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A Numerical Study of Anisotropic Crystal Growth with Bunching under Very Singular Vertical Diffusion

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Abstract

We study numerically the anisotropic bunching effect in crystal growth under curvature and a singular vertical diffusive regularization. Our assumption is that the mobility of the growth depends on the height of the given crystal. This assumption may result in overhanging crystals if approached in a naive way. Instead, we embed the profile of the crystal as the zero level set of a continuous function and study the corresponding level set evolution. To prevent "overhanging", we regularize the equation with a singular diffusion that vanishes everywhere except at the formation of "overhanging". In addition, we add the mean curvature regularization to keep the convexity of the level sets.

1 Introduction

It is observed in experiments [23] that actual crystal growth consists of different sheets, each with the same convex shape in a different orientation. The large time

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asymptotic growth shape retained in each sheet is called a Wulff shape and can be obtained from a given mobility [12]. In addition, viewing from the side, the sheets structure remains as the graph of a piecewise continuous function. The formation of jump discontinuities in this "height function" is called bunching. Our goal is to study this type of crystal growth numerically.

A single sheet crystal growth is formulated by Hamilton-Jacobi equations if the curvature effect is neglected. It is by now standard to empoly the level set method for tracking the whole evolution numerically [15] and analytically [2][3]. We refer the readers to the books of [8, 13, 18] for the level set methods and [5, 6] for recent development related to the motion by nonlocal curvatures.

The idea is to represent the regions on which the crystal resides, denoted here by Ω, by a continuous function ψ. More precisely,

$$\Omega(t) = \{x \in \mathbb{R}^n : \psi(x,t) \leq 0\}.$$

With the given mobility function γ, which determines the normal velocity of $\partial\Omega$, one can then evolve the level set equation

$$\psi_t + \gamma(\vec{n})|\nabla\psi| = 0$$

to track $\Omega(t)$ implicitly. It is shown in [14, 17] and also [20] that the asymptotic shape of $\Omega(t)$, up to dilation, is the Wulff shape contructed through the Legendre transform

$$\Omega(t) = \inf_{\theta\cdot\nu, |\theta|=1} \frac{\gamma(\theta)}{\theta\cdot\nu}.$$

The mobility function γ is a positive function of the outer normal $\vec{n}$ of Ω. As is formulated above, $\vec{n}$ corresponds to $\nabla\psi/|\nabla\psi|$ evaluated at $\partial\Omega$. Thus it can also be regarded as a positive function of $\nabla\psi$, homogeneous of degree zero; i.e. $\gamma(\vec{n}) = \gamma(\nabla\psi) = \gamma(\lambda\nabla\psi) > 0$.

Smereka [19] proposed a level set method to study the spiral growth of screw dislocations numerically. The growth model used there, as was proposed in [1], had an addition of the curvature regularization. The effect of this curvature regularization on the corner shape of the Wulff problem was investigated in [12].

In this paper, we will model the growth of multiple sheets under curvature regularization and the mobility functions that depend also on the height of the crystal; i.e. $\gamma(u(x,t), \vec{n}(x))$, where $u(x,t)$ is the function describing the profile, or the height, of the crystal, and $\vec{n}(x)$ is the ourter normal of the crystal. Let $u : \mathbb{R}^n \times \mathbb{R}^+ \mapsto \mathbb{R}$ be the height function of crystal. We assume that each l-level set of u moves with the speed as the product of the mobility $\gamma(l,\vec{n})$ and a constant plus its curvature. The corresponding equation is of the form:

$$u_t + \gamma(u, \nabla u)(C - \nabla \cdot \frac{\nabla u}{|\nabla u|})|\nabla u| = 0. \tag{1}$$

The mobility function γ determines the anisotropic motion of of the level sets of u. If γ is increasing in u, then shock may develop even if the initial data is smooth.

2 Formulation

Following the paper [9, 10] and [22], we propose a level set formulation with a singular, vertical diffusion regularization reflecting the idea of nonlocal curvature in [5]. In this formulation, the solution u to (1) is embedded as the zeros of a Lipschitz continuous function $\phi : U \times [0,T] \subseteq \mathbb{R}^{n+1} \times \mathbb{R}^+ \mapsto \mathbb{R}$; i.e. $\phi(x', u(x',t), t) = 0$ for $t \geq 0$, where $x' \in \mathbb{R}^n$. With the notation $x = (x', x_{n+1})$, $x' = (x_1, x_2, \cdots, x_n)$ and $\nabla_{x'}\phi = (\partial/\partial x_1 \phi, \partial/\partial x_1 \phi, \cdots, \partial/\partial x_n \phi)$, we have

$$\begin{aligned} \frac{d}{dt}\phi(x,u,t) &= \phi_t + \phi_{x_{n+1}}(x,u,t)u_t = 0 \\ \frac{d}{dx_j}\phi(x,u,t) &= \phi_{x_j} + \phi_{x_{n+1}}(x,u,t)u_{x_j} = 0, \;\; j = 1, \cdots, n \end{aligned}$$

near $(x, u(x,t), t)$. Thus, formally

$$\phi_t + \gamma(u, \nabla_{x'}\phi)(C - \nabla_{x'} \cdot \frac{\nabla_{x'}\phi}{|\nabla_{x'}\phi|})|\nabla_{x'}\phi| = 0,$$

assuming that $\phi_{x_{n+1}} > 0$.

As in [22], we extend the equation to the whole domain $U \times [0,T] \subseteq \mathbb{R}^{n+1} \times \mathbb{R}^+$, and add a singular diffusion term along the x_{n+1} direction,

$$\eta \frac{\partial}{\partial x_{n+1}} \frac{\phi_{x_{n+1}}}{|\phi_{x_{n+1}}|} |\nabla_{\mathbb{R}^{n+1}}\phi|,$$

where $\eta > 0$ is a suitable constant as motivated in [7, 9]. See also [4]. The level set equation that we solve numerically takes the form:

$$\phi_t + \gamma(x_{n+1}, \nabla_{x'}\phi)(C - \nabla_{x'} \cdot \frac{\nabla_{x'}\phi}{|\nabla_{x'}\phi|})|\nabla_{x'}\phi| = \eta \frac{\partial}{\partial x_{n+1}} \frac{\phi_{x_{n+1}}}{|\phi_{x_{n+1}}|} |\nabla_{\mathbb{R}^{n+1}}\phi|, \tag{2}$$

with a Lipschitz continuous data $\phi(x', x, 0)$ satisfing $\phi(x', u(x', 0), 0) = 0$, and

$$\{(x', x) \in \mathbb{R}^{n+1} : x \leq u(x', 0)\} = \{(x', x) \in \mathbb{R}^{n+1} : \phi(x', x, 0) \leq 0\}.$$

Note that the zero level set of ϕ may overturn if $\eta = 0$ or if η is sufficiently small.

2.1 Numerics

The first order derivatives in

$$\gamma(x_{n+1}, \nabla_{x'}\phi)(C - \nabla_{x'} \cdot \frac{\nabla_{x'}\phi}{|\nabla_{x'}\phi|})|\nabla_{x'}\phi|$$

is approximated by the 5th order WENO method, see [11], with Lax-Friedrichs Hamiltonian described in [16]. The curvature term,

$$\nabla_{x'} \cdot \frac{\nabla_{x'}\phi}{|\nabla_{x'}\phi|},$$

is discretized by a compact centered differencing described, e.g., in [24].

The singular diffusion term can be approximated by a compact central differencing on a regularized signum function of $\phi_{x_{n+1}}$. Here we regularize the signum function by using the tanh function or by adding a small positive number to the denominator. More precisely,

$$\frac{\partial}{\partial x_{n+1}} \frac{\phi_{x_{n+1}}}{|\phi_{x_{n+1}}|}(x)$$

is approximated by

$$\frac{1}{\Delta x}\left(S(D_+^{x_{n+1}}\phi(x)) - S(D_-^{x_{n+1}}\phi(x))\right),$$

where Δx is the spatial grid size, $S(p) = \tanh(\delta^{-1}p)$ or $(p^2/(p^2+\delta^2))^{1/2}$, for some small $\delta > 0$, and

$$D_\pm^{x_{n+1}}\phi(x) = \pm\frac{\phi(x', x_{n+1} \pm \Delta x) - \phi(x', x_{n+1})}{\Delta x}.$$

In our computations, we took $\delta = \Delta x$. We point out that a related regularization technique and the corresponding numerical issues is studied in the paper of Tornberg and Engquist [21].

The spatially discretized system is then evolved in time by the 3rd TVD Runge-Kutta scheme [16] with the Courant-Friedrichs-Levy condition $\Delta t \leq C\Delta x^3$.

3 Examples

With the singular vertical diffusion term, we have successfully prevent different sheets of a crystal structure from overhanging (the bunching effect). Our model mobility function is the following:

$$m(\theta(x_{n+1})) = 1.0 + \alpha(|\cos 2\theta(x_{n+1})| - 0.5).$$

With C and α big enough, the Wulff shape of each level set is a square of different orientation, depending on function $\theta(x_{n+1})$ that is taken to be some staircase function.

Figure 1 shows a numerical result with $\eta = 0$ in (2). It is observed that the level set of ϕ develops overhanging in the x_{n+1} direction. Figures 2, and 3 show two numerical simulations with $\eta = 1.5$. We observe in particular in Figure 3 that there is no overhanging in the x_{n+1} direction. However, without the curvature term, the convexity of the regions enclosed by each of the level sets shown is not preserved.

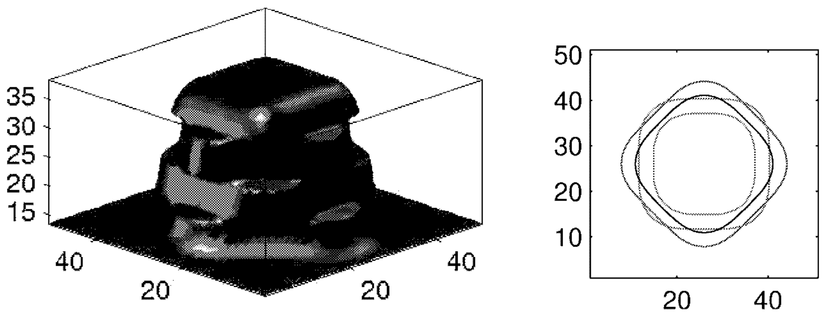

Figure 1: A crystal profile and its level contours obtained without either curvature or vertical viscosity regularization.

4 Summary

In this paper, we present a level set method to study the anisotropic bunching problem related to multiple sheets crystal growth. We show, numerically, that

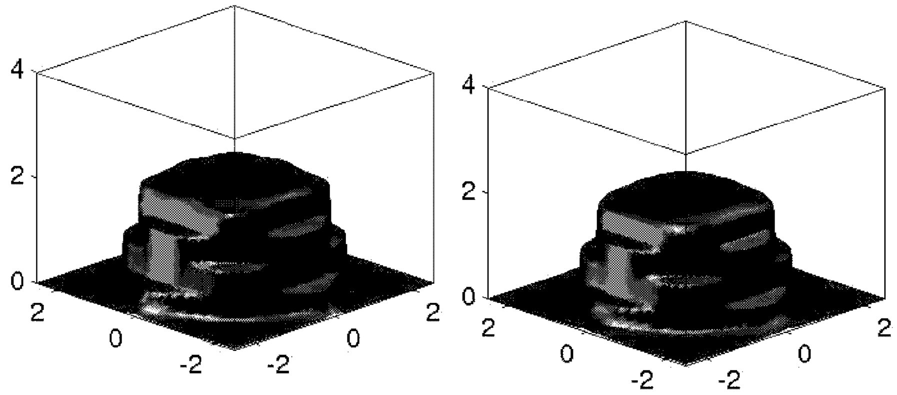

Figure 2: Two crystal profiles obtained with vertical diffusion regularization. The one one the left is obtained without curvature, while the one on the right is obtained with curvature in the mobility function.

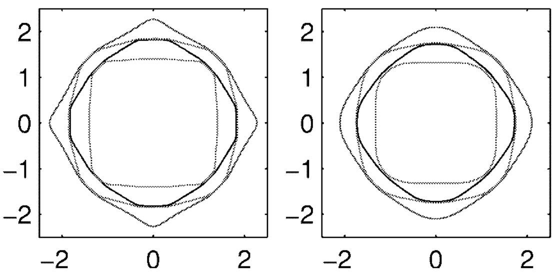

Figure 3: The level contours of the level set functions depicted in Figure 2. The one one the left is obtained without curvature, while the one on the right is obtained with curvature in the mobility function.

under the curvature regularization, the shape remains convex for all time. We also show that the singular diffusion term does prevent the overturning of the level sets.

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