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Abstracts of
Sapporo Symposium on Anisotropic Effects
in a Crystal Growth Problem and
its Mathematical Analysis (SAM)

Sapporo, January 11–15, 1999

Edited by Y. Giga and R. Kobayashi

Sapporo, 1999

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Preface

Sapporo Symposium on Anisotropic Effects in a Crystal Growth Problem and its Mathematical Analysis (SAM) was held in Sapporo from January 11 to 15, 1999. The organizing committee consisted of Y. Giga, R. Kobayashi and R. Kohn (who was unable to come to SAM). The symposium SAM focused anisotropic crystal growth phenomena with special emphasis on motion with facets. Although the topic looks not broad, there are huge variety of lectures since the lecturers include mathematical analysis, numerical analysis, experimental physicists, theoretical physicists and people working on mathematical modelling. The activity of SAM consisted of 16 lectures with 2 short presentations by experimental physicists as well as 4 organized discussion sessions. Besides these activities there is a tour to the laboratory of Professor Furukawa. There are so many interesting lectures and exciting discussions. We thank all participants for their contribution to SAM. This note includes extended abstracts of lectures as well as comments on discussion session. We thank all contributors for their submission of abstracts. We do hope this helps your further research.

We would like to thank Professor Yoshinori Furukawa who helps organization of SAM both financially and scientifically. We would like to thank also his colleague for introducing the laboratory of Professor Furukawa to participants of SAM. We would like to thank Mr. Kazuhiko Hiramatsu who showed an interesting experiment to create snow flakes in a bottle.

We would like to thank Dr. Mi-Ho Giga and Sapporo City Volunteers Ms. Y. Kataoka and Ms. K. Tamari for their practical help for visitors from abroad. We are grateful to Sapporo International Communication Plaza for their suggestion to SAM. We are also grateful to Keio Plaza Hotel for their cooperation. We would like to thank Ms. Toshiko Watanabe for her secretary work for SAM. We are grateful to Dr. K. Yokoyama, Mr. K. Yama-uchi, Mr. Y. Kohsaka for forming a very efficient reception desk. Finally, we thank undergraduate students assisting works of reception desk as well as other students helping to set up symposium room for SAM.

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Sapporo, March 1999

Yoshikazu Giga and Ryo Kobayashi

**Sapporo Symposium on
Anisotropic Effects in a Crystal
Growth Problem and its
Mathematical Analysis (SAM)**

Organizers: Y. Giga, R. Kobayashi (Hokkaido U.)
International organizer: R. Kohn (Courant Institute)
Place of symposium : January 11-14
Centennial Hall
(百年記念会館, Hyakunen-Kinen-Kaikan) (basement),
Hokkaido University
(Kita 9-Jo Nishi 5-Chome, Kita-Ku, Sapporo 060-0809)
January 15
"Rose Room", Keio Plaza Hotel (2nd floor)
(Kita 5-Jo Nishi 7-Chome, Chuo-Ku, Sapporo 060-0005)

January 11, 1999 Morning session starts from 10:30

Lecturers Y. Furukawa (Hokkaido U.)
M.-H. Giga (Hokkaido U.)

Afternoon session starts from 14:30

Lecturers J. Wettlaufer (U. Washington)
M. Uwaha (Nagoya U.)
N. Ishimura (Hitotsubashi U.)

January 12, 1999 Morning session starts from 10:00

Lecturers A. A. Wheeler (U. Sorthampton)
M. Paolini (U. Cattolica del Sacro Cuore)

Afternoon session starts from 14:00

Lecturers C. M. Elliott (U. Sussex)
A. R. Roosen (NIST)

Discussion

January 13, 1999 Morning session starts from 10:00

Lecturers P. S. Smereka (U. Michigan)
M. Suzuki (U. Electro-Communications)
(short communication)

Discussion

Afternoon: Tour to the laboratory of Prof. Furukawa

January 14, 1999 Morning session starts from 10:00

Lecturers P. Rybka (Warsaw U.)
N. A. Yip (U. Wisconsin)

Afternoon session starts from 14:00

Lecturers J. S. Warren (NIST)
R. Kobayashi (Hokkaido U.)

Discussion

January 15, 1999 Morning session starts from 10:00

Lecturers B. Mutaftschiev (Tokushima U. / U. Paris VI)
K. Tsukamoto (Tohoku U.) (short communication)

Discussion

Y. Giga (Hokkaido U.)

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Double obstacle phase field models and interfacial diffusion

C. M. Elliott (University of Sussex)

This talk considered field phase models with a bistable homogeneous 'W' energy potential of double obstacle form, i.e.

$$W(\phi) := 1 - \phi^2 \quad |\phi| \leq 1$$

$$W(\phi) := \infty \quad |\phi| > 1$$

When coupled with gradient energies via energy functionals of the form

$$\int_{\Omega} [\varepsilon A(\nabla\phi) + \frac{1}{\varepsilon} W(\phi)] dx$$

one obtains diffuse interface approximations of anisotropic surface energy with the diffuse interface, having finite thickness bounded by $C\varepsilon$, separating regions where ϕ is identically plus one or minus one. This has significant computational advantages over the smooth double well potential for which the diffuse interface is not of exactly finite width. This double obstacle phase field approach was introduced independently by, on the one hand, Elliott, Blowey and Xinfu Chen and on the other by Paolini, Verdi and Nochetto.

Numerical algorithms which exploit this idea involve storage and computation only on a narrow discrete interface. Topological changes are automatically handled. Many calculations have been performed in the context of mean curvature flow, anisotropic mean curvature flow, crystalline curvature flow, dendritic growth, phase separation etc. Convergence results have been established as $\varepsilon \rightarrow 0$ to classical sharp interface solutions (when they are valid) and to 'viscosity' solutions which have topological changes. See the works of the above names. In this talk some computations were presented. Furthermore models involving enhanced diffusion within the interface were described. Here one might consider diffusion equations of the form

$$\varepsilon u_t = \nabla(m(\phi)\nabla\mu)$$

where $m(\phi) := 1 - \phi^2$. Two systems of this type are:

- (i) Degenerate Cahn-Hilliard equation
- (ii) Phase-field model of DIGM.

In the case of (i) the limit equation is the geometric evolution law $\nu := -\pi^2/16k_{ss}$ i.e. motion by the surface Laplacian or surface diffusion.

In the case of (ii), (Diffusion induced grain boundary motion), one obtains a sharp interface model for forced mean curvature flow with a forcing coupled to diffusion along the interface. Some computations were presented which showed excellent agreement with numerical discretisation of the sharp interface models.

Pattern Formation of an Ice Dendrite

Y. Furukawa,

Institute of Low Temperature Science, Hokkaido University, Sapporo, Japan

The growth form of an ice crystal that is freely growing in supercooled bulk water changes from a circular disk to a perturbed disk and finally to a well-developed dendrite with hexagonal symmetry. Many theoretical and experimental studies about the ice crystal growth have been carried out in connection with the general theory of dendrite growth. However, many points remain unsolved and a full understanding has not yet been reached, probably most past investigations have only examined the pattern formation of ice in two dimensions.

In-situ observations of ice crystals grown in supercooled bulk water were carried out using an interferometric optical system(1). Three-dimensional patterns of ice crystals were analyzed using the interference fringes. It was found that morphological instability on the circular disk of the ice crystals starts to develop at the moment that its thickness reaches a critical value and that the instability is independent of the radius of the disk crystal.

On the other hand, one-directional growth experiments of ice crystals were also carried out and the developments of cellular patterns were observed at the interface between ice and KCl solution(2). In this experiment, the tilting of cellular patterns was observed as the functions of the growth rates and the orientations of ice crystals. The tilting of cellular patterns was analyzed on the basis of the linear theory proposed by Coriell and Sekerka(3), and the anisotropy of interfacial kinetics along the interfaces parallel to the c-axis was determined. As a result, the resistance of interfacial kinetics for the ice growth is maximum in the {1010}-faces and minimum in the {1120}-faces.

These experimental results strongly indicate that the hexagonal symmetry in the growth form of ice crystal is dominantly controlled by the anisotropy of interfacial kinetics instead of the anisotropy of interfacial free energy.

References

- (1) W. Shimada and Y. Furukawa, *J. Phys. Chem.*, B 101(1997)6171.
- (2) K. Nagashima and Y. Furukawa, *J. Crystal Growth*, 171(1997)577.
- (3) S.R. Coriell and R. F. Sekerka, *J. Crystal Growth*, 34(1976)157.

Mi-Ho Giga

This is a joint work with Yoshikazu Giga of Hokkaido University. Mathematically, an equilibrium shape of Γ of crystals can be explained by the solution of a *generalized isoperimetric* problem, which minimizes interface energy $I(\Gamma) = \int_{\Gamma} \gamma_0(\mathbf{n}) d\sigma$ by fixing area enclosed by curve Γ . Here \mathbf{n} denotes outer unit normal of Γ , and γ_0 is a given positive function defined on unit circle and corresponds to *surface energy density*. The answer is well-known *Wulff shape* and the result is valid for higher dimensional problem as proved by Taylor, Fonseca and Müller. Wulff shape of γ_0 : Wulff $\gamma_0 = \{\mathbf{p} \in \mathbf{R}^n; \mathbf{p} \cdot \mathbf{n} \leq \gamma_0(\mathbf{m}), |\mathbf{m}| = 1\}$ is the convex conjugate of *Frank diagram* of γ_0 : Frank $\gamma_0 = \{\mathbf{p} \in \mathbf{R}^n; |\mathbf{p}| \leq 1/\gamma_0(\mathbf{p}/|\mathbf{p}|)\}$, where \mathbf{R}^n is the n dimensional Euclidean space. In this talk we assume that Frank γ_0 is convex. If the temperature is higher than the critical temperature called *roughening temperature*, Frank γ_0 is smooth and strictly convex. Otherwise Frank γ_0 has corners, so that Wulff γ_0 has flat portion called *facets*. If Frank γ_0 is a convex polygon, Wulff γ_0 is also a convex polygon and γ_0 is often called *crystalline energy*.

We are interested in evolving curves Γ driven by γ_0 , when Frank γ_0 may have corners. More precisely we assume that $\gamma_0 \in \mathcal{I}$ where $\mathcal{I} = \{\gamma_0 \in C(S^1); \gamma_0 \in C^2(S^1 \setminus \mathcal{N}), \mathcal{N}$ is finite set, second derivative of γ_0 are bounded around $\mathcal{N}\}$. In a crystal growth problem it is often assumed that the free energy E consists of the sum of interface energy I and bulk free energy. The change ratio of E per unit area enclosed by curve Γ is of form

$$\frac{\delta E}{\delta \Gamma} = \Lambda_{\gamma} + C \quad \text{on } \Gamma$$

at least formally where $\Lambda_{\gamma}(\mathbf{n}) = -\text{div}_{\Gamma}(\xi(\mathbf{n}))$, $\gamma(\mathbf{p}) = \gamma_0(\mathbf{p}/|\mathbf{p}|) |\mathbf{p}|$ for $\mathbf{p} \in \mathbf{R}^2$, $\xi = \nabla \gamma$ is Cahn-Hoffman vector, and \mathbf{n} denotes the outer normal of Γ . We assume that C is a constant, which corresponds to a situation when latent heat is negligible. We are interested in well-posedness of the interface equation:

$$(I) \quad V = g(\mathbf{n}, \Lambda_{\gamma} + C) \quad \text{on } \Gamma_t \quad \text{with given initial curve } \Gamma_0,$$

when γ_0 is not necessarily C^1 . Here Γ_t denotes a closed embedded curve in the plane at time $t > 0$, V denotes the normal velocity of Γ_t in the direction of \mathbf{n} , g is a given function in $\mathcal{G} = \{g \in C(S^1 \times \mathbf{R}); g \text{ is nondecreasing in the second variable, } \limsup_{|\lambda| \rightarrow \infty} |g(\mathbf{p}, \lambda)/\lambda| < \infty\}$. If Frank γ_0 has corners it is natural to interpret Λ_{γ}

as nonlocal curvature. The validity of (I) to describe crystal growth problem is a topic of discussion session, especially when the temperature is below the roughening temperature.

To analyze motion of Γ_t we extend the *level set method* (by Chen-Giga-Goto and Evans-Spruck) for non-smooth γ_0 . An equation for a function u on $\mathbf{R}^2 \times (0, \infty)$ is called the *level set equation* of (I) if each level set of a solution u moves by (I) at least for the place where $\nabla u \neq 0$. It is formally written as

$$(L) \quad u_t - |\nabla u|g(\mathbf{n}, \Lambda_{\gamma_0}(\mathbf{n})) = 0 \quad \text{on } \mathbf{R}^2 \times (0, T)$$

with the orientation $\mathbf{n} = -\nabla u/|\nabla u|$ of level set of u . We consider initial value problem of (L) with initial data $u_0 \in \mathcal{K}_\alpha$ with $\alpha \in \mathbf{R}$, where \mathcal{K}_α is the set of continuous function z such that the support of $z - \alpha$ is compact in \mathbf{R}^2 .

For $\gamma_0 \in \mathcal{I}$ we gave a notion of generalized solution of (L) with initial data $u_0 \in \kappa_\alpha$ and showed the *existence and comparison theorem* under a suitable condition, by extending the theory of viscosity solution ([GG3], See also [GG1] and [GG2] for graph case). Moreover we showed

Convergence Theorem. Assume that $\{\gamma_0^\varepsilon\}_{0 < \varepsilon < 1} \subset \mathcal{I}$ and that $\{g_\varepsilon\}_{0 < \varepsilon < 1} \subset \mathcal{G}$. Assume that γ_0^ε converges to γ_0^0 locally uniformly and that g^ε converges to g^0 locally uniformly as ε tends to zero. For $\alpha \in \mathbf{R}$ assume that $u_0^\varepsilon \in \mathcal{K}_\alpha$ converges to $u_0^0 \in \mathcal{K}_\alpha$ locally uniformly. For $0 < \varepsilon < 1$ let u^ε be a generalized solution of (L) with $\gamma_0 = \gamma_0^\varepsilon$ and $g = g^\varepsilon$ and with initial data u_0^ε . Then $u = \lim_{\varepsilon \rightarrow 0} u^\varepsilon$ exists and the convergence is uniform in $\mathbf{R}^2 \times [0, T)$. Moreover u is a generalized solution of (L) with $\gamma_0 = \gamma_0^0$ and $g = g^0$ and with initial data u_0^0 .

As an application we see that nonlocal motion by crystalline energy γ_0^0 by Taylor and Angenent-Gurtin can be approximated by motion by approximate smooth interfacial energy $\gamma_0^\varepsilon \in \mathcal{I}$. The convergence results provides convergence of crystalline algorithm, which yields an extension of results by Girão-Kohn.

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- [GG1] M.-H. Giga and Y. Giga, Evolving graphs by singular weighted curvature, Arch. Rational Mech. Anal., 141(1998), 117-198.
- [GG2] M.-H. Giga and Y. Giga, Stability for evolving graphs by nonlocal weighted curvature, Commun. in Partial Differential Equations, to appear.
- [GG3] M.-H. Giga and Y. Giga, Motion driven by nonlocal curvature in the plane, In: Asymptotics in Nonlinear Diffusive Systems (eds. Nishiura et al), Tohoku Math. Publ. 8(1998), 75-83.

Uniform approximation for anisotropic curvature
flow by the Allen-Cahn equations

Yoshikazu Giga

This is a joint work with Reiner Schätzle of University of Freiburg (Germany). It is well-known that a solution of the mean curvature flow equation (with driving force term u)

$$V = H - u$$

is approximated by the internal layer of a solution of the Allen-Cahn equation

$$\varepsilon \partial_t \varphi_\varepsilon - \varepsilon \Delta \varphi_\varepsilon + \frac{1}{\varepsilon} W'(\varphi_\varepsilon) = c_W u$$

as $\varepsilon \rightarrow 0$, where $W(\sigma) = (\sigma^2 - 1)^2$ is a double well potential and c_W is a certain constant. Here V denotes the normal velocity in the direction of unit normal \mathbf{n} of the interface Γ_t and H denotes the mean curvature of Γ_t in the direction of \mathbf{n} . Its convergence has been proved rigorously in various settings by several authors including Chen, de Mottoni and Schatzmann, Evans, Soner and Souganidis, Bellettini and Paolini, Ilmanen. This convergence result says that the sharp interface model is well approximated by the diffuse interface model.

We now consider an anisotropic mean curvature flow of form

$$\beta(\mathbf{n})V = -\gamma(\mathbf{n})(\operatorname{div} \xi(\mathbf{n}) + u) \tag{1}$$

as a sharp interface model. Here γ denotes an interfacial energy and $\xi = D\gamma$ denote the Cahn-Hoffman vector; $\beta > 0$ denotes the mobility; $\gamma(p)$ and $\beta(p)$ is assumed to be positively homogeneous of degree one and zero on \mathbf{R}^n , respectively. The corresponding diffuse interface model is the anisotropic Allen-Cahn equation

$$\varepsilon \beta(\nabla \varphi_\varepsilon) \partial_t \varphi_\varepsilon - \varepsilon \operatorname{div}(DA(\nabla \varphi_\varepsilon)) + \frac{1}{\varepsilon} W'(\varphi_\varepsilon) = c_W u \tag{2}$$

where $A(p) = \gamma(p)^2/2$, as derived by McFadden, Wheeler and others. The convergence to the sharp interface model (1) has been established by Elliott and Schätzle (in a double obstacle form.)

Our new discovery is that the convergence is uniform with respect to γ and β provided that $\Lambda \leq \gamma(p)/|p| \leq \Lambda^{-1}$, $\Lambda \leq \beta(p) \leq \Lambda^{-1}$, $p \in \mathbf{R}^n$ with some positive constant Λ with

modification of β near $p = 0$ in (2). If we are interested in approximating (1) by (2), it is better that the diffuse interface model (2) is easy to solve. As pointed by Elliott and Schätzle, since β is discontinuous at $p = 0$ unless β is a constant, classical solvability is not expected. We consider

$$\varepsilon \beta^\chi(\nabla \varphi_\varepsilon) \partial_t \varphi_\varepsilon - \varepsilon \operatorname{div}(DA(\nabla \varphi_\varepsilon)) + \frac{1}{\varepsilon} W'(\varphi_\varepsilon) = c_W u \quad (3)$$

with

$$\beta^\chi(p) = \chi(|p|) + (1 - \chi(|p|))\beta(p)$$

where $\chi \in C_0^\infty[0, \infty)$ with $0 \leq \chi \leq 1$, $\chi \equiv 1$ on $[0, 1/2]$, $\chi \equiv 0$ on $[1, \infty)$. Then the initial value problem for (3) is easy to solve if γ and β are smooth away from $p = 0$. Our uniform convergence of (3) to (1) holds for arbitrary space dimensions n . Moreover, no control is necessary for derivatives of γ although in (3) there are derivatives of γ .

If the space dimension $n = 2$, it has been proved by Mi-Ho Giga and the author that the crystalline motion is approximated by solution for mollified γ . This is even true for solutions of level set equations. As an application of our uniform convergence, we can approximate motion by singular interfacial energy γ by the Allen-Cahn equation (3) with mollification of γ .

We do not consider (3) when γ is not C^2 . If γ is singular, say piecewise linear, the meaning of solution is not clear unless β is a constant. For constant β (3) can be interpreted by a variational inequality and the convergence to (1) has been established by Bellettini, Gogione and Novaga when the interface evolution is a classical crystalline motion.

Crystalline curvature is now known to be defined for a special class of nonsmooth curves and naturally extends ordinary curvature for smooth curves. The evolution of polygonal curves by crystalline curvature corresponds to the evolution of smooth curves by curvature, not only in the sense of normal velocity formulation, but also from the viewpoint of variational structures. It is further claimed that some physical models of crystal growth give rise to such evolution. Concerning this area of research, including basic properties and other background materials, an excellent monograph written by Gurtin should be mentioned.

Here we are concerned with the motion of spiral-shaped polygonal curves by their crystalline curvature. We consider the simplest situation described as follows: the interfacial energy has the Frank diagram which are regular n -polygons; the kinetic coefficient is set to be unity; we neglect the difference in bulk energy. As a result, we discuss the motion law given by

$$(1) \quad V_i = K_i,$$

where V_i and K_i denote respectively the normal velocity and the crystalline curvature on each line segment.

First we deal with the situation that our initial spirals are assumed to spiral out to infinity with one end being fixed at the origin. The evolution given by (1) is reduced to a system of ordinary differential equations (ODEs) of infinite order. Under reasonable assumptions on initial spirals, we show the existence and uniqueness of the solution to this ODE system by the method of approximation arguments. Contrary to real phenomena, our spirals shrink toward the origin and develop certain breakdown within finite time. The classification of singularities is not so clear and it seems to need further restrictions on the shape of initial spirals.

Next we assume that polygonal spirals we consider are symmetric with respect to the origin; at the expense of imposing the assumption of symmetry, we want to pursue the evolution beyond breakdowns. Indeed, we are able to classify the singularity in this case. It takes place at the origin where the line segments containing it vanish. By renumbering

the line segments, the solvability just after the singularity is possible; the global existence is settled. However, we are afraid that the setting is highly mathematical.

There remain topics for further investigation. Among others, 1. The crystal growth problem will be much important. 2. The bulk energies should be included so that the core of spirals may be taken into account.

The current research is joint work with Hitoshi Imai (University of Tokushima) and Takeo Ushijima (University of Tokyo).

$$(1) \quad \rho_t + \operatorname{div}(\rho v) = \rho \operatorname{div} v$$

$$(2) \quad \left[\frac{\delta W}{\delta \rho} \right] \cdot \nabla \rho = \rho v$$

where ρ is an unknown function of orientation of molecules and v is a mean velocity. In this context, Dr. J. A. Warren gave a lecture about the model from physical point of view concentrating on the energy form and the equilibrium solutions of (1) and (2). We in turn discuss the mathematical validity of the model especially the equation (2), which includes singularities. We consider the simplified equation

$$(3) \quad \left(\frac{\partial \rho}{\partial t} \right) = \rho \operatorname{div} v$$

which is derived from the energy form

$$(4) \quad E = \int_{\Omega} \rho |\nabla \rho|^2 dx$$

where $\rho(x)$ is a given positive function. Note that (3) corresponds to (2) if we take $v = \nabla \rho$ and $\rho = \rho$ and to the simplified model of faceted growth against in [2] if $\rho = \rho$. The equation (1) can be interpreted as an extended gradient system of the energy. If using the concept of subdifferential, Nonlinear semi-group theory is able to not only guarantee the mathematical validity of (3), but also give the information how the solution will behave. It tells that the solution will reach the global minimum in a finite time explaining

Mathematical Basis of the Grain Boundary Model

Ryo Kobayashi

February 16, 1999

Recently we proposed a phase field type model of the grain boundary [1]. The model equations are given by the form

$$\tau_\eta \eta_t = \nu^2 \nabla^2 \eta + 1 - \eta - 2s\eta |\nabla \theta|, \quad (1)$$

$$\tau_\theta \theta_t = \frac{s}{\eta^2} \nabla \cdot \left[\eta^2 \frac{\nabla \theta}{|\nabla \theta|} \right], \quad (2)$$

where η is an ordering parameter of orientations of molecules and θ is a mean angle. In this conference, Dr.J.A.Warren gave a lecture about this model from physical point of view concentrating on the energy form and the equilibrium solutions of (1) and (2). We, in turn, discuss the mathematical validity of this model, especially the equation (2), which includes singular diffusivities. We consider the simplified equation

$$u_t = \frac{1}{a} \left(a \frac{u_x}{|u_x|} \right)_x, \quad (3)$$

which is derived from the energy form

$$E = \int_0^1 a(x) |u_x| dx, \quad (4)$$

where $a(x)$ is a given positive function. Note that (3) corresponds to (2) if we take $a = \eta^2$ and $u = \theta$, and to the simplified model of faceted growth argued in [2] if $a \equiv 1$. The equation (3) can be interpreted as an extended gradient system of the energy (4) using the concept of subdifferentials. Nonlinear semi-group theory is able to not only guarantee the mathematical validity of (3), but also give the information how the solution will behave. It tells that the solution will reach the global minimizer in a finite time exhibiting

the elevator motions if appropriate conditions are imposed on $a(x)$ [3]. This means that our grain boundary model can describe the rotation of grains. We will demonstrate the numerical simulation of (1) and (2) under the assumption of the radial symmetry, in which shrinking and rotation of the small disk occurs simultaneously and its boundary disappears in a finite time.

References

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Strain driven periodic structures of Pb/Cu surface alloys

by

*Thomas Rosenblatt * and Boyan Mutaftschiev***

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Lead monolayers deposited on the surface of the three most compact faces of copper, (111), (100) and (110), have been largely studied since the pioneering works of Rhead et al [1, 2] some 25 years ago. The interest in their structure and phase transitions rose considerably when it was shown [3-6] that they are forming surface alloys, although lead and copper are immiscible in the bulk solid state.

In the present contribution, we recall recent experimental results obtained by helium scattering (TEAS) [4, 7] and scanning tunneling microscopy (STM) [3, 5, 6], as well as results of model calculations [8] to show that the still unexplained variety of ordered alloys on the (110)-face of copper, may be understood as due to the competition between strain energy and energy gain by mixing.

On all three studied faces of the Cu-substrate, deposited Pb-atoms form a diluted two-dimensional alloy. It may be considered that disordered surface alloys are stable so far as the difference between the atomic sizes of Pb and Cu ($d_{\text{Pb}} = 3.50 \text{ \AA}$, $d_{\text{Cu}} = 2.55 \text{ \AA}$) does not result in an important strain throughout the topmost layer of the Cu substrate. In general, the transition between surface alloy and on-top layer is always of first order, while transformations inside the alloyed layer or among on-top layers are continuous [9].

We have identified by helium scattering five different two-dimensional phases in the quite narrow interval of Pb-coverages, $0.75 < \theta < 0.80$ (0.865 to 0.923ML), namely (in the order of increasing coverage), p(4x1), p(13x1), p(9x1), p(14x1), and p(5x1) [10]. Most striking in this list of structures is that their unit cells are obtained by linear combination of the unit cells of the extreme members of the array, the p(4x1)- and the p(5x1)-structures. Two possible models have been proposed for the p(4x1)-unit cell, and one model for the p(5x1)-unit cell. In the p(4x1)AT-unit cell, the Pb-atoms are "all in the troughs" of the Cu(110) surface, under slight compression. To avoid compression, we have imagined [10] a unit cell in which every third atom has left the trough, and climbed

on the [110]-ridge of copper atoms. We proposed a similar structure also for the $p(5 \times 1)$ -unit cell.

An important step has been made with the visualization of the ordered structures of Pb/Cu(110) by atomic resolved STM [6]. The most noticeable result was that after annealing at 470 K, those layers are surface alloys with quasi periodic ordered structures, in which entire rows of Pb-atoms have replaced [100]-rows of Cu-atoms. This can be easily understood on the base of our models of the $p(4 \times 1)$ - and the $p(5 \times 1)$ -unit cells. Every third [100]-row in the case of $p(4 \times 1)$, and every fourth row in the case of $p(5 \times 1)$, supposed to climb the [110]-ridges of the Cu-surface, has in fact replaced a [100]-row of Cu-atoms. Entire [100]-rows of Pb-atoms are thus burried beneath the level of the other Pb-atoms. We called the unit cells of these two structures $p(4 \times 1)BA$ - and $p(5 \times 1)BA$ - (burried atom)-cells

The STM micrographs with atomic resolution [6], reveal some curious features of the ordered periodic $p(n \times 1)$ -structures of the Pb/Cu(110)-alloys. So, "pure" $p(4 \times 1)$ -structures composed of $p(4 \times 1)BA$ -unit cells only, have never been observed. Instead, at the same Pb-coverage, $\theta = 0.75$, there are $p(8 \times 1)BA$ - bands, composed by one $p(4 \times 1)AT$ - and one $p(4 \times 1)BA$ -unit cell. $p(12 \times 1)BA$ -bands, composed by two $p(4 \times 1)AT$ - and one $p(4 \times 1)BA$ -unit cells are also but rarely observed.

Bands of $p(5 \times 1)BA$ -unit cells are never combined with $p(4 \times 1)BA$ -bands. On the contrary, they like to be associated with $p(4 \times 1)AT$ -bands, to give $p(9 \times 1)BA$ - bands. The latter exist as "pure" $p(9 \times 1)BA$ -structures, or are combined with $p(4 \times 1)BA$ -bands [$p(13 \times 1)2BA$ -structures]. Combinations of $p(9 \times 1)BA$ - and $p(5 \times 1)BA$ -bands [$p(14 \times 1)2BA$ -bands] are often observed but do not form periodic structures. At the maximum coverage of $q = 0.8$, the surface is covered by contiguous $p(5 \times 1)BA$ -bands.

The above experimental findings have been interpreted, by the combined energy gain, due to the replacement of Cu-surface atoms by Pb-atoms (surface alloying), and the increase of strain energy due to the different size of Pb- and Cu-atoms. The "elementary bricks" of all described structures being, the $p(4 \times 1)AT$ -cell, with a positive misfit of 2.9% (compression), and the $p(4 \times 1)BA$ - and $p(5 \times 1)BA$ -unit cells with negative misfit of -10.6% and -1.0% (traction), respectively, the misfit of the others is obtained by pondered averaging of the above ones.

On should mention the case of the $p(14 \times 1)BA$ -structure, the unit cell of which has such a small misfit (+0.1%) that any order of its constituent cells [$p(9 \times 1)BA$ and $p(5 \times 1)BA$] should be equally probable. The preferred structure should be, therefore, that of high entropy (disorder) than the periodic one.

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Facet breaking of 3D crystalline mean curvature
evolution : mathematical and numerical aspects

Maurizio Paolini

Understanding the properties and even the meaning of anisotropic mean curvature flow when anisotropy degenerates to become crystalline is crucial for both theoretical and applied sciences. We propose a definition of surface evolution which should be consistent with respect to regularization of the anisotropy; namely we say that a surface $\partial A(t) \subseteq \mathbb{R}^3$ with outward unit normal ν , coupled with a vector field $n_\varphi(t) : \partial A(t) \rightarrow \mathbb{R}^3$ evolves by crystalline mean curvature if $n_\varphi \in T(\nu/\gamma(\nu))$ and $V = (-\operatorname{div} n_\varphi)n_\varphi$. Here $\varphi : \mathbb{R}^3 \rightarrow \mathbb{R}^+$ is a norm describing the anisotropy, γ is the corresponding dual norm and $T : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is the duality mapping.

A comparison principle is expected to hold, which means that of two initial surfaces are contained one into the other, then such inclusion will persist for as long as both evolutions are defined; this would imply uniqueness of the evolution. Existence, at least in 3D, is still an open problem.

We show that for such crystalline evolution initially admissible polyhedral surfaces can instantaneously undergo creation of new facets or even formation of curved regions.

A striking example of “face banding” can be constructed by fixing the Wulff shape (unit ball of φ) to be a regular hexagonal prism circumscribed to the unit sphere and centered at the origin. The initial surface is then taken to correspond to the boundary of the Wulff shape but with one of the lateral (rectangular) faces pulled out of an amount slightly less than one, and keeping fixed the support plane of all the other faces. By using the comparison principle it can be checked that the two roughly hexagonal faces must split somewhere, they cannot just move rigidly.

We suspect that the actual evolution would create a “bended” region.

Another example shows face breaking for a nonconvex admissible initial surface with the choice of a cubic Wulff shape. A first set of numerical simulations are produced using the crystalline algorithm of J. Taylor plus manual introduction of degenerate facets where break lines are expected. Such degenerate facets get wider or expected.

Crystalline evolution can be approximated by means of an anisotropic version of the Allen-Cahn equation which can be subsequently discretised by finite elements in space and forward difference in time.

Numerical simulation of the second example using this approach indeed shows automatic formation of the expected break line suggesting that a "diffused interface" approach can be feasible for crystalline curvature flow.

Understanding the properties and even the meaning of anisotropic mean curvature flow when anisotropy degenerates to become crystalline is crucial for both theoretical and applied reasons. We propose a definition of surface evolution which should be consistent with respect to regularization of the anisotropy; namely we say that a surface $\Omega(t) \subset \mathbb{R}^2$ with outward unit normal is coupled with a vector field $v_\nu(x) = \nabla \chi(x)$ on $\Omega(t)$ if v_ν is a regular mean curvature flow $v_\nu \in L^2_{loc}(\mathbb{R}^2; \mathbb{R}^2)$ and $v_\nu \cdot \nu = 1 - \text{div} \chi|_{\Omega(t)}$. Then $v_\nu \cdot \nu = 1$ if χ is not describing the anisotropy γ is the corresponding dual norm and $\chi \in W^{1,2}(\mathbb{R}^2)$ is the dual mapping.

A comparison principle is expected to hold, which means that if two initial surfaces are contained one into the other, then such inclusion will persist for as long as both evolutions are defined; this would imply uniqueness of the evolution. Existence, at least in $W^{1,2}$, is still an open problem.

We show that for such crystalline evolution initially admissible polyhedral surfaces can instantaneously undergo creation of new facets or even formation of curved regions.

A striking example of "facet bending" can be constructed by fixing the Wulff shape (with ball of radius r_0) to be a regular hexagonal prism circumscribed to the unit sphere and centered at the origin. The initial surface is then taken to correspond to the boundary of the Wulff shape but with one of the lateral (rectangular) faces pushed out of its original position by a distance δ less than one, and keeping fixed the support plane of all the other faces. By using the comparison principle it can be checked that the two roughly hexagonal faces must split somewhere; they cannot just cross rigidly.

We suspect that the actual evolution would create a "beaded" region. Another example shows (see Appendix for a nonconvex admissible initial surface) with the choice of a cubic Wulff shape. A first set of numerical simulations are presented using the crystalline algorithm of J. Taylor plus manual intervention to demonstrate facets which break first are expected. Such phenomena occur far earlier or expected.

Crystalline evolution can be approximated by means of an anisotropic version of the Allen-Cahn equation which can be interpreted as a level set method in space and forward direction in time.

Modeling silicon nitride using fully-faceted interfaces

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Enhanced mechanical properties in silicon nitride materials have been associated with their highly irregular, locally anisotropic, microstructural morphologies. At annealing temperatures around 2000 K, β -Si₃N₄ seeds grow with needle-like morphology by absorbing excess silicon nitride from the matrix. Processing for optimal properties requires a means for understanding how complex microstructures evolve. We present a two-dimensional model for microstructural development of silicon nitride growing from a seeded solution by mass diffusion. The results which are obtained are qualitatively correct for the case where a precipitate is growing out of a supersaturated solution.

The simulation technique is based on previous methods developed for simulation of fully-faceted particles. We model the liquid-solid interface as a polygon having a limited number of allowed normal directions all of which appear in the (assumed polygonal) Wulff shape. Each interfacial facet f moves according to a linear kinetic law:

$$v_f = M(\hat{n}_f)[\langle\mu\rangle_f - \mu_{eq}(f)]$$

where $M(\hat{n})$ is a mobility which depends on the facet orientation, \hat{n} . $\mu_{eq}(f) = \Gamma K$ is the equilibrium chemical potential for the facet f , which we take to be proportional to the *weighted mean curvature* K of the facet, and $\langle\mu\rangle_f$ is the chemical potential in the matrix adjacent to the facet, averaged over its length. Silicon nitride particles are observed to be faceted (in the atomically flat sense) along the long sides and rough on the short ends. This should result in much faster attachment kinetics on the rough ends than on the faceted sides. Hence, in our computations we will take the mobility to be much larger in the 'end' directions than in the 'side' directions. In contrast, equilibrium particles tend to be more equiaxed, and thus we will assume that the Wulff shape is equiaxed.

If the variation in μ is sufficiently large along an facet, the facet may split into smaller facets. Facets may also disappear if they shrink to zero length, in which case the neighboring facets are merged together. If a particle is below

a critical size and is shrinking rapidly, it is removed from the computation (with mass conservation being maintained).

The chemical potential μ evolves by diffusion in the bulk with a source term at the moving boundary.

Computations using a variety of initial conditions have been performed. In all cases, one can identify (at least) two epochs of growth. At early times, particles grow rapidly with needle-like shapes, with the growth rate being limited by diffusion of solute from the matrix. Eventually, all the free solute has been absorbed by the particle and the total solid area growth rate plateaus. The evolution of the system continues, however, with both size and shape coarsening being observed: particles tend to become large and equiaxed over long times.

The simulations mimic complex behavior which occur in physical processes and the microstructures which develop do seem to be what would qualitatively be expected from a two-dimensional simulation. Rigorous simulation of effects like percolation and interlocking of needle-like microstructures could only be carried out with three-dimensional calculations. The current results do give an indication of a computational method which could be adapted to three dimensions.

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The planar modified Stefan problem with
 kinetic undercooling and polygonal interfaces
 and its quasi-steady approximation

Piotr Rybka

We study the following problem of crystal evolution which was suggested by Gurtin and Matias.

$$\varepsilon u_t = \Delta u \quad \text{in} \quad \bigcup_{0 < t \leq T} \Omega_1(x) \cup \Omega_2(t) \quad (1)$$

$$[[\nabla u]]_{\nu_j} = -V_j, \quad j = 1, \dots, N, \quad [[u]] = 0 \quad (2)$$

$$\int_{s_i} u dl = \Gamma_i - \beta_i L_i V_i \quad i = 1, \dots, N \quad (3)$$

Here is our notation $s(t) = \partial\Omega_1(t) \cap \partial\Omega_2(t)$, $\Omega = \Omega_1(t) \cup s(t) \cup \Omega_2(t)$. We assume that the interface $s(t)$ is an admissible polygon, s_i are sides of s , $i = 1, \dots, N$. The number N remains constant throughout the evolution. V_i is the velocity of s_i into the direction of ν_i , the outer normal to s at s_i . $[[\cdot]]$ denotes the jump of a quantity across $s(t)$. $\beta_i > 0$ are kinetic coefficients and they are constants, Eq.(3) is a crystalline version of the Gibbs-Thomson relation and Γ_i/L_i is the crystalline curvature of facet s_i .

We consider $\varepsilon \geq 0$, the case $\varepsilon = 0$ is called the quasi-steady approximation of the problem.

We define a proper notion of weak solution to (1-3). (for $\varepsilon \geq 0$). We show that a weak solution exists and it is unique for $\varepsilon \geq 0$. Details of proof for $\varepsilon = 0$ and $\varepsilon > 0$ are different but the idea to use the representation in terms of Green function is common. We also study properties of solutions. For this purpose we prove some auxiliary geometric results. We show that if for a convex admissible polygon γ , the isoperimetric quotient of γ is only slightly larger than the isoperimetric quotient of the Wulff shape, then

$$\frac{\max L_i}{\min L_i} \leq \kappa < \infty$$

is bounded with κ independent of γ . Here we assume that the Wulff shape is a regular polygon.

This result permits us to show that if $\beta_i \equiv \beta$, $i = 1, \dots, N$, so has small isoperimetric quotient $|s_0| \equiv \sum L_i$ is small, $u_0 \leq 0$, then: the isoperimetric quotient of $s(t)$ decreases;

$V_i < 0$, $u(t) < 0$, and $s(t)$ goes to a point in finite time. We can show this by comparing the motion of $s(t)$ to solutions of the system of weighted crystalline curvature flow.

We can also show a priori bounds for $\|u\|_{L^\infty}$ but the bound may explode for $\varepsilon \rightarrow 0$.

Finally we show that the limits $\lim_{\varepsilon \rightarrow 0} u^\varepsilon(t) = u^0(t)$, $\lim_{\varepsilon \rightarrow 0} s^\varepsilon(t) = s^0(t)$ exist in an appropriate sense and the limiting objects $u^0(t)$, $s^0(t)$ satisfy the limiting equation i.e. (1-3) for $\varepsilon = 0$.

I left the issue of breaking or stability of facets open. I hope that the discussions we have held here at SAM will bring us closer to a solution of this problem.

Dynamics of Faceted Polycrystals

P. Smereka

In the first part of this talk I discuss joint work with D. Srolovitz on the development of a mean field theory to model the evolution of a large number of crystals. We consider the two dimensional situation where the crystals are regular polygons initially placed on a flat substrate. Numerical experiments show that as the system evolves it coarsens, further the number of uncovered seeds, $N(t)$, decays like $t^{-1/2}$ as $t \rightarrow \infty$. This is because the seeds which are pointed upwards grow faster. We are able to develop an expression for the number density of seeds, $n(\theta, t)$, with a given orientation, θ . We find:

$$\frac{\partial n(\theta, t)}{\partial t} = -\frac{n(\theta, t)\theta}{\nu} \int_{-\theta}^{\theta} n(\alpha, t) d\alpha, \quad (1)$$

with $\nu = \cos(\pi/M)$ and $M =$ number of sides of the polygon. Furthermore we show that Eq. (1) has the following solution

$$\eta(\theta, t) = B \operatorname{sech}^2 \left(\theta \sqrt{\frac{2Bt}{2}} \right) \quad (2)$$

where B is a constant determined by the initial conditions. It follows from Eq. (2) that

$$N(t) \sim \frac{K}{\sqrt{t}} \quad \text{as } t \rightarrow \infty.$$

In the second part of my talk I describe joint work with G. Russo and S. Li on the development of a level set method to complete the motion of faceted polycrystals in three dimensions. We modify the traditional level set method to keep the corners sharp by adding a tangential component to the normal velocity. This causes a shock to form thereby giving sharp corners.

Numerical results are presented showing the evolution of a large number of seeds with applications to diamond thin films. Results are also shown for needle-shaped crystals using our narrow band level set method. This algorithm saves considerable memory and time.

Effect of crystal anisotropy on wandering
instabilities of a step

Makio Uwaha, Masahide Sato and Yukio Saito

In vapor growth of a crystal, steps moving in a surface diffusion field of adsorbed adatoms (adatoms) control surface morphology. Asymmetry in the surface diffusion field on the upper and the lower terraces of a step causes various instabilities [1]. In the case of asymmetric step kinetics, when supersaturation exceeds a critical value determined by the step stiffness, long wavelength fluctuations grow rapidly and step wanders [2-4]. To predict the behavior of an unstable step, nonlinear effects are essential. By using the reductive perturbation method, Bena et al. [3] have shown that the step obeys the Kuramoto-Sivashinsky (KS) equation

$$\frac{\partial H}{\partial T} = -\frac{\partial^2 H}{\partial X^2} - \frac{\partial^4 H}{\partial X^4} + \frac{1}{2} \left(\frac{\partial H}{\partial X} \right)^2.$$

The solution of the KS equation exhibits spatiotemporal chaos, and chaotic motion of the step is expected. A crystal anisotropy may change this wandering pattern. The strong anisotropy in the step stiffness suppresses the chaotic behavior and keeps the step pattern periodic [5]. If the step lies in a symmetry orientation, the system has the inversion symmetry, $x \rightarrow -x$. Then the anisotropy in the stiffness adds a nonlinear term proportional to $\varepsilon^2 H_X^2 H_{XX}$ to the KS equation, where ε is the distance from the critical point. The solution of the new equation becomes regular and periodic if the coefficient of this term is positive and large [5].

If the inversion symmetry is absent and the stiffness depends on the inclination ζ_x as $\tilde{\beta} = \tilde{\beta}_0(1 + a\zeta_x)$, a term $H_X H_{XX}$ is added to the KS equation since the stiffness appears with the curvature ($\sim \zeta_{xx}$). The evolution equation should have the form

$$\frac{\partial H}{\partial T} = -\frac{\partial^2 H}{\partial X^2} - \frac{\partial^4 H}{\partial X^4} + \frac{1}{2} \left(\frac{\partial H}{\partial X} \right)^2 + v \frac{\partial H}{\partial T} \frac{\partial^2 H}{\partial X^2},$$

where $v \sim \varepsilon^{1/2}$. The pattern obtained is, not completely regular and irregular motion remains. Both with and without the inversion asymmetry, the anisotropy effect of the stiffness becomes weak near the threshold of instability. With anisotropy in step kinetics,

the kinetic coefficient K in general depends on the inclination of the step as $K = K_0 + K_1 \zeta_x$ to the first order. Then the nonlinear evolution equation can be written as

$$\frac{\partial H}{\partial T} = -\frac{\partial^2 H}{\partial X^2} - \delta \frac{\partial^3 H}{\partial X^3} - \frac{\partial^4 H}{\partial X^4} + \frac{1}{2} \left(\frac{\partial H}{\partial X} \right)^2,$$

where $\delta \propto K_1/(K_0\sqrt{\varepsilon})$. This is a form of the Benny equation which interpolates the KS equation (when $\delta = 0$), and the Korteweg-de Vries (KdV) equation¹ (when $\delta \rightarrow \infty$). When $|\delta| \ll 1$, the solution of the Benny equation is spatiotemporal chaos like that of the KS equation as shown in Fig. 1a. When $|\delta| \geq 1.2$, however, the solution produces a regular pattern. Near the threshold of the instability where $\varepsilon = 0$, the value of δ becomes very large. Therefore if the anisotropy in the step kinetics is present, $\delta \gg 1$ near the threshold, and the step will show the regular pattern.

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Modeling Grain Boundaries using a Phase Field Technique

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We propose a two dimensional frame-invariant phase field model of grain impingement and coarsening. One dimensional analytical solutions for a stable grain boundary in a bicrystal are obtained, and equilibrium energies are computed. We are able to calculate the rotation rate for a free grain between two grains of fixed orientation. For a particular choice of functional dependencies in the model the grain boundary energy takes the same analytic form as the microscopic (dislocation) model of Read and Shockley [1].

Previously we presented a new model [2] and [3] and phase-field simulations of the simultaneous processes of solidification, impingement, and coarsening of arbitrarily oriented crystals. In earlier models of this phenomenon, a finite number of crystalline orientations are allowed with respect to the fixed coordinate reference frame. Morin et al.[4], and Lusk [5] constructed a free energy density having N minima by introducing a rotational (orientation) variable in the homogeneous free energy. Chen and Yang[6] and Steinbach

et al.[7] assigned N order parameters to the N allowed orientations. In these approaches, the free energy density depends on the orientation of the crystal measured in the fixed frame—a property which is not physical.

In [2] and [3] (KWC, WCK) the model introduced was invariant under rotations of the reference frame. A similarly motivated approach has also been developed by Lusk [8]. Herein, we present a completely general formulation of a new class of models which allow for accurate, physical modeling of grain boundary formation by impingement and subsequent motion.

We focus on a completely solid system with grain boundaries present. The model parameters η and θ represent a coarse-grained measure of the degree of crystalline order, and the crystalline orientation, respectively. To define η and θ , consider a fixed subregion of solid material. At the atomic scale we can define a discrete variable θ_i which represents the orientation of an atomic bond (lattice vector) with respect to some fixed laboratory frame. For this subregion, we define η and θ such that

$$(\eta \cos \theta, \eta \sin \theta) = \frac{1}{N} \sum_{i=1}^N (\cos \theta_i, \sin \theta_i), \quad (1)$$

where $N \rightarrow \infty$ is the number of bonds in the subregion. Then, the variable η is an order parameter for the degree of crystalline orientational order, where $\eta = 1$ signifies a completely oriented state and $\eta = 0$ a state where no meaningful value of orientation exists in the subregion, and $0 \leq \eta \leq 1$ always holds. The variable θ is an indicator of the mean orientation of the crystalline subregion. Note, that when symmetrically equivalent crystalline

directions exist, θ may not be uniquely defined. However, the point group symmetry operations can be used to map each of the θ_i into a subdomain of $(0, 2\pi)$ where they are unique.

Given the order parameters η and θ we need to construct a free energy which is invariant under rotations of the reference frame. We start from the expression

$$F = \int \left[f(\eta) + s\mu(\eta)G(|\nabla\theta|) + \frac{\nu^2}{2}|\nabla\eta|^2 \right] dV, \quad (2)$$

where ν and s are constants, $f(\eta)$ is the homogeneous free energy and $G(|\nabla\theta|)$ is specified below. The function $\mu(\eta)$ should have the property $\mu(0) = 0$ and should increase monotonically with η . The constants s and ν are parameters which set the strength of the penalties for gradients in misorientation and degree of crystalline orientation, respectively. The total free energy is frame invariant since it includes the variable θ only in the form $\nabla\theta$. For this work we assume that only ordered phase is stable, so $f(\eta)$ has a single-well at $\eta = 1$.

For a bicrystal (a single grain boundary) with Dirichlet boundary conditions, the spatial extent of the grain boundary is determined by $G(|\nabla\theta|)$ and the coupling to η . The customary choice of square gradient, $G(|\nabla\theta|) = \nabla\theta \cdot \nabla\theta$, *cannot* be physically correct, since it leads to a diffusion equation for θ and therefore the region of misorientation spreads indefinitely. In order to properly determine the form for G , it is useful to determine the energetic contribution of terms with the form $|\nabla\theta|^\alpha$; where α is a positive number.

If the gradient is completely spread out over a one dimensional domain of length L and η is uniform, then $\nabla\theta \equiv \Delta\theta/L$, where $\Delta\theta$ is the change in angle across the domain (grain boundary misorientation). If $\eta \equiv \bar{\eta}$ where $\bar{\eta}$ gives a minimum of $f(\eta) + s\mu(\eta)|\nabla\theta|^\alpha$, and L is taken to be large, the total excess energy (associated with $\Delta\theta \neq 0$) is given by

$$\Delta F_{\alpha,L} = \int_{-\frac{L}{2}}^{\frac{L}{2}} [\Delta f(\bar{\eta}) + s\mu(\bar{\eta})|\nabla\theta|^\alpha] dx = O(L^{1-\alpha}),$$

where $\Delta f(\eta) \equiv f(\eta) - f(1)$. In particular, for $\alpha > 1$

$$\lim_{L \rightarrow \infty} \Delta F_{\alpha,L} = 0. \quad (3)$$

Thus, there is *no* form for $\alpha > 1$ leading order behavior in G which has a globally stable, non-diffuse solution, since a completely diffuse boundary has an energy which can always be made smaller than any other configuration.

However, the form of $\Delta F_{\alpha,L}$ suggests that the choice of $\alpha = 1$ may admit solutions for equilibrium grain boundaries of finite spatial extent. If $\alpha < 1$ then the derived evolution equation is completely singular in the region where $\nabla\theta = 0$. Thus, $\alpha = 1$ ($G(|\nabla\theta|) = |\nabla\theta|$ to leading order) *is the only possible choice.*

Therefore, the dimensionless energy takes the following form:

$$F = \int_{\Omega} \left[f(\eta) + \frac{\nu^2}{2} |\nabla\eta|^2 + s\mu(\eta)|\nabla\theta| \right] dV, \quad (4)$$

The equilibrium solutions $\eta(x)$ and $\theta(x)$ must satisfy the following equations:

$$0 = \nu^2 \eta_{xx} - \frac{\partial f}{\partial \eta} - s \frac{\partial \mu}{\partial \eta} |\theta_x|, \quad (5)$$

$$0 = s \left[\mu \frac{\theta_x}{|\theta_x|} \right]_x, \quad (6)$$

where the subscript x indicates differentiation with respect to x . Dirichlet boundary conditions $\theta(\pm\infty) = \theta_{\pm}$ are applied as well as the condition $0 \leq \eta(x) \leq 1$. Here, let us consider the equilibrium solution which corresponds to a bicrystal. Without loss of generality, the center of the grain boundary is located at $x = 0$. If $\eta(x)$ has only one minimum, it can be shown that the solution for $\theta(x)$ is a step function at the point where η takes minimum [9].

So we can take θ as

$$\theta(x) = \begin{cases} \theta_- & -\infty < x < 0; \\ \theta_+ & 0 < x < \infty. \end{cases} \quad (7)$$

Note that $|\theta_x| = \Delta\theta \delta(x)$, where $\Delta\theta = |\theta_+ - \theta_-|$ and $\delta(x)$ is the Dirac delta function. Eqn. 5 gives

$$\nu^2 \eta_x^2 = 2f(\eta), \quad x \neq 0 \quad (8)$$

using this result we can find $\eta_0 = \eta(0)$ by integration of Eqn. 5 through the discontinuity in θ :

$$\sqrt{8\nu^2 f(\eta_0)} = s \left. \frac{\partial \mu}{\partial \eta} \right|_{\eta=\eta_0} \Delta\theta. \quad (9)$$

The energies of low-misorientation tilt grain boundaries have been approximated by summing the energy of distribution of edge dislocations [1]. Here we discuss a method for reproducing the same energetic dependence on misorientation. Using the above results we may compute the surface energy

to be

$$\gamma = 2\nu \int_{\eta_0}^1 \sqrt{2f(\eta)} d\eta + 2\mu(\eta_0)\Delta\theta. \quad (10)$$

If we choose $f = (1 - \eta)^2/2$ (a very plausible choice), and a somewhat unusual choice for μ of

$$\mu(\eta) = -2 \ln(1 - \eta) \quad (11)$$

then we find

$$\gamma = s\Delta\theta \left(1 - \ln \frac{s\Delta\theta}{\nu}\right) \quad (12)$$

holds. Eqn. 12 is the Read-Shockley energy of a low angle tilt grain boundary [1]. This is a very useful result, as it allows us to mimic the physical picture of a grain boundary as a collection of dislocations using a macroscopic (coarse grained) free energy for small misorientations.

To summarize, we have derived a class of models which can describe the solidification, impingement and coarsening of grains. These models are rotationally invariant, and can be modified in a straightforward manner to include a variety of physics. All of these models are analytically tractable in one dimension, which makes study of their behavior particularly direct. If we choose the coupling carefully we are able to derive a grain boundary energy identical to the Read-Shockley low misorientation tilt grain boundary energy.

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J.S. Wettlaufer

Two qualitatively different growth laws can be brought to bear on the study of arbitrary initial shapes of crystalline material. These can be broadly distinguished based on (a) whether they depend in an explicit manner on the surface free energy (b) whether the initial shape of interest is the equilibrium crystal shape, and (c) the goals of the study. A growth law embodying (a) is generally motivated by the desire to obtain the equilibrium crystal shape (ECS) as a solution in the zero velocity limit. It is well known that the ECS can be fully faceted (everywhere smooth on the scale of the lattice parameter), completely rough (possessing a hill and valley structure on the scale of the lattice parameter), or contain both types of surface. Hence, the detailed nature of the interfacial structure, and thus the symmetry of the ECS, is reflected in the anisotropy of the mechanisms by which molecules attach to the surface, i.e., the growth kinetics. Therefore, we can envisage a growth law that satisfies criterion (b) above, but does not seek the ECS as a solution in the zero speed limit. We call such a law "kinematic", relying on a physical understanding of how the anisotropy of the ECS manifests itself in the anisotropy of the growth kinetics. Because the ECS can always serve as an initial condition, a kinematic growth law is broadly applicable to a host of physically realizable initial value problems in crystal growth (1-3). Specific features of the polygonalization of partially faceted ECS's are predicted by such models, and they are well suited for analysis. Nevertheless, strictly thermodynamic models are necessary to capture the shape preserving growth of crystals growing asymptotically close to equilibrium. Connecting kinematic and thermodynamic models is an important goal for the future.

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On the Theory of generalised Cahn-Hoffman ξ -vectors

A. A. Wheeler

We discuss recent developments that combine two of areas; diffuse interface theory of interfaces and the ξ -vector for the description of interfacial surfaces with anisotropic surface energy. We show how a connection can be made between anisotropic diffuse interface models of interfaces and the ξ -vector formalism by a natural generalisation of the ξ -vector originally conceived by Hoffman and Cahn [1, 2] for sharp interfaces. We show that the generalised ξ -vector plays a central rôle in the theory of anisotropic diffuse interface models from describing the equilibrium interface shape, to representing the entropy flux of a moving interface, as well as describing the notion of stress in the interface through its rôle in contributing to the reversible part of the stress tensor.

The equilibrium shape of an isothermal interface of a pure material may be found by minimising the total energy of the system which is comprised of the energy of the interface due to its surface energy plus the energy of each of the bulk phases, subject to the constraint that the volume enclosed by the interface is constant. A simple calculation gives that

$$\gamma\mathcal{K} = -\Delta f. \quad (1)$$

Here \mathcal{K} is the mean curvature of the interface and Δf is the free energy difference (per unit volume) between the two interfaces given by $L(T - T_M)/T_M$, where T is the temperature of the system, T_M the melting temperature of a planar interface, and L the latent heat per unit volume. Eq. (1) may be expressed as

$$T = T_M - \gamma \frac{T_M}{L} \mathcal{K}, \quad (2)$$

the so-called Gibbs-Thomson equation. It is satisfied in two dimensions by a circular interface shape.

When the surface energy is anisotropic the same procedure in two dimensions gives that

$$T = T_M - [\gamma(\theta) + \gamma''(\theta)] \frac{T_M}{L} \mathcal{K}, \quad (3)$$

where θ is the angle subtended by the normal to the interface with a fixed direction.

In three dimensions this procedure results in a much more complicated formula, and is best described compactly by adopting the Hoffman Cahn ξ -vector defined by

$$\xi^i = \frac{\partial \gamma(\vec{p})}{\partial p^i}$$

where $\gamma(\vec{p})$ is the homogeneous degree one extension of $\gamma(\vec{n})$ and \vec{n} is the unit normal to the interface. The Gibbs-Thomson equation is then

$$T = T_M - \nabla_S \cdot \vec{\xi}$$

where $\nabla_S \cdot \vec{\xi}$ is the surface divergence of $\vec{\xi}$ on the interface S .

The description of equilibrium shapes of interfaces with anisotropic surface energy dates back to the Gibbs-Wulff construction [3, 4] which describes a geometric procedure to determine the equilibrium shape based upon the γ -plot; a polar plot in which $r = \gamma(\vec{e}_r)$, where (\vec{e}_r) is the unit radial vector. A review of this classical area of theory is given by Frank [5] and Mullins [6]. The Cahn-Hoffman ξ -vector theory developed in the 1970's encompasses these ideas and places them in an elegant and relatively simple framework.

In contrast to sharp interface models, diffuse interface theories recognise that in reality the interfaces have a small, but finite, thickness in which physical quantities vary between their values in the bulk phases. Quantities in the sharp interface formulation which are viewed as localised in the interfacial surface are, in the diffuse interface treatment, identified as being distributed throughout the interfacial region. For example, the surface energy of the interface is derived from the raised Helmholtz free energy density associated within the interfacial region.

We review both the Cahn-Hoffman ξ -vector and diffuse interface theories of interfaces. In particular, we discuss recent developments which allow diffuse interface models to describe interfaces with anisotropic surface energy. Subsequently, we show how these two complementary approaches may be unified by a generalised Cahn-Hoffman ξ -vector. We go on to describe its use in a range of different diffuse interface models associated with both solid-liquid and solid-solid phase transitions. We illustrate its utility in the context of anisotropic phase-field models of solid-liquid interfaces where it may be used in their sharp interface asymptotic analysis, determination of the type of the anisotropic Allen-Cahn equation differential equations, as well as contributing to both the entropy flux and reversible part of the stress tensor that emerges in the derivation of the phase-field model in the setting of irreversible thermodynamics.

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Continuum Limits of Step Flow Models

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This work (done jointly with Weinan E and Robert Kohn) studies the continuum limits of the one-dimensional Burton-Cabrera-Frank step flow model with the possibility of nucleations. We arrive at certain Hamilton-Jacobi and singular parabolic equations. Our goal is to understand in what spatial and parameter regimes these equations are valid. We believe that such passage from microscopic dynamics to meso(macro)-scopic motion laws are of profound physical and mathematical importance.

We consider the evolution of a general one-dimensional surface consisted of horizontal terraces (of length l) connected by vertical steps (of constant height δ). Atoms are uniformly deposited onto the terraces. They diffuse and then attach to the steps. Under the assumption of no evaporation, the velocity of an arbitrary step is computed as

$$v = \alpha_+ l_+ + \alpha_- l_- \quad (1)$$

where l_+ and l_- are the lengths of the lower and upper terraces adjacent to the step and α_+ and α_- are the Schwoebel coefficients normalized so that $\alpha_+ + \alpha_- = 1$.

In the region where the step profiles are monotonically decreasing or increasing, the continuum limits of the above step flows (in the sense of letting $\delta \rightarrow 0$) is given by

$$\frac{\partial h}{\partial t}(x, t) = 1 \quad (2)$$

where $h(x, t)$ is a continuous function approximating the actual terrace-step profile.

If we use the second order Taylor expansion of l in terms of h_x and h_{xx} , the following singular parabolic equation is obtained for h

$$h_t = 1 + \delta \left(\frac{\alpha_+ - \alpha_-}{2} \right) \frac{h_{xx}}{h_x^2} = 1 - \delta \left(\frac{\alpha_+ - \alpha_-}{2} \right) \frac{\partial}{\partial x} \left(\frac{1}{h_x} \right) \quad (3)$$

Note that the above equation is well-posed only when $\alpha_+ > \alpha_-$. The equation is singular at the maximum or minimum of h where $h_x = 0$ or is undefined.

At the maximum of h , i.e. the top terrace, we allow the possibility of nucleations using the following deterministic rule – a new step is introduced at the center of the top terrace when its length reaches N_0 which is an *a priori* chosen fixed parameter.

Numerical experiments are performed using the above step dynamics and nucleation criterion with a wide range of N_0 . We observe a distinctive plateau type tip structure near the nucleation site. Its size is of $O(\delta)$ and is an increasing function of N_0 . We have tried to describe this structure by two methods:

1. using the second order equation (??) with appropriate boundary condition at the maximum height. The results are quite accurate when N_0 is small compared with δ .
2. looking for time invariance (traveling wave) step profile. Numerical experiments indicate the existence of such a structure. However, the matching of this traveling wave with the rest of the step profiles far away from the nucleation sites remains unclear.

This work provides an example (among many others) of the subtlety of obtaining continuum limits from microscopic evolutions when there are nonlinear effects (such as nucleations in the present case). A better understanding of such procedures we believe can give more hints to the validity of various macroscopic motion laws.

Further works include the incorporations of step atom detachments, bulk diffusions and multiple species. Some kind of interfacial diffusive motion laws are anticipated.

Proposed topics of organized discussions

1. Sharp interface model for motion with facets. Kinetic anisotropy vs. anisotropy in interfacial energy (Y. Giga)
2. Diffusion induced grain boundary motion in thin polycrystalline film (C. M. Elliott)
3. Backward and forward parabolic problems (M. Paolini and N.-K. Yip)
4. Facet splitting, Mathematics vs. Physics (Y. Giga, M. Paolini and A. Roosen)

We do not intend to write a summary of these topics because it is not in a stage to be summarized. We just mention natures of problems of each topics. First and fourth topics are closely related so we shall discuss later.

The second topic is to find a reasonable model to describe motion of grain boundary in a polycrystalline thin film surrounded by vapour of other materials. Typical example is a Fe thin film surrounded by Zn vapour. Here Zn only diffuse on the grain boundary. There is a model proposed by Cahn, Fife and Penrose (Acta Metal '97) which is a phase field type taking some kind of elastic energy into account. However, the model needs an assumption that the grain boundary moves monotonically. It is desirable to have a new model. The problem is difficult from a physical point of view.

A typical example concerning the third topic is an understanding of $u_t = (W'(u_x))_x$ where $W(p)$ has two minima and W'' changes signs twice, i.e., double well function. A typical example is $W(p) = (1 - p^2)^2$. Such type of problem arises when we consider a macroscopic model of motion by nonconvex interfacial energy. Since the problem has a feature of backward parabolic problem, it is not well-posed in usual sense. It is known (at least for piecewise quadratic W) that there are infinitely many solutions (Hollig, Nohel, Slemrod, ...). There are at least two ways to regularize. The first one is to replace W by its convexification W^{**} . The second one is to add fourth order term $-\varepsilon u_{xxxx}$ in the right hand side or similar higher order effects, where $\varepsilon > 0$ is small. This is exactly the Cahn-Hilliard equation. The choice of approximation should depend on what physics we consider. For convexified problem we know the well-posedness for initial value problem in viscosity sense. For higher order approximation we get a Young measure solution as a limit of $\varepsilon \rightarrow 0$. However, its characterization is not enough to guarantee the uniqueness of the limit. There are more examples of backward-forward parabolic problem including image processing (see, e.g. Kawohl and Kutev, Math. Ann. '98). It is desirable to have a suitable notion of solution depending upon physics.

We are now going back to the first and the fourth topic.

Kinetic anisotropy vs. anisotropy in interfacial energy. In an interface controlled model motion of phase boundary Γ_t is often of form

$$V = M(\vec{n})(-\text{div } \xi(\vec{n}) + C) \quad \text{on } \Gamma_t.$$

Here V represents the normal velocity of Γ_t in the direction of the unit normal \vec{n} and $\xi = \text{grad } \gamma$ (the Chan-Hoffman vector), where γ is the homogenization of interfacial energy density γ_0 , i.e., $\gamma(p) = |p|\gamma_0(p/|p|)$. The coefficient $M > 0$ is called mobility and is given. The mobility M may depend on \vec{n} . The anisotropy of M is called kinetic anisotropy to distinguish it from the anisotropy of γ . The term C represents a driving force and it is given. Two anisotropies are often confused since their symmetric structure is the same. Kinetic anisotropy contributes a rough shape of growing large crystal. If C is constant and the sign is taken so that crystal is growing, then its large time behaviour is asymptotically approximated by the Wulff shape of M . Anisotropy in interfacial energy effects local shape of a crystal. In the theory of crystal growth it is reflected in the equilibrium shape. Mathematically, the solution is a Wulff shape of γ and it satisfies $-\text{div } \xi(\vec{n}) = C$. Experimental physics distinguish two anisotropies by checking equilibrium shape.

However, mathematically, $-\text{div } \xi(\vec{n}) = C$ is unstable (with one unstable mode). Mathematicians are curious to have equilibrium shape. In experiments especially in crystal growth they get equilibrium sphere by controlling C bigger or smaller depending on time as commented by M. Suzuki. As noted by C. Elliott this Wulff shape is stable as a solution of the quasi-steady Stefan type problem with Gibbs-Thomson effects.

In conclusion we should be careful to distinguish two anisotropies both theoretically and experimentally.

Sharp interface model for motion with facets. The question whether there is a macroscopic model to explain motion with facets in low temperature triggers a very exciting discussion among physicists and mathematicians. Physicists pointed out that growth law on a molecularly flat facet is different from rough portion. The velocity V is no longer proportional to the thermodynamical driving force $\frac{\partial F}{\partial \Gamma} = -\text{div } \xi(\vec{n}) + C$. It should depend on $\partial F / \partial \Gamma$ nonlinearly, say $V = g(\vec{n}, \delta F / \delta \Gamma)$ where $X \mapsto g(\vec{n}, X)$ is nondecreasing with $\frac{\partial g}{\partial X}(\vec{n}, 0) = 0$, $g(\vec{n}, 0) = 0$ where \vec{n} is the normal of facets.

However, such facets also appear in equilibrium shape of crystal so that the Frank diagram of γ has a corner in \vec{n} direction. The quantity $-\text{div } \xi(\vec{n})$ has no meaning

in naive sense γ is not differentiable in the direction of \vec{n} . However, according to study of M.-H. Giga and Y. Giga, there is a notion of solution of $V = g(\vec{n}, \partial F/\delta\Gamma)$ can be approximated by motion by smooth interfacial energy at least when the space dimension is two and C is constant. It qualitatively agrees with microscopic explanation by understanding that $-\text{div } \xi(\vec{n})$ is a nonlocal curvature. Physicists prefer microscopic explanation to macroscopic explanation especially when real facets appear since there was no macroscopic explanation. Arguments so far do not exclude the possibility that the macroscopic sharp interface model explain motion with facets by taking g in appropriate way. Also, relation among microscopic of macroscopic models should be investigated. Further study of macroscopic model is necessary to these purposes.

Facet splitting. In macroscopic formulation facets may split when Γ_t is a surface or Γ_t is curve but C depends on the spatial variable. The way of splitting is given by calculating the minimal section of energy at least formally. However, it is not so explicit that further study is necessary. It is also important whether this describes the phenomena of facet breaking in a crystal growth problem. It is a good idea to explain faceted dendritic growth by using sharp interface model coupled with bulk equations.

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