

## A Stefan type problem arising in modeling ice crystals growing from vapor

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**Abstract.** This paper is concerned with a quasi-steady Stefan problem with the Gibbs-Thomson relation and a kinetic term applied to model ice crystals growing from vapor. Our goal is to expose a number of properties of solutions to the system. Here we survey our earlier work [GR1]–[GR4] and announce new results, [GR5].

### 1 Presentation of the problem

Our goal is to study geometric properties of simple surfaces  $S(t)$  evolved according to the driven mean weighted curvature flow

$$\beta V = \kappa_\gamma + \sigma. \quad (1.1)$$

We would immediately like to expose the main features of the problem. Namely, they are:

- (a) the lack of smoothness of  $S(t)$ , i.e.  $S(0)$  is a straight, circular cylinder;
- (b)  $\kappa_\gamma$  is the crystalline curvature of  $S(t)$  (see (1.4) and Proposition 2.1 below);
- (c) the driving force  $\sigma$  is the coupling to another equation.

The motivation to study such problems comes from physics. More precisely, we are interested in growth of ice crystals in the air. Depending on the controlling temperature one can observe a variety of shapes from hexagonal; prism to needles, and to snowflakes (see [Ne]). In particular, large columnar ice crystals can be not only collected in nature but they have also been grown in a laboratory (see e.g. [GoG]).

The mathematical model whose part is (1.1), is supposed to handle naturally non-smooth  $S(t)$ . At the same time we are convinced that the Gibbs-Thomson relation is important and should be included, see [G]. Finally, the model we come up with should allow us to study stability of facets. We will say that a facet is *stable* at time  $t$  if it neither bends nor breaks at that time instant.

We have in mind an evolution system stemming from the work by Seeger (see [Se]) on planar polygonal crystals, which was further developed to deal with three-dimensional crystal by Kuroda *et al.*, see [KIO]. Namely, we consider,

$$0 = \Delta\sigma \quad \text{in } \bigcup_{0 < t < T} \mathbb{R}^3 \setminus \Omega(t), \quad \sigma(\infty) = \sigma^\infty > 0 \quad (1.2)$$

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

$$-\sigma = -\operatorname{div}_S \xi - \beta V, \quad \text{on } S(t). \quad (1.4)$$

In this system  $\sigma(t, x)$  is the supersaturation outside of crystal  $\Omega(t)$ . The mass is transported by diffusion, which is much faster than the interface  $S(t) = \partial\Omega(t)$  whose speed is denoted by  $V$ . Hence the form of equation (1.2) follows. The second equation of the above system is a properly rescaled mass conservation law, where  $V$  is the speed of  $S(t)$ , (see [GR3]). Here, the outer normal to  $\Omega(t)$  is denoted by  $\mathbf{n}$ .

The last equation is in fact the Gibbs-Thomson relation, where  $\xi$  is the Cahn-Hofmann vector and  $\operatorname{div}_S \xi$  is its surface divergence. However, in the earlier papers [Se], [KIO] the curvature term was omitted. We shall recall the definition of  $\operatorname{div}_S \xi$ , namely suppose that  $\xi$  defined in  $U$  a neighborhood of  $S_i$

$$\operatorname{div}_S \xi = \operatorname{trace} (\operatorname{Id} - \mathbf{n} \otimes \mathbf{n}) \nabla \xi, \quad \text{for } x \in S,$$

where  $\mathbf{n}$  is an outer normal to the surface. This definition is independent of the extension of  $\xi$  to  $U$  (see [Si]).

Crucial for the definition of  $\xi$  is the surface energy density  $\gamma$ . If  $\gamma$  were smooth, then we would take  $\xi = \nabla \gamma(\mathbf{n}(x))$ , but  $\gamma$  is only Lipschitz continuous. This definition of  $\xi$  does not make sense because the normals to  $\Omega$  belong to the set of points where  $\gamma$  is not differentiable. We will define  $\xi$  in a proper way in §2 below.

As we mentioned earlier, the hexagonal prisms are quite common ice shapes but we will make simplifications frequently applied in the physics literature (e.g. see [Ne], [YSF]). Namely, we shall assume that  $\Omega(t)$  is a straight circular cylinder, i.e.  $\Omega(t) = \{(x_1, x_2, x_3) : x_1^2 + x_2^2 \leq R^2(t), |x_3| \leq L(t)\}$ .

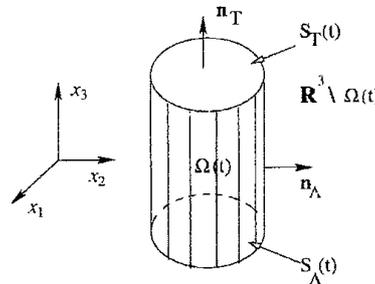


Fig. 1. Evolving crystal

We distinguish three parts of  $S(t)$ : top  $S_T$ , bottom  $S_B$ , and the lateral part  $S_\Lambda$ . The normal to  $S_i$  is denoted by  $\mathbf{n}_i$ ,  $i = \Lambda, B, T$ . We assume that the super-saturation  $\sigma$  shares the symmetries of  $\Omega$ . i.e. it is axially symmetric and it enjoys symmetry with respect to the plane  $x_3 = 0$ , i.e.

$$\sigma(x_1, x_2, x_3) = \sigma(\sqrt{x_1^2 + x_2^2}, |x_3|). \quad (1.5)$$

We may now spell out the main question:

Suppose that  $\gamma$  is so chosen that straight circular cylinders are admissible. What are the conditions which will guarantee that  $\Omega(t)$  evolving according to (1.2)–(1.4) will retain stability of facets on time interval  $[0, T_0)$ . In other words, what are the conditions on  $\Omega(0)$ ,  $\sigma^\infty$  which prohibit bending and braking of facets of  $\Omega(t)$ .

Here we will give a preliminary answer to this questions, details will appear elsewhere, see [GR5].

## 2 On Cahn-Hoffmann vector $\xi$ .

We here summarize the common properties of the surface energy density function  $\gamma$ . Namely, we assume that function  $\gamma$  is:

- (1) Lipschitz continuous;
- (2) convex;
- (3) 1-homogeneous.

Thus,  $\gamma$  is differentiable a.e., but this is not enough, because the normals to  $\partial\Omega(t)$  fall into the set of points where  $\gamma$  is not differentiable. For this reason we must turn our attention to objects which are defined for all  $\mathbf{n} \in \mathbb{R}^3$ . Namely, its subdifferential  $\partial\gamma(\mathbf{n})$  is defined everywhere. We recall that if  $\gamma : \mathbb{R}^n \rightarrow \mathbb{R}$  is convex, then we set

$$\gamma(v) = \{w \in \mathbb{R}^n : \gamma(v+h) - \gamma(v) \geq w \cdot h \text{ for all } h \in \mathbb{R}^n\}.$$

Subsequently, we shall require

$$\xi(x) \in \partial\gamma(\mathbf{n}(x)). \quad (2.1)$$

This condition amends the evolution equations (1.2)–(1.4).

We shall consider a specific form of  $\gamma$ , consistent with our problem

$$\gamma(x_1, x_2, x_3) = r\gamma_\Lambda + |x_3|\gamma_{TB}, \quad \gamma_\Lambda, \gamma_{TB} > 0, \quad (2.2)$$

where  $r^2 = x_1^2 + x_2^2$  and  $\gamma_\Lambda, \gamma_{TB}$  are positive constants.

Hence, the Frank diagram,  $F_\gamma$ , and Wulff shape of  $\gamma$ ,  $W_\gamma$  are

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

$$W_\gamma = \{x \in \mathbb{R}^3 : \forall \mathbf{n} \in \mathbb{R}^3, |\mathbf{n}| = 1, x \cdot \mathbf{n} \leq \gamma(\mathbf{n})\} = \{x \in \mathbb{R}^3 : x_1^2 + x_2^2 \leq \gamma(\mathbf{n}_\Lambda), |x_3| \leq \gamma(\mathbf{n}_T)\}.$$

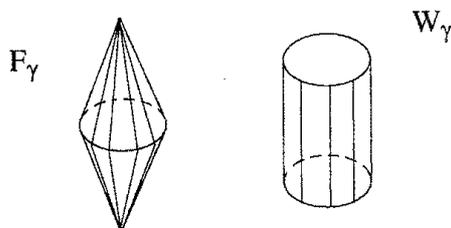


Fig. 2. Frank diagram  $F_\gamma$  and Wulff shape  $W_\gamma$

Thus, all straight, circular cylinders will be called *admissible*. However, we shall not go more deeply into the notion of admissibility of sets.

Since at normals to  $W_\gamma$  the set  $\partial\gamma$  is not a singleton we have some freedom of choosing  $\xi$ . Thus, we can rephrase our goal: To find conditions guaranteeing existence of a section  $\xi$  such that

$$\sigma - \operatorname{div}_S \xi \equiv \operatorname{const}_i = \beta_i V_i \quad \text{on } S_i, \quad i = \Lambda, B, T. \quad (2.3)$$

However, at the moment we do not know how to solve (1.2)–(1.4), (2.1). Such a task at the moment is possibly too broad. For this reason we will make another simplification.

We notice that after averaging (1.4) (or (2.3)) we can see

$$\beta V = \frac{\beta_i}{|S_i|} \int_{S_i} V dS = \frac{1}{|S_i|} \int_{S_i} \sigma dS - \frac{1}{|S_i|} \int_{S_i} \operatorname{div}_S \xi dS.$$

This formula is well-defined if

$$\operatorname{div}_S \xi|_{S_i} \in L^2(S_i) \text{ and } \xi \in L^\infty(S_i), \quad i \in \{\Lambda, T, B\}. \quad (2.4)$$

Conditions (2.4) imply that the trace  $\xi \cdot \nu$  on  $S_i$  is well-defined ( $\nu \in TS_i$  and  $\nu$  is the normal to  $\partial S_i$ ). Combining this with

$$\partial\gamma(\mathbf{n}_\Lambda) \cap \partial\gamma(\mathbf{n}_T) = \{\gamma_{TB}\mathbf{n}_T + \gamma_\Lambda\mathbf{n}_\Lambda\}$$

implies

$$\xi|_{S_i \cap S_j} \in \partial\gamma(\mathbf{n}_i) \cap \partial\gamma(\mathbf{n}_j). \quad (2.5)$$

It turns out that the averages of  $\operatorname{div}_S \xi$  over facets are independent of the choice of  $\xi$ .

**Proposition 2.1.** (Proposition 2.1. in [GR4]) *Let us suppose that  $\gamma$  is defined by (2.2), and  $\Omega$  is a straight circular cylinder. If  $\operatorname{div}_S \xi|_{S_i} \in L^2(S_i)$ ,  $\xi \in L^\infty(S_i)$  as well as (2.1), i.e.  $\xi(x) \in \partial\gamma(\mathbf{n}(x))$ , and (2.5) hold, then*

$$\int_{S_i} \operatorname{div}_S \xi = -\kappa_i |S_i|,$$

where

$$\kappa_\Lambda = -2 \frac{\gamma(\mathbf{n}_\Lambda)}{R}, \quad \kappa_T = -\frac{\gamma(\mathbf{n}_L)}{R} - \frac{\gamma(\mathbf{n}_T)}{L}. \quad (2.6)$$

We shall call the numbers  $\kappa_T = \kappa_B, \kappa_\Lambda$  *crystalline curvatures* of the top, bottom, and the lateral surfaces, respectively.

The proof of this fact depends just on integration by parts. This becomes more tricky on  $S_\Lambda$  whose mean Euclidean curvature is non-zero, (see [Si]).

This Proposition will help us to simplify the problem by replacing (1.4) with its averaged form

$$-\int_{S_i} \sigma dS = \kappa_i |S_i| - \beta_i V_i, \quad i = L, T, B. \quad (2.7)$$

Let us note that  $V_\Lambda, V_B = V_T$  are easily expressed in terms of time derivatives of  $R, L$ , i.e.  $V_\Lambda = \dot{R}$ ,  $V_T = \dot{L}$ , then (2.7) turns into an ODE,

$$\mathcal{A}(L, R) \begin{bmatrix} \dot{L} \\ \dot{R} \end{bmatrix} = \mathbf{B}(L, R), \quad L(0), R(0) \text{ are given.} \quad (2.8)$$

Here  $\mathcal{A}(L, R)$  is a symmetric, positive definite matrix, it is Lipschitz continuous in  $L, R$ , (see [GR1]) and

$$\mathbf{B} = (B_\Lambda, B_T), \quad B_i = (\sigma^\infty + \kappa_i) |S_i|, \quad i = \Lambda, T.$$

In the process of reducing (2.7) to (2.8) we obtain a representation formula for  $\sigma$ :

$$\sigma(t, x) = \sigma^\infty - [(f_T(t, x) + f_B(t, x))V_T(t) + f_\Lambda(t)V_\Lambda(t)], \quad (2.9)$$

where the functions  $f_T, f_B$  and  $f_\Lambda$  are solutions to a Neumann problem for Laplace equation in the outer domain  $\mathbb{R}^3 \setminus \Omega(t)$ , (see §3 in [GR1]). We can summarize it as follows.

**Proposition 2.2.** (Theorem 1 in [GR1]) *There exists  $(R(t), L(t), \sigma(t, x))$  a unique weak solution to*

$$\begin{aligned} \Delta\sigma &= 0 \quad \text{in } \mathbb{R}^3 \setminus \Omega(t), & \lim_{|x| \rightarrow +\infty} \sigma(x) &= \sigma^\infty; \\ \frac{\partial\sigma}{\partial\mathbf{n}} &= V \quad \text{on } \partial\Omega(t) & & \\ -\int_{S_i} \sigma &= \kappa_i |S_i| - \beta_i V_i |S_i| & & \end{aligned} \quad (2.10)$$

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

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

The notion of weak solutions here is fairly natural, for a rigorous definition see [GR1]. In order to make the notation more concise we shall write  $(\Omega, \sigma)$  in place of  $(R(t), L(t), \sigma(t, x))$ .

We may wonder what is the relation of solution of the original system and the averaged one. Fortunately we have an easy answer.

**Theorem 2.3.** (Theorem 2.3 in [GR4]) *The original system (1.2)–(1.4), (2.1) and the averaged one (i.e., (2.10)) are equivalent in the class of solutions satisfying*

$$\sigma - \operatorname{div}_S \xi = \text{const} \quad \text{on each } S_i.$$

Then our original question takes the following form:

Can we construct solutions to (1.2)–(1.4), (2.1) such that  $\sigma - \operatorname{div}_S \xi$  is constant on each facet? Alternatively, can we solve (2.10) and then find  $\xi$  satisfying all the constraints?

### 3 A variational principle for selecting $\xi$

The proper choice of  $\xi$  is crucial for our tasks. We will postulate a variational principle for its selection. Namely, we can claim that

$$\sigma - \operatorname{div}_S \xi = \text{const} \quad \text{on each } S_i, \quad i = \Lambda, T, B \quad (3.1)$$

are three Euler-Lagrange equations of energy functionals  $\mathcal{E}_i$ ,  $i = \Lambda, T, B$ . Thus, selecting the right Cahn-Hoffman vector amounts to choosing  $\xi$  with minimal energy. This idea was justified by [FG] for the graph evolution and it was further developed in [GG]. Similar ideas were used by Bellettini, Novaga and Paolini, (see [BNP1]–[BNP3]) as well as in [GPR]. We define these three functionals

$$\mathcal{E}_i(\xi) = \frac{1}{2} \int_{S_i} |\operatorname{div}_S \xi - \sigma|^2 d\mathcal{H}^2, \quad i = \Lambda, T, B$$

on

$$\mathcal{D}_i = \{ \xi \in L^\infty(S_i) : \operatorname{div}_S \xi \in L^2(S_i), \xi(x) \in \partial\gamma(\mathbf{n}(x)), \xi|_{S_i \cap S_j} \in \partial\gamma(\mathbf{n}_\Lambda) \cap \partial\gamma(\mathbf{n}_T) \}.$$

Thus, we **postulate**: the right motion is such that at each time instance  $\xi$  is a solution to

$$\mathcal{E}_i(\xi) = \min\{\mathcal{E}_i(\zeta) : \zeta \in \mathcal{D}_i\}, \quad i = \Lambda, T, B. \quad (3.2)$$

It is obvious from the definition that these functionals are strictly convex, hence  $\operatorname{div}_S \xi$  is uniquely defined. It is also fairly easy to see that indeed the Euler-Lagrange equation of  $\mathcal{E}_i$  is (3.1). Moreover, all solutions to (3.2) inherit the symmetry of  $\Omega$ , namely, we can show:

**Proposition 3.1.** (Proposition 3.1 in [GR4].) *Let us assume that  $\sigma \in L^2(S_i)$  and that it satisfies the symmetry relations (1.5);  $\xi \in \mathcal{D}_i$ ,  $i \in I$ , is a solution to the minimization problem (3.2). Then:*

(a) *There exists a rotationally invariant vector field  $\bar{\xi} \in \mathcal{D}_i$  i.e. for any rotation  $Q_\alpha$ , around the  $x_3$  axis by the angle  $\alpha \in (0, 2\pi)$ ,*

$$Q_{-\alpha} \bar{\xi}(Q_\alpha x) = \bar{\xi}(x), \quad (3.3)$$

$\bar{\xi}$  is a minimizer of  $\mathcal{E}_i$ ,  $i = T, \Lambda, B$ , and

$$\operatorname{div}_S \bar{\xi} = \operatorname{div}_S \xi.$$

(b) There exists  $\tilde{\xi} \in \mathcal{D}_i$  a minimizer of  $\mathcal{E}_i$ ,  $i = T, \Lambda, B$ , which satisfies

$$\tilde{\xi}(x_1, x_2, -x_3) = \tilde{\xi}(x_1, x_2, x_3)$$

and

$$\operatorname{div}_S \tilde{\xi} = \operatorname{div}_S \xi.$$

**Sketch of proof:** We can simply write formulas for  $\bar{\xi}$  and  $\tilde{\xi}$ , namely

$$\bar{\xi}(x) = \frac{1}{2\pi} \int_0^{2\pi} Q_{-\alpha} \xi(Q_\alpha x) d\alpha, \quad \tilde{\xi}(x) = \frac{1}{2} (\xi(x_1, x_2, -x_3) + \xi(x_1, x_2, x_3)).$$

It is easy to check that they have the desired properties.  $\square$

Simply by dropping the divergence free part of  $\xi$  a further simplification of the structure of  $\xi$  is possible. Namely, we deduce the following result.

**Proposition 3.2.** (Proposition 3.3 in [GR4]) *Let us suppose that  $\xi \in \mathcal{D}_i$  is a minimizer of  $\mathcal{E}_i$ ,  $i \in I$ . Then, there exist  $\varphi, \psi : \mathbb{R} \rightarrow \mathbb{R}$ ,  $\varphi, \psi \in H_{loc}^2(\mathbb{R})$ , such that*

$$\tilde{\xi} = \nabla(\varphi(r) + \psi(|x_3|)) \in \mathcal{D}_i, \quad i = T, B, \Lambda, \quad (3.4)$$

where  $r^2 = x_1^2 + x_2^2$  and

$$\operatorname{div}_S \tilde{\xi} = \operatorname{div}_S \xi \quad \text{on } S_\Lambda, S_T, S_B. \quad \square$$

## 4 Necessary and sufficient conditions for the stability of facets

If we interpret (3.1) as Euler-Lagrange equation, then it should satisfy a number of constraints and we face the question: whether we can solve the following problem

$$\begin{aligned} \sigma - \operatorname{div}_S \xi &= \text{const on } S_i, \\ \xi &\in \partial\gamma(\mathbf{n}), \quad x \notin S_i \cap S_j, \\ \xi &\in \partial\gamma(\mathbf{n}_i) \cap \partial\gamma(\mathbf{n}_j), \quad x \in S_i \cap S_j? \end{aligned} \quad (4.1)$$

Once we solve it we wish to know what is the relation of solutions to Euler-Lagrange equations to minimizers? We can give the answer to this question which corresponds to our expectations.

**Proposition 4.1.** (Proposition 4.5 in [GR4]) *Let us suppose that  $\xi \in \mathcal{D}_i$  is a solution to (4.1). Then,  $\xi$  is a minimizer of  $\mathcal{E}_i$ .*

**Proof.** Let us take any  $\bar{\xi} \in \mathcal{D}_i$ . Then,  $\bar{\xi} = \xi + h$ , where  $h$  satisfies  $h \cdot \nu_i = 0$  on  $S_i \cap S_j$  in an appropriate sense (this is explained in detail in §2 of [GR4]). We will see that  $\mathcal{E}_i(\bar{\xi}) \geq \mathcal{E}_i(\xi)$ . Indeed,

$$\mathcal{E}_i(\xi + h) = \mathcal{E}_i(\xi) - \int_{S_i} (\sigma - \operatorname{div}_S \xi) \operatorname{div}_S h \, d\mathcal{H}^2 + \frac{1}{2} \int_{S_i} (\operatorname{div}_S h)^2 \, d\mathcal{H}^2.$$

Now, we recall  $\sigma - \operatorname{div}_S \xi = V_i \beta_i$ . We will consider only  $i = T, B$ . The integration by parts yields

$$\int_{S_i} (\sigma - \operatorname{div}_S \xi) \operatorname{div}_S h \, d\mathcal{H}^2 = V_i \beta_i \int_{\partial S_i} h \cdot \nu \, d\mathcal{H}^1 = 0.$$

The Proposition follows for  $i = T, B$ . A slightly more involved argument is valid for  $S_\Lambda$ , the details are omitted.  $\square$

Indeed, we can solve (4.1). We consider only  $S_T$ , because the analysis in the other case is similar. We take  $\xi(x_1, x_2, x_3) = \nabla(\varphi(r) + \psi(x_3))$ . Thus, we look only for  $\varphi(r)$  on  $S_T$ , since  $\psi_{x_3}(L) = \gamma(\mathbf{n}_T)$  there. Finally, (4.1) takes the form,

$$\sigma - \beta_T V_T = \frac{1}{r}(r\varphi_r)_r.$$

This equation is augmented with boundary data

$$\varphi_r(R) = \gamma(\mathbf{n}_\Lambda), \quad \varphi_r(0) = 0.$$

This problem may be easily solved. Finally,

$$\varphi_r(r) = \frac{1}{r} \int_0^r s\sigma(s, L) ds + \frac{r}{R} \left( \gamma(\mathbf{n}_\Lambda) - \frac{1}{R} \int_0^R s\sigma(s, L) ds \right). \quad (4.2)$$

A similar reasoning leads to a formula for  $\psi_z$  on  $S_\Lambda$ ,

$$\psi_z(z) = \int_0^z \sigma(R, s) ds - \frac{z}{L} \int_0^L \sigma(R, s) ds + \frac{\gamma(\mathbf{n}_T)}{L} z. \quad (4.3)$$

□

We may summarize what we know.

**Theorem 4.2.** (Theorem 4.6 in [GR4]) (**Necessary and sufficient conditions for facet stability**) *Let us suppose that  $\sigma$  is given by Proposition 2.2, thus in particular  $\sigma|_{S_i} \in L^2(S_i)$ . If  $\xi \in \mathcal{D}_i$  is a solution to (4.1), then there exists  $\bar{\xi} \in \mathcal{D}_i$  another minimizer of  $\mathcal{E}_i$ , which is of the form (3.4), i.e.  $\bar{\xi}(x_1, x_2, x_3) = \nabla(\varphi(r) + \psi(|x_3|)) \in \mathcal{D}_i$ ,  $i \in I$ , where  $\varphi_r$  is given by (4.2) and  $\psi_z$  by (4.3), and*

$$\operatorname{div}_S \xi = \operatorname{div}_S \bar{\xi}.$$

Moreover,

(i) *Facet  $S_T$  (and  $S_B$ ) is stable if and only if*

$$\varphi_r(r) \in [-\gamma(\mathbf{n}_\Lambda), \gamma(\mathbf{n}_\Lambda)], \quad \forall r \in [0, R], \quad \varphi_r(0) = 0, \quad \varphi_r(R) = \gamma(\mathbf{n}_\Lambda).$$

(ii) *Facet  $S_\Lambda$  is stable if and only if*

$$\psi_{x_3}(x_3) \in [-\gamma(\mathbf{n}_T), \gamma(\mathbf{n}_T)], \quad \text{for all } x_3 \in [-L, L], \quad \psi_{x_3}(0) = 0, \quad \psi_{x_3}(L) = \gamma(\mathbf{n}_T).$$

**Proof.** (i) *Necessity.* The stability implies that  $\operatorname{div}_S \bar{\xi} - \sigma = \beta_T V_T$  and we can solve (4.1). Its only solution is given by formula (4.2). Since  $\bar{\xi} \in \mathcal{D}_i$ , we obviously have that  $\varphi_r(r) \in [-\gamma(\mathbf{n}_\Lambda), \gamma(\mathbf{n}_\Lambda)]$ ,  $\varphi_r(R) = \gamma(\mathbf{n}_\Lambda)$ , while  $\varphi_r(0) = 0$  is a consequence of smoothness of  $\varphi$ .

(ii) *Sufficiency.* This is the content of Proposition 4.1. □

So far our results are general, we wish to see more specific ones. For this purpose we rewrite  $\varphi_r, \psi_z$  in a cleaner way, and we introduce

$$\bar{\sigma}_r := \frac{1}{|S_T \cap \{x_1^2 + x_2^2 \leq r^2\}|} \int_{S_T \cap \{x_1^2 + x_2^2 \leq r^2\}} \sigma(x) d\mathcal{H}^2(x),$$

$$\bar{\sigma}_z := \frac{1}{|S_\Lambda \cap \{|x_3| \leq z\}|} \int_{S_\Lambda \cap \{|x_3| \leq z\}} \sigma(x) d\mathcal{H}^2(x).$$

As above, we will present the main points for  $S_T$  because the case  $S_\Lambda$  can be handled in a similar manner. Thus, (4.2) takes the form:

$$\varphi_r(r) = \frac{r}{R} \gamma(\mathbf{n}_\Lambda) + \frac{r}{2} (\bar{\sigma}_r - \bar{\sigma}_R).$$

and we have to make sure that  $\varphi_r(r) \in [-\gamma(\mathbf{n}_\Lambda), \gamma(\mathbf{n}_\Lambda)]$ .

The analysis of behavior of  $\bar{\sigma}_r - \bar{\sigma}_R$  relies on the knowledge of the signs of  $V_i$ 's, namely we have:

**Lemma 4.3.**

- (a) If  $V_\Lambda > 0$ , then  $\bar{\sigma}_R - \bar{\sigma}_r > 0$  for all  $r \in (0, R]$ .
- (b) If  $V_\Lambda < 0$ , then  $\bar{\sigma}_R - \bar{\sigma}_r < 0$  for all  $r \in (0, R]$ .
- (c) If  $V_\Lambda = 0$ , then  $\bar{\sigma}_R \equiv \bar{\sigma}_r$  for all  $r \in (0, R]$ .

We shall see that the proof of this result depends on so-called Berg's effect. Namely, Berg has observed (see [Be]) that supersaturation enjoys some monotonicity on the crystal surface. We shall state this below in a rigorous form.

**Theorem 4.4.** (Berg's effect, Theorem 1 in [GR2]) *Let us suppose that  $\sigma$  is a unique solution to*

$$\begin{aligned} 0 &= \Delta \sigma \quad \text{in } \mathbb{R}^3 \setminus \Omega, \quad \sigma(\infty) = \sigma^\infty > 0, \\ \frac{\partial \sigma}{\partial \mathbf{n}} &= V_i \quad \text{on } S = \partial \Omega, \end{aligned}$$

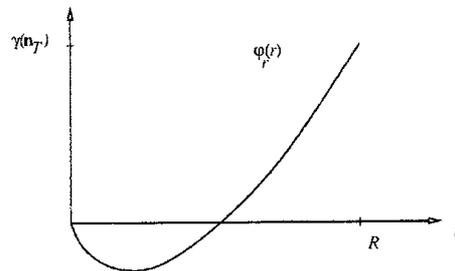
where  $V_i > 0$  are constants, and  $\sigma = \sigma(\sqrt{x_1^2 + x_2^2}, |x_3|)$ . Then,

- (a)  $\frac{\partial \sigma}{\partial x_3} > 0$  (resp.  $< 0$ ) on  $S_\Lambda \cap \{x_3 > 0\}$ , (resp.  $< 0$ );
- (b)  $\frac{\partial \sigma}{\partial r} > 0$  on  $S_T, S_B$ ; (c)  $\sigma < \sigma^\infty$ .

An analogous statement is valid if we reverse the signs of  $V_i$ 's. □

**Proof of Lemma 4.3.** (a) By Berg's effect we deduce  $\frac{\partial \sigma}{\partial r} > 0$ , hence  $\bar{\sigma}_R > \bar{\sigma}_r$  for all  $r < R$ . Similarly we deduce (b). Basically, (c) is a direct consequence of (a) and (b).

In fact, Lemma 4.3 implies that some of the inequalities in Theorem 4.2, i.e.  $\varphi_r(r) \in [-\gamma(\mathbf{n}_\Lambda), \gamma(\mathbf{n}_\Lambda)]$ , are satisfied automatically, e.g. for  $V_\Lambda > 0$  we have the following picture.



**Fig. 3.** A sketch of  $\varphi_r$

**Lemma 4.5.** We assume that  $\xi = \nabla(\varphi(r) + \psi(z))$ , where  $\varphi_r$  and  $\psi_z$  are given by (4.2) and (4.3), respectively. Then,

- (a) if  $V_\Lambda < 0$ , then  $\varphi_r(r) > -\gamma(\mathbf{n}_\Lambda)$ , for all  $r \in [0, R]$ ;
- (b) if  $V_\Lambda > 0$ , then  $\varphi_r(r) < \gamma(\mathbf{n}_\Lambda)$ , for all  $r \in [0, R]$ ;
- (c) if  $V_T < 0$ , then  $\psi_z(z) > -\gamma(\mathbf{n}_T)$ , for all  $z \in [0, L]$ ;
- (d) if  $V_T > 0$ , then  $\psi_z(z) < \gamma(\mathbf{n}_T)$ , for all  $z \in [0, L]$ .

But we do not know if all the constraints are fulfilled. If we keep our focus on  $S_T$  then, for instance, if  $V_\Lambda > 0$  the question is: when it is true that

$$\varphi_r(r) > -\gamma(\mathbf{n}_\Lambda), \quad \text{for all } r \in (0, R)?$$

The above inequality is equivalent to

$$\frac{r}{2}(\bar{\sigma}_R - \bar{\sigma}_r) < \gamma(\mathbf{n}_\Lambda)\left(1 + \frac{r}{R}\right).$$

By the representation formula for  $\sigma$ , (2.9), we can see

$$\bar{\sigma}_R - \bar{\sigma}_r = aV_T \mathcal{F}_1(\rho, \theta, \tau), \quad (4.4)$$

where

$$\rho = \frac{L}{R}, \quad \theta = \frac{r}{R}, \quad \tau = \frac{V_\Lambda}{V_T}, \quad a(t) \text{ is the scale at time } t$$

$$\mathcal{F}_1(\rho, \theta, \tau) = \text{a complicated expression.}$$

This looks bad. It gets simpler if  $\frac{V_\Lambda}{V_T} = \text{const}$  and  $\frac{L}{R} = \text{const}$ , because  $\mathcal{F}_1$  is then a function of one variable. Indeed, we can have it for *self-similar motion*, i.e. if  $\Omega(t) = a(t)\Omega_0$ .

Self-similar motion is a special, important kind of solutions. But more basic ones are steady states. Let us notice that  $V \equiv 0$  is equivalent to  $\Omega = \frac{2}{\sigma^\infty} W_\gamma$ , where  $W_\gamma$  is the Wulff shape, i.e.  $\frac{2}{\sigma^\infty} W_\gamma$  is the only steady state.

We have seen in Lemmas 4.3. and 4.5 that a lot depends on signs of velocities. Deciding the sign of  $V_T, V_\Lambda$  is another story. At the moment it is enough to say that for a self-similar motion they have the sign of  $\sigma^\infty + \kappa(t)$ , where  $\kappa(t)$  is the constant curvature of  $a(t)W_\gamma$ .

Let us finally state the result guaranteeing existence of self-similar solutions.

**Theorem 4.6.** (Theorem 4.8 in [GR3]) *There exists a choice of  $\beta$  and  $\gamma$  satisfying*

$$\beta \cdot \gamma = \text{const},$$

for which  $\Omega(t) = a(t)W_\gamma, a(0) = 1$  is a solution to (2.10).

We are now in a position to state our first specific stability result:

**Theorem 4.7.** (Theorem 4.8 in [GR4]) *Let us suppose that  $\gamma, \beta$  are as above and  $\Omega(t) = a(t)W_\gamma$  is a self-similar solution. To fix attention, we assume that  $\sigma^\infty + \kappa > 0$ , where  $\kappa$  is the curvature of  $\Omega(0) = W_\gamma$ .*

(i) *The stability of  $S_T$  at time  $t$  is equivalent to*

$$\frac{a(t)(\sigma^\infty a(t) - 2)c_T}{\beta_T + a(t)c_T} \leq \bar{d}_T, \quad (4.5)$$

where  $c_T$  and  $\bar{d}_T$  are constants depending only on  $W_\gamma$ .

(ii) *A similar statement holds for  $S_\Lambda$ .*

It is apparent from (4.4), i.e.  $\bar{\sigma}_R - \bar{\sigma}_r = aV_T \mathcal{F}_1(\rho, \theta, \tau)$ , that the proof of Theorem 4.6 depends on estimates of  $V_T$ . Indeed, we have.

**Lemma 4.8.** *Let us assume that  $\gamma$  and  $\beta$  are such that they admit self-similar evolution. Moreover,  $\Omega(t)$  is a self-similar solution, and  $\Omega(0) = W_\gamma$ . Then,*

$$V_T(t) = \frac{\sigma^\infty - 2/a(t)}{\beta_T + a(t)c_T}, \quad V_\Lambda(t) = \frac{\sigma^\infty - 2/a(t)}{\beta_\Lambda + a(t)c_\Lambda}. \quad (4.6)$$

Here,  $c_T, c_\Lambda$  are constants.

**Idea of the proof of Lemma 4.8:** We use the averaged Gibbs-Thomson and the representation formula for  $\sigma$ ,

$$V_T(t) \left( \beta_T + \int_{S_T} ((f_T^a + f_B^a)\alpha_T + f_\Lambda^a \alpha_\Lambda) d\mathcal{H}^2 \right) = \sigma^\infty + \kappa(t),$$

where  $\alpha_T = 1, \alpha_\Lambda = \frac{V_\Lambda(t)}{V_T(t)} = \text{const}$ . □

The proof of the facet stability result, **Theorem 4.7**, amounts to checking if the inequality

$$\theta a(t)V_T(t)\mathcal{F}_1(\rho_0, \theta, \rho_0) \leq 1 + \theta$$

holds. The calculations are based on the fact that  $V_\Lambda/V_T$  is constant and they use explicit formulas for  $V_T$  and  $V_\Lambda$ .  $\square$

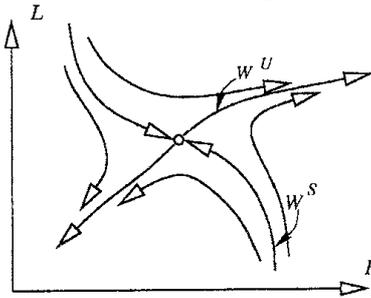
**Remark.** We will succeed in general, if we can bound  $\frac{V_\Lambda(t)}{V_T(t)}$ . For this purpose we draw a general picture of the phase portrait of the ODE system (2.10).

## 5 Phase portrait

Let us denote the unique equilibrium of (2.10) by  $z_0 = \frac{2}{\sigma_\infty}(R_0, L_0)$ , where  $R_0$  is the radius and  $L_0$  is half-height of  $W_\gamma$ .

**Theorem 5.1.** *There exists a neighborhood  $\mathcal{U}$  of  $z_0$  in the first quarter of the plane and orthogonal projections  $P, Q : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ , such that  $\dim \text{Im } P = 1$ ,  $\dim \text{Im } Q = 1$ . They are such that  $W^U(z_0, \mathcal{U})$  (respectively,  $W^S(z_0, \mathcal{U})$ ) exists and it is a  $C^1$  curve over  $P\mathbb{R}^2$  (respectively,  $Q\mathbb{R}^2$ ) which is tangent at  $z_0$  to  $P\mathbb{R}^2$  (respectively  $Q\mathbb{R}^2$ ).*

This statement is an application of standard results from dynamical systems like that exposed in Hale's book [Ha], details will be presented elsewhere, see [GR5].



**Fig. 4.** The phase portrait

Once we know the phase portrait we can draw other conclusions related to behavior of the system near  $z_0$ . The first observation is,

**Corollary 5.2.** There exists an open set  $\mathcal{W}$  in  $B(z_0, r_0) \subset \mathbb{R}^2$  for some  $r_0 > 0$ , such that

$$0 \leq \frac{|V_\Lambda|}{|V_T|} < \bar{\varrho} < \infty \quad \text{in } \mathcal{W}.$$

The point is that the manifolds  $W^U(z_0) \cap B(z_0, r_0)$  and  $W^S(z_0) \cap B(z_0, r_0)$  are contained in  $\mathcal{W}$  which generalizes the situations described earlier.

Finally, our preliminary, facet stability result is here.

**Theorem 5.3.** Let us assume that  $(R, L)$  is in the subset  $\mathcal{W}$  of the phase plane. Then,

(a) there exists  $U_T$ , a neighborhood of  $z_0$ , such that for all points  $(R, L) \in \mathcal{W} \cap U_T$  the facets  $S_T, S_B$  are stable.

(b) there exists  $U_\Lambda$ , a neighborhood of  $z_0$ , such that for all points  $(R, L) \in \mathcal{W} \cap U_\Lambda$  the facet  $S_\Lambda$  is stable.

The proof is based on the same ideas as in the proof of Theorem 4.7. That is, we have to check (for  $V_T > 0$ ) if the inequality

$$\theta a(t)V_T(t)\mathcal{F}_1(\rho, \theta, \tau) \leq 1 + \theta$$

holds. However, the calculations are more involved, they depend upon the bound stated in Corollary 5.2. and the fact that in  $\mathcal{W}$  the aspect ratio of cylinder with radius  $R$  and half-height  $L$ , where  $(R, L) \in \mathcal{W}$  is bounded. The details of a more precise result will be presented elsewhere, see [GR5].  $\square$

**Remark.** Lemma 4.3 suggests that the set of facet stability is large, because if  $V_\Lambda = 0$ , then  $\varphi_r(r) = \frac{r}{R}\gamma(\mathbf{n}_\Lambda)$ .

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