An Analysis of Crystalline Surface Diffusion Using a Subdifferential Framework

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Outline

1. **Motivation** and **Examples**
2. **Crystalline Motion of Polygonal Curves**
3. **Subdifferential Formulation** and **Canonical Restriction** for One-Dimensional Crystalline Motion: **Motion by Mean Curvature** and **Surface Diffusion**
4. **Splitting Phenomena**
5. Some Open Problems

Motivation

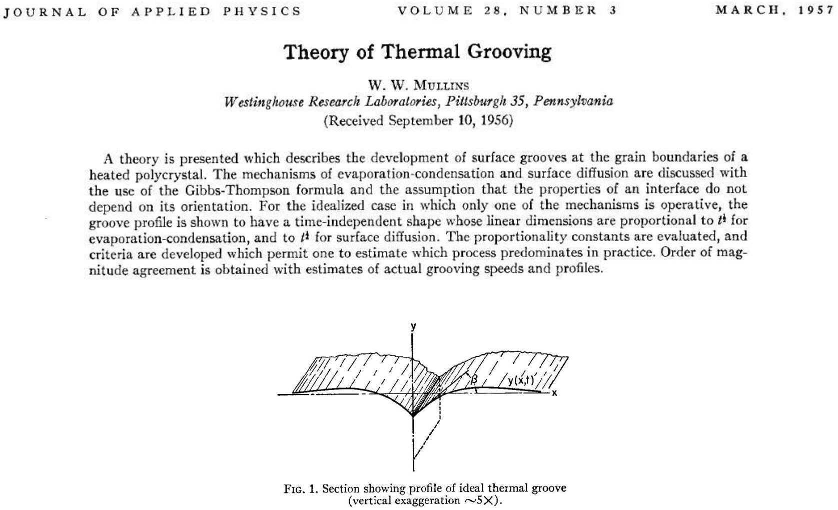
- Curvature type motion apprears in many applications, e.g. geometry, image processing and materials science.
- In terms of applications, two common ones are motion by mean curvature and surface diffusion.
- **Motion by mean curvature (MMC)**:

$$\mathbf{V_n} = \mathbf{H} \quad (L^2\textbf{-gradient flow of surface area}).$$

- **Surface Diffusion (SD)**:

$$\mathbf{V_n} = -\triangle_{\mathbf{s}}\mathbf{H} \quad (H^{-1}\textbf{-gradient flow of surface area}).$$

Mullins Thermal Grooving



JOURNAL OF APPLIED PHYSICS VOLUME 28, NUMBER 3 MARCH, 1957

Theory of Thermal Grooving

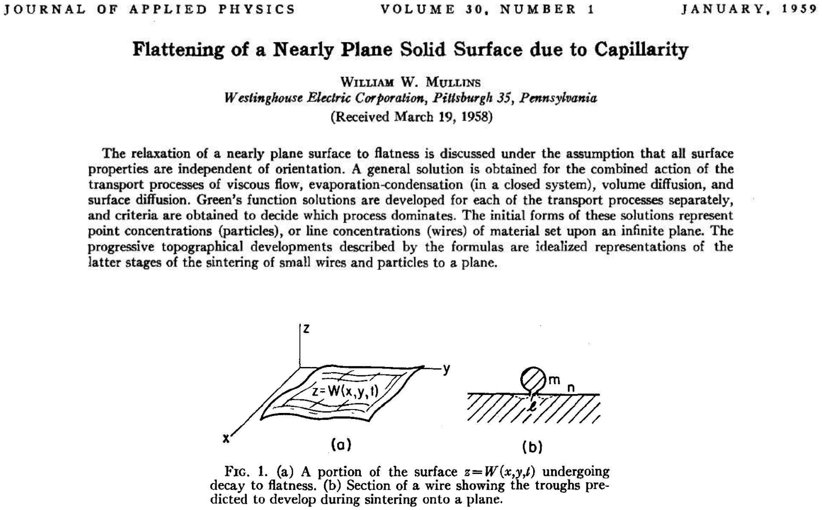
W. W. MULLINS
Westinghouse Research Laboratories, Pittsburgh 35, Pennsylvania

(Received September 10, 1956)

A theory is presented which describes the development of surface grooves at the grain boundaries of a heated polycrystal. The mechanisms of evaporation-condensation and surface diffusion are discussed with the use of the Gibbs-Thompson formula and the assumption that the properties of an interface do not depend on its orientation. For the idealized case in which only one of the mechanisms is operative, the groove profile is shown to have a time-independent shape whose linear dimensions are proportional to $t^{\frac{1}{2}}$ for evaporation-condensation, and to $t^{\frac{1}{4}}$ for surface diffusion. The proportionality constants are evaluated, and criteria are developed which permit one to estimate which process predominates in practice. Order of magnitude agreement is obtained with estimates of actual grooving speeds and profiles.

FIG. 1. Section showing profile of ideal thermal groove (vertical exaggeration ~5×).

Mullins Thermal Grooving



JOURNAL OF APPLIED PHYSICS VOLUME 30, NUMBER 1 JANUARY, 1959

Flattening of a Nearly Plane Solid Surface due to Capillarity

WILLIAM W. MULLINS
Westinghouse Electric Corporation, Pittsburgh 35, Pennsylvania

(Received March 19, 1958)

The relaxation of a nearly plane surface to flatness is discussed under the assumption that all surface properties are independent of orientation. A general solution is obtained for the combined action of the transport processes of viscous flow, evaporation-condensation (in a closed system), volume diffusion, and surface diffusion. Green's function solutions are developed for each of the transport processes separately, and criteria are obtained to decide which process dominates. The initial forms of these solutions represent point concentrations (particles), or line concentrations (wires) of material set upon an infinite plane. The progressive topographical developments described by the formulas are idealized representations of the latter stages of the sintering of small wires and particles to a plane.

FIG. 1. (a) A portion of the surface $z=W(x,y,t)$ undergoing decay to flatness. (b) Section of a wire showing the troughs predicted to develop during sintering onto a plane.

Physical Derivation of Surface Diffusion

- **Conservation law: (*J* is the flux)**

$$\mathbf{V_n}(\mathbf{t}) = -\frac{\partial}{\partial \mathbf{x}}\mathbf{J}(\mathbf{x},\mathbf{t})$$

- **Fick's Law:**

$$\mathbf{J}(\mathbf{x},\mathbf{t}) = -\mathbf{D}\frac{\partial}{\partial \mathbf{x}}\mu(\mathbf{x},\mathbf{t})$$

  where $\mu(\mathbf{x},\mathbf{t})$ is the **chemical potential** on the surface and D is the surface diffusion coefficient.

- **Chemical Potential = the mean curvature *H*:**

$$\mu = \mathbf{H}$$

- The above leads to the following **Surface Diffusion Equation**:

$$\mathbf{V_n} = -\mathrm{div}(\mathbf{D}\nabla\mathbf{H}) \sim -\triangle_{\mathbf{S}}\mathbf{H}$$

Gradient Flows: L^2 vs H^{-1}

Given a **surface energy integrand** $\gamma : \mathbf{S^1} \to \mathbb{R}^+$, and a **set** $\mathbf{K} \subset \mathbb{R}^{\mathbf{2}}$,

Surface (Area) Energy:

$$\mathbf{E}(\partial\mathbf{K}) = \int_{\partial\mathbf{K}} \gamma(\hat{\mathbf{n}})\,\mathbf{ds}$$

First Variation of E: (g is some test function.)

$$\delta\mathbf{E}(\partial\mathbf{K})(\mathbf{g}) = \frac{\mathbf{d}}{\mathbf{dt}}\mathbf{E}(\partial\mathbf{K} + \mathbf{tg})\Big|_{\mathbf{t=0}} = \int_{\partial\mathbf{K}} \langle -\mathbf{H}_\gamma\hat{\mathbf{n}}, \mathbf{g}\rangle\,\mathbf{ds},$$

i.e.

$$\text{“}\delta\mathbf{E}(\partial\mathbf{K}) = -\mathbf{H}_\gamma\text{”}$$

Gradient Flows: L^2 vs H^{-1} (J. Taylor)

L^2-**Gradient of Energy**:

$$\delta\mathbf{E}(\partial\mathbf{K})(\mathbf{g}) = \int_{\partial\mathbf{K}} \langle -\mathbf{H}_\gamma \hat{\mathbf{n}}, \mathbf{g}\rangle \, \mathbf{ds} = \langle -\mathbf{H}_\gamma \hat{\mathbf{n}}, \mathbf{g}\rangle_{\mathbf{L^2(\partial K)}}$$

Identify:

$$\langle \nabla_{\mathbf{L^2}}\mathbf{E}, \mathbf{g}\rangle_{\mathbf{L^2(\partial K)}} = \langle -\mathbf{H}_\gamma \hat{\mathbf{n}}, \mathbf{g}\rangle_{\mathbf{L^2(\partial K)}}$$

which gives

$$\nabla_{\mathbf{L^2}}\mathbf{E} = -\mathbf{H}_\gamma.$$

L^2-**Negative Gradient Flow:**

$\mathbf{V_n} = -\nabla_{\mathbf{L^2}}\mathbf{E} = \mathbf{H}_\gamma$: **Motion by Mean Curvature (MMC)**

(Evaporation-condensation mechanism)

Gradient Flows: L^2 vs H^{-1} (J. Taylor)

H^{-1}-Gradient of Energy: **identify**

$$\delta \mathbf{E}(\partial \mathbf{K})(\mathbf{g}) = \langle -\mathbf{H}_\gamma, \mathbf{g}\rangle_{\mathbf{L^2(\partial K)}} = \langle \nabla_{\mathbf{H^{-1}}}\mathbf{E}, \mathbf{g}\rangle_{\mathbf{H^{-1}(\partial K)}},$$

where

$$\langle \mathbf{f}, \mathbf{g}\rangle_{\mathbf{H^{-1}}} = \int \langle \nabla^{-1}\mathbf{f}, \nabla^{-1}\mathbf{g}\rangle = \int \left((-\triangle^{-1})\mathbf{f}\right)\mathbf{g}$$

which gives

$$\langle \nabla_{\mathbf{H^{-1}}}\mathbf{E}, \mathbf{g}\rangle_{\mathbf{H^{-1}(\partial K)}} = \left\langle (-\triangle)^{-1}(\nabla_{\mathbf{H^{-1}}}\mathbf{E}), \mathbf{g}\right\rangle_{\mathbf{L^2(\partial K)}} = \langle -\mathbf{H}_\gamma, \mathbf{g}\rangle_{\mathbf{L^2(\partial K)}}.$$

$$(-\triangle)^{-1}(\nabla_{\mathbf{H^{-1}}}\mathbf{E}) = -\mathbf{H}_\gamma, \quad \text{i.e.} \quad \nabla_{\mathbf{H^{-1}}}\mathbf{E} = \triangle \mathbf{H}_\gamma.$$

H^{-1}-Negative Gradient Flow

$$\mathbf{V_n} = -\nabla_{\mathbf{H^{-1}}}\mathbf{E} = -\triangle \mathbf{H}_\gamma : \qquad \textbf{Surface Diffusion (SD)}.$$

Gradient Flows: L^2 vs H^{-1}

L^2-Gradient Flow (Motion by Mean Curvature)

- $\mathbf{V_n} = -\nabla_{\mathbf{L^2}}\mathbf{E} = \mathbf{H}_\gamma$.
- $\frac{d}{dt}E(\partial K_t) = -\int_{\partial K} H_\gamma^2 ds < 0$ (energy decreasing in time)
- The equation is 2^{nd}-order, quasi-linear parabolic.
- The equation enjoys maximum principle.

Grayson-Hamilton, Gage, . . . : curves in $\mathbf{R}^2$;
Ecker-Huisken, . . . : surfaces, graphs, singularity characterization;
Almgren-Taylor-Wang, Luckhaus-Sturzenhacker: variational approach

Gradient Flows: L^2 vs H^{-1}

H^{-1}-**Gradient Flow (Surface Diffusion)**

- $\mathbf{V_n = -\nabla_{H^{-1}} E = -\triangle_s H_\gamma}$.
- $\frac{d}{dt}E(\partial K_t) = -\int_{\partial K} |\nabla_s H_\gamma|^2 ds < 0$. (energy decreasing in time)
- $\frac{d}{dt}\mathrm{Area}(K_t) = \int_{\partial K} V_n \, ds = \int_{\partial K} -\triangle H \, ds = 0$ (area preserving).
- The equation is 4th-order, quasi-linear parabolic.
- The equation does not satisfy maximum principle.

Elliott-Garcke, Escher-Simonett: local existence;
Cahn-Elliott-Novick-Cohen: phase field formulation;
Bertozzi-Bernoff-Witelski:
simulation (axisymmetric) of singularity formation;
Chung: variational approach

Crystalline Motion of Polygons

Now we restrict our attention to the:

Motion of Polygonal Shapes in $\mathbb{R}^2$:

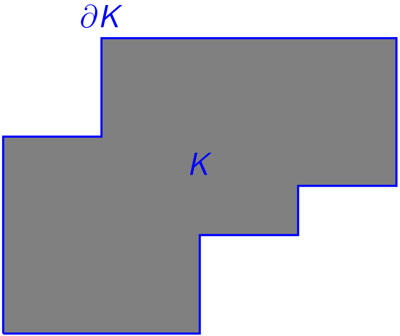


Figure: Example of a Polygonal Shape.

Crystalline Motion of Polygons

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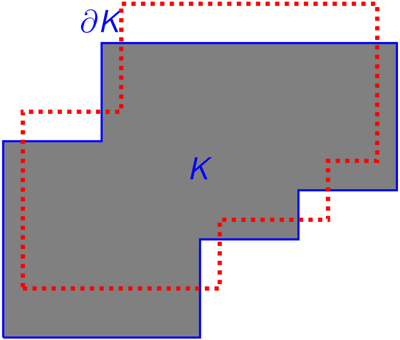
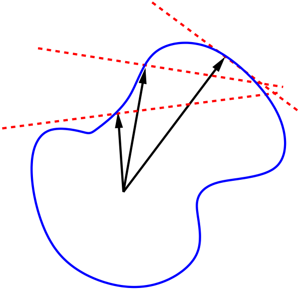


Figure: Example of a Crystalline Motion.

Surface Energy and Wulff Shape

Surface Energy: $\mathbf{E}_\gamma(\partial\mathbf{K}) = \int_{\partial\mathbf{K}} \gamma(\hat{\mathbf{n}})\,\mathbf{ds}$

Wulff Shape: $\mathbf{W}_\gamma = \{\mathbf{x} : \langle \mathbf{x}, \hat{\mathbf{n}}\rangle \ \leq \ \gamma(\hat{\mathbf{n}}) \text{ for all } \hat{\mathbf{n}}\}$.

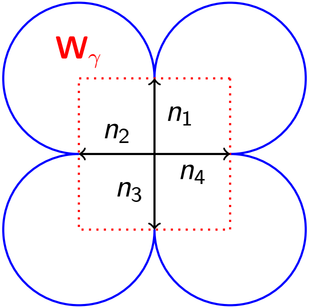


(Rescaled) W_γ **solves the (anisotropic) isoperimetric problem**:

$$\min_{\partial\mathbf{K}} \mathbf{E}_\gamma(\partial\mathbf{K}) \ \text{ with } \ \mathbf{Area}(\mathbf{K}) = \mathbf{1}.$$

Crystalline Wulff Shape

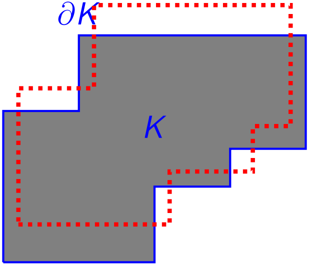
Often the **surface energy integrand** γ can have **deep inward cusps**. In this case, the **Wulff shape** W_γ **will be facetted**. For example,



where $\{\mathbf{n_i}\}$ is a set of **low energy directions** for E.

Crystalline Motion

Hence we expect that the **low energy directions will be preserved during motions**:



Question: How to formulate such a motion in a mathematically consistent way?

Total Variation Flow (TV flow)

Consider a graph given by a function $u(x, t)$.

Total Variation (TV) Norm:

$$\mathbf{E}(\mathbf{u}) = \int_{\mathbf{\Omega}} |\nabla \mathbf{u}| \ \mathbf{dx}.$$

L^2 **TV-flow** (Rudin-Osher-Fatemi, Giga-Kobayahi):

$$\mathbf{u_t} = -\nabla_{\mathbf{L^2}} \mathbf{E}(\mathbf{u}) = \mathrm{div}\left(\frac{\nabla \mathbf{u}}{|\nabla \mathbf{u}|}\right)$$

H^{-1} **TV-flow** (Giga-Kohn, Giga-Giga, Kashima, Osher-Sole-Vese):

$$\mathbf{u_t} = -\nabla_{\mathbf{H^{-1}}} \mathbf{E}(\mathbf{u}) = -\triangle\left(\mathrm{div}\frac{\nabla \mathbf{u}}{|\nabla \mathbf{u}|}\right)$$

Subdifferential and Canonical Restriction

Let X be a real Banach space and X^* be its the dual space. $\langle f, x\rangle$ is the duality pairing of X^* and X for $f \in X^*$ and $x \in X$.

Definition

Given $E : X \longrightarrow (-\infty, +\infty]$, a convex function. For $u \in X$,

Subdifferential of E at u, denoted by $\partial \mathbf{E}(\mathbf{u})$, is defined by

$$\partial E(u) = \{f \in X^* \mid E(u+x) - E(u) \geq \langle f, x\rangle \quad \text{for all } x \in X\}$$

Canonical Restriction of $\partial E(u)$, denoted by $\partial^{\mathbf{c}}\mathbf{E}(\mathbf{u})$, is the element with the minimum norm:

$$||\partial^c E(u)|| = \min_{f \in \partial E(u)} ||f||.$$

General Theory of Negative Gradient Flow

Consider the equation:

$$\begin{cases} u_t \in -\partial E(u) & , \\ u_{|_{t=0}} = u_0 \end{cases}$$

From the general theory of nonlinear semigroup, there is a unique solution satisfying

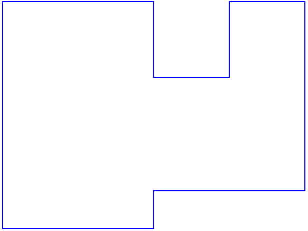
$$\begin{cases} u_t = -\partial^c E(u) & , \\ u_{|_{t=0}} = u_0 \end{cases}$$

Goal: to identify $\partial^c E(u)$.

Crystalline Motion by Mean Curvature (L^2-Gradient Flow)

Assume the **Wulff shape W_γ is a unit square**.

$\mathbf{K} \subset \mathbb{R}^2$:



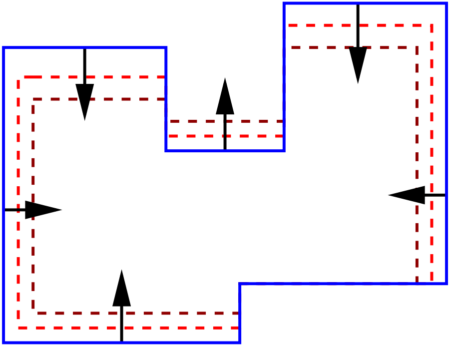
(Angenent-Gurtin, Taylor)

Crystalline Curvature: $\kappa_i = -\dfrac{\sigma_i}{L_i}$.

Motion by Mean Crystalline Curvature: $v_i = \kappa_i = \dfrac{\sigma_i}{L_i}$,

$$\text{where} \quad \sigma_i = \begin{cases} 1\ (-1), & \text{if the } i^{th} \text{ facet is convex (concave),} \\ 0, & \text{otherwise.} \end{cases}$$

Crystalline Motion by Mean Curvature (L^2-Gradient Flow)



- Convex facet moves in;
- Concave facet moves out;
- Staircase facet does not move;
- **No splitting of facets** (in $\mathbf{R}^2$)

Crystalline Surface Diffusion (H^{-1}-Gradient Flow)

Heuristic Derivation of Motion (Carter-Roosen-Cahn-Taylor)

- **Conservation law: (J is the flux)**

$$\mathbf{v_i(t)} = -\frac{\partial}{\partial \mathbf{x}}\mathbf{J_i(x,t)} = \text{constant}(\text{t})$$

  Velocity on each facet is assumed to be a constant.

- **Fick's Law:**

$$\mathbf{J_i(s,t)} = -\mathbf{D_i}\frac{\partial}{\partial \mathbf{s}}\mu_{\mathbf{i}}\mathbf{(s,t)}$$

  where $\mu_{\mathbf{i}}\mathbf{(s,t)}$ is the **chemical potential** of the i^{th} facet, and $D_i =$ the surface diffusion coefficient.

- **Average chemical potential** $\mu_i =$ **crystalline curvature,** i.e.

$$\frac{\mathbf{1}}{\mathbf{L_i}}\int_{\mathbf{0}}^{\mathbf{L_i}}\mu_{\mathbf{i}}\mathbf{(s)dx} = \kappa_{\mathbf{i}} = \frac{\sigma_{\mathbf{i}}}{\mathbf{L_i}}$$

- **Continuity of flux and chemical potential across corners.**

Crystalline Surface Diffusion (H^{-1}-Gradient Flow)

Heuristic Derivation of Motion (Carter-Roosen-Cahn-Taylor)

The above formulation gives the following explicit formula for the velocity:

$$\mu_i(s,t) = \mu_i - \frac{J_i}{D_i}s + \frac{v_i}{2D_i}s^2.$$

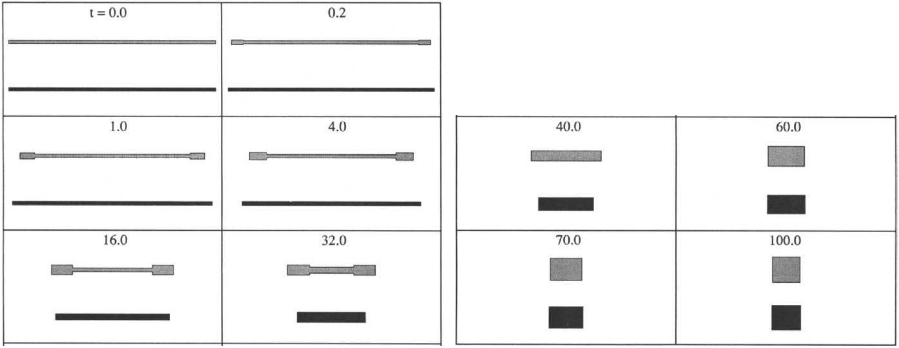
$$\mu_{i+1} = \mu_i - \frac{J_i}{D_i}L_i + \frac{v_i}{2D_i}L_i^2, \quad J_{i+1} = J_i - v_i L_i,$$

$$\mathbf{v_i} = \frac{\mathbf{6D_i}(\kappa_{\mathbf{i}}^{\gamma} - \mu_{\mathbf{i}}) + \mathbf{3J_iL_i}}{\mathbf{L_i^2}}.$$

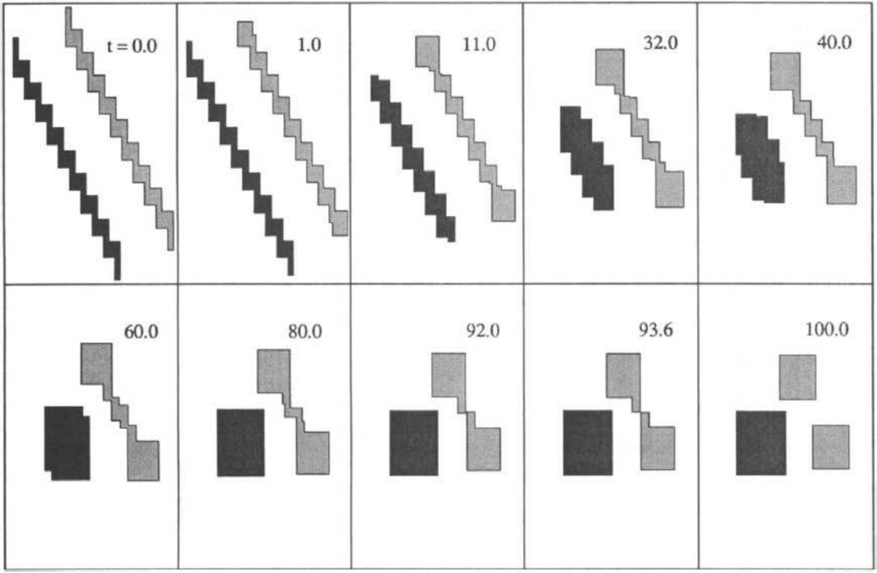
Note: $\sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{v_i L_i} = \mathbf{0}$ (**area preserving**).

Crystalline Surface Diffusion (H^{-1}-Gradient Flow)

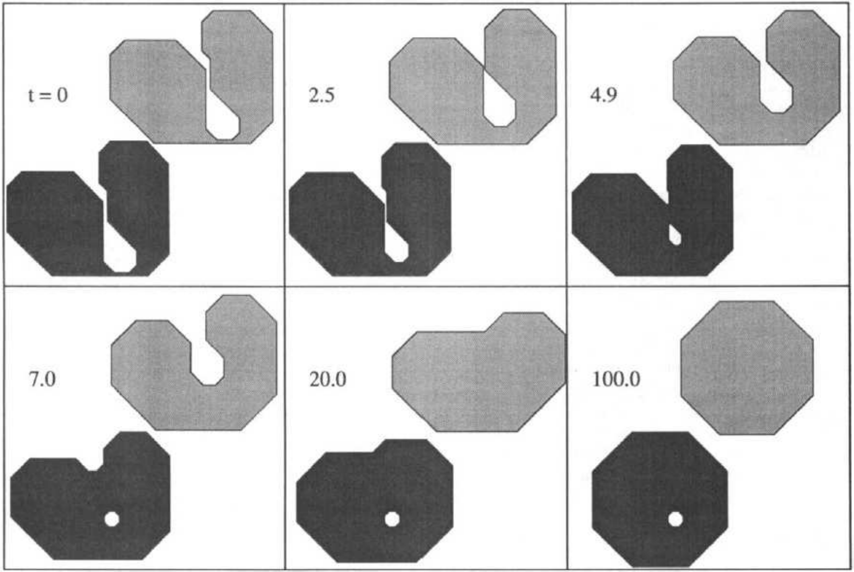
Examples of Crystalline Surface Diffusion (CRCT)



Crystalline Surface Diffusion (H^{-1}-Gradient Flow)



Crystalline Surface Diffusion (H^{-1}-Gradient Flow)



Subdifferential of Crystalline Surface Energy

Assume the **Wulff shape W_γ is a unit square**.

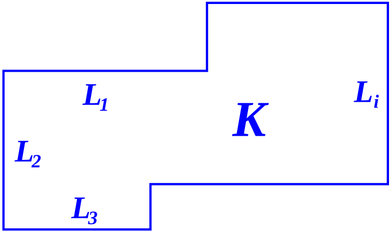
Then the **Surface Energy w.r.t γ** is defined by

$$\mathbf{E}(\partial \mathbf{K}) = \int_{\partial \mathbf{K}} \gamma(\hat{\mathbf{n}})\, \mathbf{ds}$$

For a **polygon ∂K with N facets**, $\mathbf{E}(\partial \mathbf{K})$ is simply (proportional to) the **length of ∂K**:

$$\mathbf{E}(\partial \mathbf{K}) = \frac{1}{2}\sum_{i=1}^{N} \mathbf{L_i}$$

where L_i is the length of the i^{th} facet.



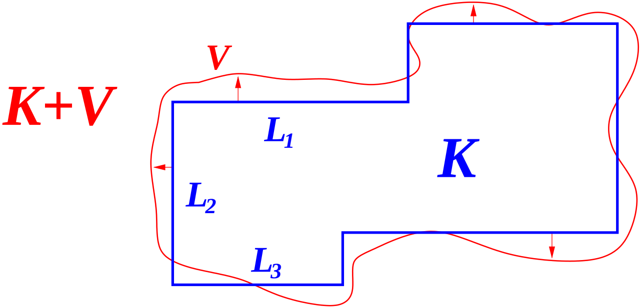
Subdifferential of Crystalline Surface Energy

Recall

$$\mathbf{f} \in \partial_{\mathbf{H}^{-1}} \mathbf{E}(\partial \mathbf{K}) \Longleftrightarrow \mathbf{E}(\partial \mathbf{K} + \mathbf{V}) - \mathbf{E}(\partial \mathbf{K}) \geq \langle \mathbf{f}, \mathbf{V} \rangle_{\mathbf{H}^{-1}}$$

for all $V \in H^{-1}(\partial K)$. (Note that $\int_{\partial K} V$ and $\int_{\partial K} f$ are both zero.)

As a simplification, we consider **both V and f can be written as a graph over ∂K**:



Subdifferential of Crystalline Surface Energy

Then

$$\mathbf{E}(\partial\mathbf{K}+\mathbf{V})-\mathbf{E}(\partial\mathbf{K}) \approx \frac{1}{2}\left[\sum_{i=1}^{N}\int_{(0,L_i)}|(\mathbf{V}_i)_x|\,ds+\sigma_i^0\mathbf{V}_i(0)+\sigma_i^1\mathbf{V}_i(L_i)\right]$$

(where $\sigma_i^{0,1}=1\ (-1)$ if it is a convex (concave) corner.)

Hence $\mathbf{f}\in\partial_{H^{-1}}\mathbf{E}(\partial\mathbf{K})$ if and only if for all V,

$$\frac{1}{2}\left[\sum_{i=1}^{N}\int_{(0,L_i)}|(\mathbf{V}_i)_x|\,ds+\sigma_i^0\mathbf{V}_i(0)+\sigma_i^1\mathbf{V}_i(L_i)\right]\geq\ \langle\mathbf{f},\mathbf{V}\rangle_{H^{-1}}$$

(note the appearance and similarity to the TV-norm.)

Characterization of $\partial_{H^{-1}} E(\partial K)$

Define:

$$\mathbf{\Phi(V) = \frac{1}{2}\left[\sum_{i=1}^{N}\int_{(0,L_i)} |(V_i)_x| ds + \sigma_i^0 V_i(0) + \sigma_i^1 V_i(L_i)\right]}$$

i.e. we identify $\partial_{\mathbf{H}^{-1}}\mathbf{E}(\partial\mathbf{K})$ with $\partial_{\mathbf{H}^{-1}}\mathbf{\Phi}(\mathbf{0})$.

Theorem

$f \in \partial_{H^{-1}}\Phi(0) \iff \exists\{\tilde{\eta}_i\}$, $\tilde{\eta}_i$ *defined on the* i^{th} *facet such that*

1) $f = (\tilde{\eta}_i)_{xxx}$ *on* $[0, L_i]$.
2) $\tilde{\eta}_i(0) = \sigma_i^0, \quad \tilde{\eta}_i(L_i) = -\sigma_i^1$.
3) $|\tilde{\eta}_i(x)| \leq 1$ *on* $[0, L_i]$.
4) $(\tilde{\eta}_i)_x(L_i) = (\tilde{\eta}_{i+1})_x(0)$.

Characterization of $\partial_{H^{-1}} E(\partial K)$

- $(\tilde{\eta}_i)_x$ is the chemical potential;
- $(\tilde{\eta}_i)_{xx}$ is the flux along the facet;
- $(\tilde{\eta}_i)_{xxx} = f$ is the normal velocity of the facet;
- $(\tilde{\eta}_i)_x(L_i) = (\tilde{\eta}_{i+1})_x(0)$ gives the continuity of chemical potential across each corner.

Characterization of $\partial^c_{H^{-1}} E(\partial K)$

Let $f^0 = \partial^c_{H^{-1}} E(\partial K)$. Then $f^0_i = (\tilde{\eta}_i)_{xxx}$ and

$$\|\mathbf{f^0}\|^2_{\mathbf{H^{-1}}} = \min_{\tilde{\zeta}} \sum_{\mathbf{i=1}}^{\mathbf{N}} \|(\tilde{\zeta}_{\mathbf{i}})_{\mathbf{xxx}}\|^2_{\mathbf{H^{-1}}} = \min_{\tilde{\zeta}} \sum_{\mathbf{i=1}}^{\mathbf{N}} \|(\tilde{\zeta}_{\mathbf{i}})_{\mathbf{xx}}\|^2_{\mathbf{L^2}}.$$

Note that $\tilde{\zeta}_i$'s satisfy the following **boundary conditions**:

$$\tilde{\zeta}_{\mathbf{i}}(\mathbf{0}) = \sigma^{\mathbf{0}}_{\mathbf{i}}, \ \ \tilde{\zeta}_{\mathbf{i}}(\mathbf{L_i}) = -\sigma^{\mathbf{1}}_{\mathbf{i}}, \ \ |\tilde{\zeta}_{\mathbf{i}}(\mathbf{x})| \leq \mathbf{1}, \quad [\tilde{\zeta}_{\mathbf{x}}]_{\mathbf{i}} = \mathbf{0}.$$

The **minimzer** $\{\tilde{\eta}_i\}$ **satisfies the "Euler-Lagrange Condition"**:

$$(\tilde{\eta}_{\mathbf{i}})_{\mathbf{xxxx}} \text{``}=\text{''} \mathbf{0}$$

together with the B.C. and $\{-\mathbf{1} \leq \tilde{\eta}_{\mathbf{i}}(\mathbf{x}) \leq \mathbf{1}\}$.

"Regularity" Properties of $\partial^c_{H^{-1}} E(\partial K)$

Let K **be a (finite) polygonal shape**.

Then we have the following properties for $\partial^{\mathbf{c}}_{\mathbf{H^{-1}}}\mathbf{E}(\partial\mathbf{K}) = \tilde{\eta} = \{\tilde{\eta}_{\mathbf{i}}\}$:

1. Existence and uniqueness of $\partial^c_{H-1}E(u)$.
2. The function $\tilde{\eta}_{xx}$ is continuous throughout the whole ∂K, in the interior of each facet and also across each corner. i.e. $[\tilde{\eta}_{xx}] = 0$. (Continuity of flux)
3. **If on a facet, $\{-\mathbf{1} < \tilde{\eta}_{\mathbf{i}}(\mathbf{x}) < \mathbf{1}\}$, then $\tilde{\eta}_i$ is a single cubic polynomial on that facet**:

$$(\tilde{\eta}_{\mathbf{i}})_{\mathbf{xxxx}} = \mathbf{0} \quad \Longrightarrow \quad \tilde{\eta}_{\mathbf{i}} = \mathbf{A}\mathbf{x}^{\mathbf{3}} + \mathbf{B}\mathbf{x}^{\mathbf{2}} + \mathbf{C}\mathbf{x} + \mathbf{D}$$

The Case with No Splitting $(-1 < \tilde{\eta}_i(x) < 1)$

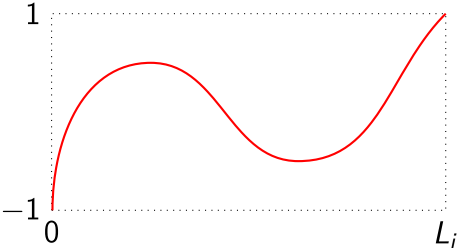
Recall $\mathbf{f^0} = \partial^{\mathbf{c}}_{\mathbf{H}^{-1}}\mathbf{E}(\partial\mathbf{K}) = (\tilde{\eta}_{\mathbf{i}})_{\mathbf{xxx}}$ so that

$-(\tilde{\eta}_i)_{xxx}$ is the velocity of each facet.

If $\{-\mathbf{1} < \tilde{\eta}_{\mathbf{i}}(\mathbf{x}) < \mathbf{1}\}$, then $\tilde{\eta}_i$ is a single cubic polynomial on a facet:

$$\tilde{\eta}_{\mathbf{i}} = \mathbf{Ax^3} + \mathbf{Bx^2} + \mathbf{Cx} + \mathbf{D}$$

implying that the **whole facet moves with one single speed**, i.e. **there is no splitting of the facet**:



$\tilde{\eta}(0) = -1$ and $\tilde{\eta}(L_i) = 1$

The Case with No Splitting $(-1 < \tilde{\eta}_i(x) < 1)$

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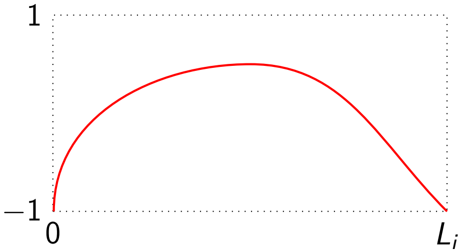
implying that the **whole facet moves with one single speed**, i.e. **there is no splitting of the facet**:



$\tilde{\eta}(0) = -1$ and $\tilde{\eta}(L_i) = -1$

Connection to Carter-Rooson-Taylor-Cahn

1. Let $\mu = \frac{1}{2}\tilde{\eta}_{\mathbf{x}}$ (**chemical potential**). Then

$$\int_0^{L_i} \mu\, dx = \int_0^{L_i} -\frac{1}{2}(\tilde{\eta}_i)_x\, dx = 1 \quad \text{(as an example)}$$

$$\text{so that} \quad \frac{1}{L_i}\int_0^{L_i} \mu\, dx = \frac{1}{L_i} = \kappa_i$$

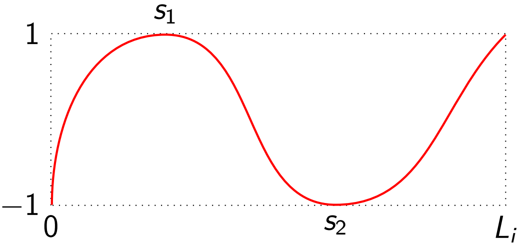
2. Let $\mathbf{J} = -\mu_{\mathbf{x}}$ (**flux**).
3. Then $\mathbf{v} = -\mathbf{J}_{\mathbf{x}} = -\mu_{\mathbf{xx}} = -\tilde{\eta}_{\mathbf{xxx}}$ is the **velocity of the facet**.

   (If $\tilde{\eta}$ is a single cubic polynomial on the whole facet, then **the velocity is a constant on the facet, i.e. no splitting**.)

Splitting Phenomena ($\tilde{\eta} = \pm 1$)

However, it is possible that on some facet,

there exists an $s \in (0, L_i)$ such that $\tilde{\eta}_i(s) = 1$ or $\tilde{\eta}_i(s) = -1$.



In this case, $\tilde{\eta}$ might not be a single cubic polynomial. Then $(\tilde{\eta}_i)_{xxx}$ **can be discontinuous at the s_i's, so that splitting can occur**.

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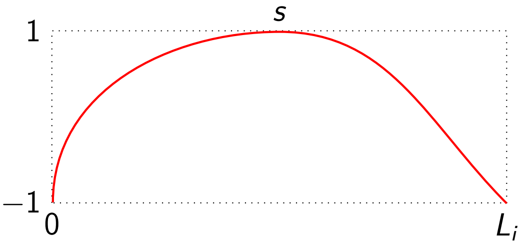
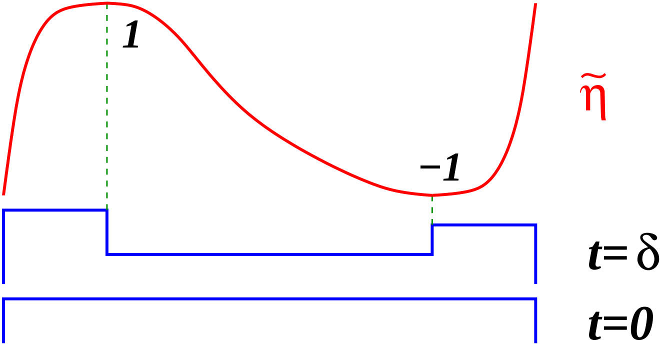


In this case, $\tilde{\eta}$ might not be a single cubic polynomial. Then $(\tilde{\eta}_i)_{xxx}$ **can be discontinuous at the s_i's, so that splitting can occur**.

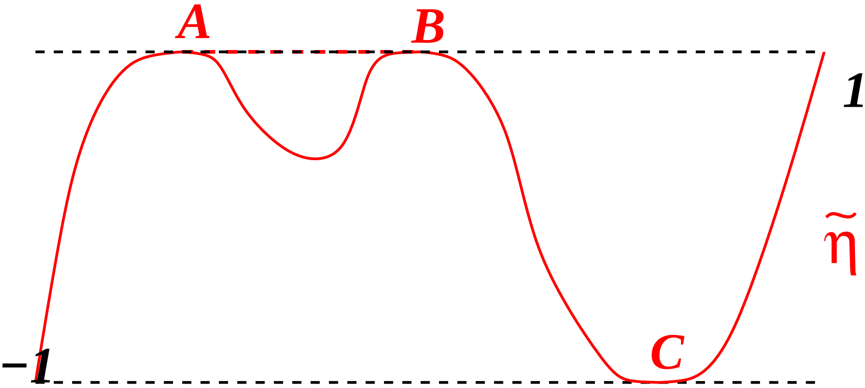
Properties at Splitting Points: $\tilde{\eta}(s) = \pm 1$

- $\tilde{\eta}_x(s) = 0$ and $\tilde{\eta}_{xx}(s^+) = \tilde{\eta}_{xx}(s^-)$.
- If $\tilde{\eta}_i(s) = 1$, then $-\tilde{\eta}_{xxx}(s^-) \geq -\tilde{\eta}_{xxx}(s^+)$.
- If $\tilde{\eta}_i(s) = -1$, then $-\tilde{\eta}_{xxx}(s^-) \leq -\tilde{\eta}_{xxx}(s^+)$.



Properties at Splitting Points: $\tilde{\eta}(s) = \pm 1$

- There can be **at most two** splitting locations on each facet.



Further Properties of $\partial^c_{H^{-1}} E(\partial K)$

1. If all the lengths of polygons are all positive, then $\mathbf{\partial^c_{H^{-1}} E(\partial K)}$ is **stable** in the following sense:

$$\|\partial^c_{H^{-1}} \mathbf{E}(\partial \mathbf{K}_1) - \partial^c_{H^{-1}} \mathbf{E}(\partial \mathbf{K}_2)\| \leq \mathbf{C} \, \|\partial \mathbf{K}_1 - \partial \mathbf{K}_2\|$$

2. If at the splitting location, $\tilde{\eta}_{\mathbf{xx}}(\mathbf{s}) \neq \mathbf{0}$, then there is **no "avalanche"** of splitting. Hence in a sense, **the splitting phenomena is stable**.

3. In principle, if $\tilde{\eta}_{\mathbf{xx}}(\mathbf{s}) = \mathbf{0}$, then there can be a **continuum sequence** of splitting events.

Some Open Problems

Time-Stepping Variational Scheme.

Given $\partial \mathbf{K_i}$, find $\partial \mathbf{K_{i+1}} = \partial \mathbf{K_i} + \mathbf{v_{i+1}}$ such that $\mathbf{v_{i+1}}$ minimizes the following energy functional:

$$\min_{\mathbf{v}} \mathbf{E}(\partial \mathbf{K_i} + \mathbf{v}) + \frac{1}{2\triangle t}\|\mathbf{v}\|^2_{\mathbf{H}^{-1}}$$

This gives a sequence $\mathbf{K_0} \to \mathbf{K_1} \to \mathbf{K_2} \to \dots$

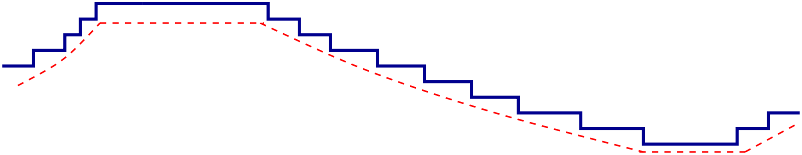
Establish the convergence and the connection to the subdifferential formulation and canonical restriction.

- The convergence of the above scheme and its connection to the subdifferential formulation are fairly well established for motion by mean curvature
  (Almgren-Taylor-Wang, Luckhaus-Sturzenhacker).
- But for surface diffusion, it is quite open (Chung).

Some Open Problems

Surfaces in Three Dimensions. In this case, the structure and regularity of $\partial^c_{H^{-1}} E$ can be quite intricate. Even for motion by mean curvature, continuum splitting of facets can occur.

Connection and Derivation from Microscopic Models, such as epitaxial thin film growth.
(Spohn, Margetis, Kohn, Schulze, E, Xiang, Yip, ...)



Thank you for your attention.