)}{V_\Lambda(0)} = \rho = \frac{\frac{1}{|S_T|} \int_{S_T} \sigma d\mathcal{H}^2 + \kappa_T}{\frac{1}{|S_\Lambda|} \int_{S_\Lambda} \sigma d\mathcal{H}^2 + \kappa_\Lambda} \cdot \frac{\beta_\Lambda}{\beta_T}.$$

Effectively, due to representation of σ in terms of speeds, this is an equation for the initial speeds, where the role of β_Λ and β_T has to be clarified. We shall see momentarily that the relation between β_Λ and β_T is set by another necessary condition of the self-similar motion.

Proposition 4.2 *Let us suppose that $(\Omega(t), \sigma(t))$ is a self-similar solution to (2.2)–(2.4), then*

$$\frac{\beta_\Lambda}{\beta_T} = \frac{V_T}{V_\Lambda} = \rho.$$

Remark. Combining this Proposition with (4.2) and the definition of the Wulff shape W_γ leads us to the conclusion that the relation

$$\beta\gamma = \text{const.}$$

is a necessary condition for existence of self-similar solutions.

Proof of Proposition 4.2. Let us suppose that $(\Omega(t), \sigma(t))$ is a self-similar solution. We can then express the supersaturation

$$\sigma(t) = - \sum_{i \in \{\Lambda, T, B\}} f_i(t) V_i(t) + \sigma^\infty$$

in terms of $f_i(\cdot) \equiv f_i(0, \cdot)$, $V_i(0)$, $i = T, B, \Lambda$. In §2.2 we showed that if

$$\Omega(t) = a\Omega(0),$$

then

$$\sigma = - \sum_{i \in \{\Lambda, T, B\}} f_i^{a(t)}(t) V_i(t) + \sigma^\infty,$$

Where f_i^a satisfy (2.10) and

$$f_i^{a(t)}(t, y) \equiv a(t) f_i\left(\frac{y}{a(t)}\right)$$

thus, we can rewrite both sides of

$$\int_{S_i(t)} \sigma(t, x) d\mathcal{H}^2(x) = (-\kappa_i(t) + \beta_i V_i) |S_i(t)| \quad (4.5)$$

in the following way

$$\begin{aligned} LHS &= \int_{S_i} \left(- \sum_{j \in I} V_j(t) f_j^{a(t)} + \sigma^\infty \right) d\mathcal{H}^2 \\ &= -a(t) \int_{S_i(t)} \sum_{j \in I} z_j(0) f_j^{a(t)} d\mathcal{H}^2 + \sigma^\infty |S_i(t)| \\ &= -\frac{a(t)}{\dot{a}(0)} \sum_{j \in I} \int_{a(t)S_i(0)} \dot{a}(0) z_j(0) a(t) f_j \left(\frac{y}{a(t)} \right) d\mathcal{H}^2(y) + \sigma^\infty a^2(t) |S_i(0)|. \end{aligned}$$

We change variable $x = y/a$, then

$$\begin{aligned}
LHS &= -\frac{\dot{a}(t)}{\dot{a}(0)} \sum_{j \in I} a^3(t) \int_{S_i(0)} V_j(0) f_j(x) d\mathcal{H}^2(x) + \sigma^\infty a^2 |S_i(0)| \\
&= \frac{\dot{a}(t) a^3(t)}{\dot{a}(0)} \left(\int_{S_i(0)} \sigma(0, x) d\mathcal{H}^2(x) - \sigma^\infty |S_i(0)| \right) + \sigma^\infty a^2 |S_i(0)| \\
&= \frac{\dot{a}(t) a^3(t)}{\dot{a}(0)} |S_i(0)| (\beta_i V_i(0) - \kappa_i - \sigma^\infty) + \sigma^\infty a^2 |S_i(0)|.
\end{aligned}$$

We now calculate the *RHS* of (4.5)

$$\begin{aligned}
RHS &= \int_{aS_i(0)} -\frac{\kappa_i(0)}{a(t)} d\mathcal{H}^2(y) + \beta_i \dot{a}(t) a^2(t) |S_i(0)| z_i(0) \\
&= -a(t) \kappa_i |S_i(0)| + \beta_i \dot{a}(t) a^2(t) |S_i(0)| z_i(0).
\end{aligned}$$

After dividing by $|S_i(0)|$ we see that

$$\sigma^\infty a^2(t) + \frac{\dot{a}(t)}{\dot{a}(0)} a^3(t) (-\kappa_i(0) - \sigma^\infty + \beta_i V_i(0)) = -\kappa_i(0) a(t) + \beta_i \dot{a}(t) a^2(t) z_i(0).$$

Further simple manipulations based on (4.5) yield

$$\dot{a}(t) a^2(t) ((-\kappa_i(0) - \sigma^\infty) a(t) + \beta_i V_i(0) (a(t) - 1)) = -\dot{a}(0) (\sigma^\infty a^2(t) + \kappa_i(0) a(t)).$$

If we assume that $\Omega(0) = W_\gamma$, then the formula for crystalline curvatures yields

$$\kappa_i(0) = \kappa (\equiv -2), \quad i \in \{\Lambda, B, T\}$$

If we plug this result into equations above, we obtain

$$\dot{a}(t) = \frac{\dot{a}(0) (\sigma^\infty a(t) + \kappa)}{a(t) ((\sigma^\infty + \kappa) a(t) + \beta_i V_i(0) (1 - a(t)))}, \quad i \in \{\Lambda, B, T\} \quad (4.6)$$

Of course, we have to assume that $\sigma^\infty + \kappa \neq 0$, for otherwise we would have a stationary solution.

If the left-hand side is to be independent of i , then we conclude that

$$\beta_T V_T(t) = \beta_\Lambda V_\Lambda(t),$$

as desired. □

On the way, we established the equation which $a(t)$ has to fulfill, namely equation (4.6). This equation has to be augmented with an initial condition, *i.e.*

$$a(0) = 1$$

and we have to supply $\dot{a}(0)$ calculated from (4.5). Namely, (4.5) may be rewritten as

$$\sum_{j \in I} V_j(0) (f_i, f_j) + \beta_i |S_i| V_i(0) = (\sigma^\infty + \kappa_i(0)) |S_i|.$$

Before we proceed, we make a simplifying assumption. Due to the scaling formula of §2.2 without loss of generality, we may assume

$$L = \rho \quad \text{and} \quad R = 1. \quad (4.7)$$

If we use this simplification, Cramer's formula applied to (2.8) yields

$$\frac{V_T(0)}{V_\Lambda(0)} = \frac{\|f_\Lambda\|^2 + 4\beta_\Lambda\pi\rho - 8\rho(f_\Lambda, f_T)}{4\rho(f_T, f_T + f_B) + 4\pi\rho^2\beta_T - 2(f_\Lambda, f_T)}.$$

Combining this with

$$\frac{V_T(0)}{V_\Lambda(0)} = \rho,$$

we obtain an equation for ρ , where we use also $\beta_\Lambda/\beta_T = \rho$.

After some simple algebraic manipulations the equation for ρ reduces to

$$4\rho^2(f_T, f_T + f_B) + 6\rho(f_T, f_\Lambda) = \|f_\Lambda\|^2. \quad (4.8)$$

We notice that β_Λ, β_T miraculously cancel out.

We stress here that f_T, f_B, f_Λ depend only on ρ and they are independent of σ^∞ .

This is an equation for the constant in time proportions of the self-similar, evolving cylinder. It guarantees that

$$\frac{L(0)}{R(0)} = \frac{V_T(0)}{V_\Lambda(0)} = \frac{\beta_\Lambda}{\beta_T} = \rho.$$

We will show that (4.8) has at least one solution. We will achieve our goal after calculating behavior of both sides of (4.8) for large and small ρ . This will be done in a series of Lemmata. We do not pretend to show optimal estimates here. We are content to conclude that they are sufficient for showing existence of solutions.

Lemma 4.3 *There exists a universal constant C_1 independent of ρ such that*

$$\|f_\Lambda\| \leq C_1 \rho^{\frac{1}{2}}(1 + \rho^{\frac{1}{3}}), \quad \forall \rho \in \mathbb{R}_+$$

and $\|f_\Lambda\| \leq C_1 \rho^{\frac{3}{4}}$ for small ρ .

Proof. Let us choose a cut-off function $\eta : [0, \infty) \rightarrow [0, 1]$, such that $\eta(1) = 1$ and

$$\eta(r) = \begin{cases} \frac{R+l-r}{l}, & r \in [R, R+l], \\ 0, & r > R+l, \\ 1, & r \in [0, R]. \end{cases}$$

Of course $R = 1$ due to our scaling, but for the sake of clarity we shall stress it anyway. Let us note that

$$\|f_\Lambda\|^2 = \int_{S_\Lambda} f_\Lambda(x) d\mathcal{H}^2(x) = 2 \int_0^{2\pi} \int_0^\rho f_\Lambda(x) R dx_3 d\theta,$$

where (r, θ, x_3) are cylindrical coordinates.

Let us set $D = (B(0, R + l) \setminus B(0, R)) \times (-\rho, \rho)$, then due to the definition of η we can see,

$$\begin{aligned} \|f_\Lambda\|^2 &= 2 \int_0^{2\pi} \int_0^\rho [f_\Lambda(x)R\eta(R) - f_\Lambda(x)(R+l)\eta(R+l)] dx_3 d\theta \\ &= -2 \int_0^{2\pi} \int_0^\rho \int_R^{R+l} \frac{\partial}{\partial r}(\eta(r)r f_\Lambda(x)) dx_3 d\theta dr \\ &= - \int_D \left(\frac{\partial}{\partial r} \eta f_\Lambda + \eta \frac{\partial f_\Lambda}{\partial r} + \frac{\eta}{r} f_\Lambda \right) dx. \end{aligned}$$

We notice that $|D| = 2\rho\pi(2R+l)l$ and $\eta/r \leq 1$ for $r \geq R = 1$. Now, by Hölder inequality we come to

$$\|f_\Lambda\|^2 \leq (1 + \frac{1}{l})|D|^{\frac{5}{6}} \left(\int_D f_\Lambda^6 \right)^{\frac{1}{6}} + |D|^{\frac{1}{2}} \left(\int_D |\nabla f_\Lambda|^2 \right)^{\frac{1}{2}}.$$

The first integral may be estimated by Sobolev inequality for unbounded domains (see e.g. [HK, Theorem 5]) i.e. we obtain

$$\|f_\Lambda\| \leq c\rho^{\frac{5}{6}}(l^{\frac{5}{6}} + l^{-\frac{1}{6}})(1+l)^{\frac{5}{6}} + c\rho^{\frac{1}{2}}l^{\frac{1}{2}}(1+l)^{\frac{1}{2}},$$

where c is a constant. When we choose $l = 1$, then

$$\|f_\Lambda\| \leq c\rho^{\frac{1}{2}}(1 + \rho^{\frac{1}{3}}), \quad \forall \rho \in \mathbb{R}_+.$$

For small ρ it is advantageous to balance power of the ingredients, for this reason we take $l = \rho^{\frac{1}{2}}$. Hence,

$$\|f_\Lambda\| \leq c\rho^{\frac{5}{6} - \frac{1}{12}} + c\rho^{\frac{1}{2} + \frac{1}{4}} =: C_1\rho^{\frac{3}{4}}$$

for sufficiently small $\rho > 0$, as desired. \square

A similar reasoning leads us to

Lemma 4.4 *There exists a constant C_2 independent of ρ such that*

$$\|f_T\| \leq C_2. \quad \square$$

We need also good lower bounds on $\|f_\Lambda\|$.

Lemma 4.5 *There exists $C_3 > 0$ such that for all sufficiently small ρ the following estimate holds*

$$\|f_\Lambda\| \geq C_3\rho^{\frac{5}{6}}.$$

Proof. We shall exploit the fact that for any function η , with $\nabla\eta \in L^2$ and being equal to 1 on S_Λ , we have

$$4\pi R\rho = \int_{S_\Lambda} 1 d\mathcal{H}^2 = \int_{\mathbb{R}^3 \setminus \Omega} \nabla\eta \cdot \nabla f_\Lambda \leq \|f_\Lambda\| \cdot \|\eta\|.$$

We shall take $\eta = \psi(r)\varphi(x_3)$, where $r^2 = x_1^2 + x_2^2$ and $\varphi(z)$ is even. Namely, we choose

$$\psi(r) = \begin{cases} 1 & r \in [0, R], \\ \frac{R+l-r}{l} & r \in (R, R+l], \\ 0 & r \geq R+l, \end{cases}$$

$$\varphi(z) = \begin{cases} 1 & z \in [0, \rho], \\ \frac{\rho + \lambda - z}{L} & z \in (\rho, \rho + \lambda], \\ 0 & z > \rho + \lambda, \end{cases}$$

where $\ell, \lambda > 0$ shall be picked later. Obviously

$$\nabla \eta = \psi_r \varphi \cdot \vec{e}_r + \psi \varphi_{x_3} \vec{e}_{x_3},$$

where $\vec{e}_r = (x_1, x_2, 0)/r$, $\vec{e}_{x_3} = (0, 0, 1)$ and $|\nabla \eta|^2 = \psi_r^2 \varphi^2 + \psi^2 \varphi_{x_3}^2$. We set now

$$D = [B(0, R + \ell) \setminus B(0, R)] \times [-\rho, \rho],$$

$$P = B(0, R + \ell) \times [\rho, \lambda + \rho] \cup B(0, R + \ell) \times [-\lambda - \rho, -\rho],$$

$$X = [B(0, R + \ell) \setminus B(0, R)] \times ([-\lambda - \rho, -\rho] \cup [\rho, \rho + \lambda]).$$

Then with these definitions, we see

$$\int_{\mathbb{R}^3 \setminus \Omega} |\nabla \eta|^2 dx = \int_D \psi_r^2 \varphi^2 dx + \int_P \psi^2 \varphi_{x_3}^2 dx + \int_X \psi_r^2 \varphi^2 dx.$$

We shall treat each term separately. On D we clearly have $\psi_r = -\ell^{-1}$, hence

$$\int_D \varphi^2 \psi_r^2 dx \leq \frac{1}{\ell^2} |D| = \frac{2\pi\rho}{\ell} (2R + \ell).$$

On P we have $|\varphi_{x_3}| = \frac{1}{\lambda}$, and

$$\int_P \varphi_{x_3}^2 \psi^2 dx \leq \frac{\pi}{\lambda^2} (R + \ell)^2$$

and finally we calculate the integral over X

$$\int_X \psi_r^2 \varphi^2 dx \leq \frac{2\pi}{\ell} \lambda (2R + \ell).$$

Combining those results we arrive at

$$\|\eta\| \leq c \left(\frac{3}{\ell} (1 + \ell) + \frac{(1 + \ell)^2}{\lambda} + \frac{\lambda}{\ell} (1 + \ell) \right)^{\frac{1}{2}}$$

Again, we want to balance all the terms, we put $\ell = \rho^\alpha$, $\lambda = \rho^{-\beta}$, $\alpha, \beta > 0$, The constraint of equal powers of all terms yields $\beta = 1/3$, $\alpha = 2/3$, and finally

$$\|\eta\| \leq c \rho^{\frac{1}{6}}.$$

Hence $\|f_\Lambda\| \geq C_3 \rho^{\frac{5}{6}}$, for all $\rho > 0$. □

The argument used above yields also

Lemma 4.6 *There exists $C_4 > 0$ such that for all $\rho > 0$*

$$\|f_T\| \geq C_4,$$

i.e. $\|f_T\|$ is bounded below by a positive constant. □

We are now ready to study equation (4.8).

Theorem 4.7 Equation (4.8) has at least one positive solution ρ_0 .

Proof. Both sides of (4.8) are continuous functions of ρ . We shall estimate the growth of both sides at ∞ and near 0.

For $\rho > 1$ due to Lemmata 4.3 and 4.6 we have

$$\begin{aligned} RHS &\leq C_U \rho^{5/6} \\ LHS &\geq 4\rho^2 \|f_T\| \geq C_L \rho^2, \end{aligned}$$

where we also used positivity of (f_T, f_B) and (f_T, f_Λ) . Hence, $LHS > RHS$ for sufficiently large ρ .

Now, for small $\rho > 0$, because of Lemmata 4.5, 4.3 and 4.4 we see

$$\begin{aligned} RHS &\geq c_1 \rho^{5/3} \\ LHS &\leq c \left(\rho^2 + \rho \rho^{3/4} \right) \end{aligned}$$

It is obvious that

$$LHS < RHS, \quad \text{for sufficiently small } \rho > 0.$$

Hence, for some $\rho_0 > 0$ both sides of (4.8) must be equal, because they are continuous functions of ρ . \square

What we have done so far is: we have determined the proportions of the Wulff shape and the proportions of the kinetic coefficients $\rho_0 = \beta_\Lambda / \beta_T$. The number ρ_0 is special and may not be unique.

We are now ready to establish existence of self-similar evolution.

Theorem 4.8 Let us suppose that ρ_0 is a solution of (4.8) and $\Omega(0)$ is the Wulff shape of γ i.e., $\Omega(0) = W_\gamma$ and $L/R = \rho_0$. We also assume that

$$\frac{\beta_\Lambda}{\beta_T} = \rho_0.$$

Then the evolution of $\Omega(0)$ is self-similar.

Proof. We have to show that $\Omega(t) = a(t)\Omega(0)$. We have already shown in the course of proof of Proposition 4.2 that $a(t)$ satisfies the ODE (4.6)

$$\begin{aligned} \dot{a} &= \frac{\dot{a}(0)(\sigma^\infty a(t) + \kappa)}{a(t)((\sigma^\infty + \kappa)a(t) + \beta_T V_T(0)(1 - a(t)))} \\ a(0) &= 1, \end{aligned} \tag{4.9}$$

where $\beta_T V_T(0) = \beta_\Lambda V_\Lambda(0)$ by our choice of ρ_0 and $\kappa = \kappa_T = \kappa_\Lambda$. Similarly,

$$\dot{a}(0) = \frac{V_\Lambda}{R} = \frac{V_T}{L},$$

Equation (4.9) has a unique solution, because the right-hand-side of (4.9) is Lipschitz continuous with respect to a and the denominator never vanishes. This is so due to

$$\begin{aligned} (\sigma^\infty + \kappa)a - \beta_T V_T(0)a + \beta_T V_T(0) &= a(\sigma^\infty + \kappa - \beta_T V_T(0)) + \beta_T V_T(0) \\ &= \int_{S_T} \sum_{i \in I} \beta_i V_i(0) f_i d\mathcal{H}^2 + \beta_T V_T(0) \neq 0 \end{aligned}$$

as long as $\sigma^\infty \neq -\kappa$ and V_i 's have the same sign.

We have to check that

$$(V_\Lambda, V_T) := (\dot{a}z_\Lambda, \dot{a}z_T) \equiv \dot{a} \cdot (R, L)$$

and

$$\sigma := - \sum_{i \in I} \dot{a}z_i f_i^a + \sigma^\infty$$

satisfy (2.2)–(2.4). Of course

$$\Delta\sigma = 0 \quad \text{in} \quad \mathbb{R}^3 \setminus \Omega(t) \quad \text{and} \quad \lim_{|x| \rightarrow \infty} \sigma(x) = \sigma^\infty$$

and

$$\frac{\partial\sigma}{\partial\mathbf{n}} = V_i \quad \text{on} \quad \partial\Omega$$

due to properties of f_i^a , see Proposition 2.2. Moreover,

$$\int_{S_i} \sigma = \int_{S_i} (\beta_i V_i - \kappa_i) d\mathcal{H}^2$$

holds by the very definition of $\dot{a}(t)$. □

Let us remark that if $V_i > 0$, then $a(t)$ is defined for all $t \geq 0$. On the other hand, if $\Omega(t)$ shrinks, *i.e.* $V_i < 0$, then it is easy to see from (4.9) that the solution dies out in finite time. We leave this calculation to the interested reader.

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