

Geometric Interfacial Motion: Coupling Surface Diffusion and Mean Curvature Motion

V. Derkach, J. McCuan, A. Novick-Cohen and A. Vilenkin

Abstract Mean curvature motion as well as surface diffusion both constitute geometric interfacial motions which have received considerable attention. However in many applications a complex coupling of surfaces occurs whose evolution may be described using both these types of motion. A variety of such physical problems are described. While sometimes an anisotropic formulation might seem to be preferable, often an isotropic formulation is helpful to consider. Some analytic and numerical results are being presented, with some supporting experimental evidence. Many open questions remain.

Keywords Surface diffusion · Mean curvature motion · Microstructure Numerical simulations · Coupled geometric motions

While arguably motion by mean curvature and motion by surface diffusion, as well as systems describable by coupling these motions, may all be traced back to a series of papers by W. Mullins from 1956–1958 [35–37], our interest in these directions began some 40 years later and is reflected in a series of papers, in part in collaboration with J. Cahn, R. Dal Passo, C. Elliott, L. Giacomelli, J. Kanel, L. Peres-Hari, E. Rabkin, O. Zelekman-Smirin, and A. Zigelman, [12–19, 29–33, 38–41, 43, 51–53].

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Below is a partial list of some of relevant physical problems.

1. Polycrystalline films are material layers composed of a number of individual crystals, or grains. When these films are thin, the effects of their exterior surface can affect the stability of the film. Since thin films are in common use in numerous technological applications, the interest in their stability is considerable.
2. Sintering is a technology with a long history, which is still in active use to this day. In this process, a collection of metallic particles, produced previously by evaporation and condensation, are placed into a mold. Under pressure, the collections of particles can be made to combine to yield one solid metallic block with some specific shape.
3. Under appropriate compositional conditions, ordering can be induced in a previously homogenous material. If the composition differs slightly from these conditions, the excess composition can emerge as droplets along the boundaries between the ordered regions. This phenomena can be modeled with some success by a coupled Allen-Cahn/Cahn-Hilliard system of equations with degenerate mobilities.

In all of the above applications, the coupled motion of surface diffusion with motion by mean curvature appears quite naturally. In each of these applications, there are additional effects which are often neglected and which arguably should be included. However, the coupled motion, in and of itself, is not overly well understood, so it is reasonable to isolate it and study it, even given its limitations. So we shall first define motion by mean curvature and motion by surface diffusion, then return to consider some systems coupling these motions.

1 Motion by Mean Curvature

Initially let us take

$$\Gamma(t) := \{X(\alpha, t) : [0, 1] \times [0, T] \rightarrow \mathbb{R}^2\}, \quad (1)$$

to be a smooth (and smoothly parameterized) embedded curve in $\mathbb{R}^2$. For $\alpha \in (0, 1)$, we may define $\hat{n}$, the unit normal to $\Gamma(t)$ at α , and we may define κ , the mean curvature of $\Gamma(t)$ at α , via the inscribed circle at α . Then setting $\hat{V} := \frac{\partial}{\partial t} X$ for $(\alpha, t) \in (0, 1) \times (0, T)$, the motion known as motion by mean curvature is given by

$$V_n = \mathcal{A}\kappa, \quad (2)$$

where $V_n := \hat{n} \cdot \hat{V}$ is the normal velocity, and $\mathcal{A}$ is a dimensional parameter, known as the reduced mobility whose dimensions are given by $[\mathcal{A}] = L^2/T$. It is straightforward to later extend the above definition to smooth (and smoothly parameterized) embedded hypersurfaces in $\mathbb{R}^3$, taking κ to be the sum of the principle curvatures. An early reference, if not the earliest reference, to motion by mean curvature is

Mullins 1956 [35]. In the mathematical literature, early references include Brakke 1978 [11], Huisken 1984 [27], Grayson 1987 [25]. For surveys, see Giga 2006 [22] and Bellettini 2013 [9].

2 Motion by Surface Diffusion

To define motion by surface diffusion, we may proceed as above and let us initially consider $\Gamma(t) := X(\alpha, t)$ to be a smooth and smoothly parameterized embedded curve in R^2 prescribed as in (1), with $\hat{n}$, κ , $\hat{V}$, V_n defined as above for $(\alpha, t) \in (0, 1) \times (0, T)$. Taking $s (= s(t))$ to be an arc-length parametrization of $\Gamma(t)$, e.g. $s := \int_0^\alpha |\frac{\partial}{\partial \alpha} X(\tilde{\alpha}, t)| d\tilde{\alpha}$, the motion known as motion by surface diffusion is given by $V_n = -\mathcal{B} \frac{\partial^2 \kappa}{\partial s^2}$, where $\mathcal{B}$ is a dimensional kinetic coefficient with dimensions $[\mathcal{B}] = L^4/T$. The above definition of surface diffusion may be extended to smooth (and smoothly parameterized) embedded hypersurfaces in R^3 , by defining κ as the sum of the principle curvatures and by replacing the operator $\frac{\partial^2}{\partial s^2}$ with the Laplace-Beltrami operator Δ_s , yielding that

$$V_n = -\mathcal{B} \Delta_s \kappa. \quad (3)$$

The Laplace-Beltrami operator on a smooth hypersurface may be defined as $\Delta_s := \sum_{i=1}^2 \frac{\partial^2}{\partial s_i^2}$, where s_i $i = 1, 2$ are locally defined arc-length parameterizations in the directions of the principle curvatures; in this sense Δ_s indeed generalizes $\frac{\partial^2}{\partial s^2}$. An early reference, if not the earliest reference, to surface diffusion in the literature is Mullins 1957 [36]. Unlike motion by mean curvature, convex curves evolving by surface diffusion can later lose convexity [24]. Pinch off of embedded curves may also occur [23]. Some recent references include [3, 34].

3 Coupling the Two Motions

Why couple the two motions discussed above? Let us focus on the first problem in the list given earlier, that of polycrystalline films. Because the microstructure of polycrystalline materials, namely the way in which the individual crystals or grains are arranged within the specimen, strongly influences the material properties, it has attracted many studies since Mullins' 1956 [35] work on the dynamics of grain boundaries, and earlier static discussions by Smith [45] and Herring [26]. Much emphasis has been placed on considering grain boundaries within the material, especially in large systems and on the distribution of grain boundary properties, see e.g. [7]. Many additional effects have been included, such anisotropy, elastic effects, and defects [44].

When a polycrystalline specimen is thin enough to be considered a film, or more specifically a thin film, the exterior surface is nowhere too far from the grain boundaries within, and the effects of the dynamics of the exterior surface on the structural

stability of the specimen need to be taken into account. A classical though somewhat simplistic model for the evolution of the exterior surface, due to Mullins 1957 [36], predicts that it evolves by surface diffusion. While many of the grain boundaries lie totally within the interior of the material, some continue on up until they intersect the exterior surface. This gives rise a system in which numerous grain boundaries are coupled with the exterior surface, which we assume for simplicity to evolve by mean curvature and by surface diffusion, respectively. As there is much to be studied in regard to these coupled motion, a possible simplification is to consider some special simple geometries.

4 Some Special Geometries

In polycrystalline specimens with *bamboo structure*, the specimen is one grain thick throughout. Accordingly all of the grains intersect the exterior surface at least twice, once above and once below. Within the interior of the specimen, triple junctions form where three-grain boundaries intersect. On the exterior surface, where three intersecting grain boundaries intersect with the exterior surface, quadruple junctions form. Although assuming bamboo structure simplifies the analysis somewhat, it still is quite complicated. A further possible simplification is to consider the 2D symmetric thermal grooving geometry proposed by Mullins [36], described below. Other special geometries are possible to consider, some of which will be described a bit further on.

5 A Phase Field Approach

One approach to modeling this type of coupled motions is to embed the problem description within a phase field approach, and one way to accomplish this is to consider certain types of Allen-Cahn/Cahn-Hilliard system with degenerate mobility. Such a system was derived to describe the dynamics of simultaneous order-disorder and phase transitions, as the formal continuum limit of discrete lattice dynamics, in the context of the Krzanowski instability [12]. For the resultant system, it was possible to formally derive the coupled motion by mean curvature and surface diffusion by considering an appropriately defined long time asymptotic limit [39, 40].

6 The Mullins' Sharp Interface Approach

Mullins considered a geometrically simple exterior surface-grain boundary configuration with important experimental implications and outlined a dynamic problem for its evolution [36], following the general thermodynamic framework outlined by Gibbs. The geometry which he considered consisted of an initially flat exterior

surface of infinite extent, coupled with an initially flat grain boundary of semi-infinite extent which intersected the exterior surface perpendicularly. The exterior surface was assumed to evolve by surface diffusion, and the grain boundary, which in theory could evolve by motion by mean curvature, could be expected to remain flat due to symmetry considerations. Although this reflects a 3D problem, its dynamics reduce to a 2D problem due to the uniform cross-section of its geometry. To complete the problem formulation, boundary conditions are required at the triple junction, in addition to far-field and initial conditions. The following conditions were proposed by Mullins: 1) persistence, meaning that the grain boundary remained attached to the exterior surface, 2) balance of mechanical forces, known also as Herring's law or Young's law for isotropic systems, 3) continuity of the chemical potential, which, based on thermodynamic considerations of Gibbs, implies continuity of the mean curvature, 4) balance of mass flux along the exterior surface, assuming that there is no mass flux along the grain boundary. While Mullins formulated the conditions above within the framework of a linearized approximation for surface diffusion, the same physical conditions can be readily formulated within a fully nonlinear framework [31]. Assuming asymptotic planarity and fixing the initial location of the exterior surface along the x -axis and the initial location of the grain boundary to lie along the negative y -axis, yields the following problem formulation for the evolution of the exterior surface,

$$\left\{ \begin{array}{l} y_t = -\mathcal{B} \left[\frac{\kappa_x}{\sqrt{1+y_x^2}} \right]_x, \quad \kappa = \frac{y_{xx}}{(1+y_x^2)^{3/2}}, \quad x \in (-\infty, 0) \cup (0, \infty), \quad t \in (0, \infty), \\ y(0^+, t) = y(0^-, t), \quad t \in (0, \infty), \\ \arctan(y_x(0^+, t)) = \arctan(y_x(0^-, t)) + 2 \arcsin(m/2), \quad t \in (0, \infty), \\ \kappa(0^+, t) = \kappa(0^-, t), \quad t \in (0, \infty), \\ \frac{\kappa_x}{\sqrt{1+y_x^2}}|_{(0^+, t)} = \frac{\kappa_x}{\sqrt{1+y_x^2}}|_{(0^-, t)}, \quad t \in (0, \infty), \\ y(\pm\infty, t) = y_x(\pm\infty, t) = 0, \quad t \in (0, \infty), \\ y(x, 0) = 0, \quad x \in (-\infty, 0) \cap (0, \infty), \end{array} \right. \quad (4)$$

where

$$m = \gamma_{\text{exterior}} / \gamma_{\text{gb}}. \quad (5)$$

Here γ_{exterior} , γ_{gb} denote the surface free energies of the exterior surfaces and of the grain boundaries, respectively. The physically natural energy for the coupled systems is $E = \gamma_{\text{exterior}} A_{\text{exterior}} + \gamma_{\text{gb}} A_{\text{gb}}$, where A_{exterior} , A_{gb} denote the total area of the exterior surfaces and of the grain boundaries, respectively. It is convenient to normalize the energy by setting $E_{\text{exterior}} := A_{\text{exterior}}$, $E_{\text{gb}} := A_{\text{gb}}$, and defining

$$E_w = E_{\text{exterior}} + m E_{\text{gb}}, \quad (6)$$

as the *weighted energy*. For the coupled systems a natural restriction on m is that

$$m \in [0, 2), \quad (7)$$

since when $m = 2$, the energy of two exterior surface equals that of one-grain boundary, so that two exterior surfaces coupling with a grain boundary *wet* the grain boundary.

Mullins assumed that $0 < m \ll 1$, which is physically reasonable, and linearized the system in (4) about $y \equiv 0$. For the resultant linear system, known in the literature as *Mullins' small slope approximation*, he found a self-similar solution of the form $y(x, t) = \frac{m}{\sqrt{4-m^2}}(\mathcal{B}t)^{1/4}Y(\xi)$ where $\xi = x/(\mathcal{B}t)^{1/4}$, and derived a series formula for the dimensionless function $Y(\xi)$ which allowed him to predict that $y(0, t) = a_0 m(\mathcal{B}t)^{1/4}$ with $a_0 \approx -0.39$. The quantity $y(0, t)$ is known as the *thermal groove depth*, since the kinetic coefficient, $\mathcal{B}$, increases with temperature. Based on the linearization of the equation in (4), he also identified a traveling wave [37] describing a groove which steadily translates along the exterior surface with speed $V_0 = \mathcal{B}(m/3d)^3$, where d is the thermal groove depth.

Despite the years which have passed, many questions remain regarding the non-linear problem formulation given in (4). For example, it is not yet known whether it possesses self-similar solutions, although a positive answer has been demonstrated for (4) with partially linearized boundary conditions [3]. In the next two sections we outline some of what is known regarding traveling wave solutions for problem formulations related to (4).

7 Traveling Wave Solutions

In [29–32], together with J. Kanel we considered a configuration in which a grain boundary is attached at a thermal groove to an exterior surface in a *quarter loop geometry*. The quarter loop geometry refers to a two grain system which may be assumed to be of semi-infinite extent, in which the exterior surface is asymptotically flat, and where there is one internal grain boundary, which intersects the exterior surface and partitions the specimen into two grains, then asymptotes to one side, say to the right, to some specific depth below the exterior surface, say $-H$. If we assume that the profiles of both the exterior surface and the grain boundary can be described by graphs of functions, say by $h = h(x, t)$ and by $u = u(x, t)$, then we may obtain a problem formulation, much as in (4) above, except that now we need to consider $x \in (-\infty, s(t)) \cup (s(t), \infty)$, where $s = s(t)$ with $s(0) = 0$ since the groove can move, and we need to amplify the resultant equations with equations governing the motion for the grain boundary, such as

$$\begin{cases} u_t = \mathcal{A}\kappa, & \kappa = u_{xx}(1 + u_x^2)^{-3/2}, & x \in (-\infty, s(t)) \cup (s(t), \infty), & t \in (0, \infty), \\ y(s(t)^-, t) = u(s(t)^+, t), & & t \in (0, \infty), \\ \arctan(u_x(0^+, t)) = -\frac{\pi}{2} + \frac{1}{2}[\arctan(y_x(0^+, t)) + \arctan(y_x(0^-, t))], & & t \in (0, \infty), \\ u(\infty, t) = -H, & & t \in (0, \infty), \\ u(x, 0) = u_0(x), & & x \in (0, \infty), \end{cases} \quad (8)$$

where $u_0(x)$ needs to be prescribed. In [30] it was demonstrated that there indeed exists a traveling wave solution to the resultant system if $0 < m$ is sufficiently small.

It turns out that the restriction on m resulted from looking for traveling wave solutions which could be described as graphs of functions. The restriction could be removed by formulating the traveling wave problem in terms of the angles, $\Phi(s_1)$ and $\Psi(s_2)$, where $\Phi(s_1)$ and $\Psi(s_2)$ denote respective the angles between the tangent to the grain boundary and the exterior surface and the x -axis, and where s_1, s_2 are respective arc-length parameterizations for $\Phi(s_1)$ and $\Psi(s_2)$, with $s_1 \in (0, \infty)$, $s_2 \in (-\infty, 0) \cup (0, \infty)$, and with the thermal groove as the location where $s_1 = s_2 = 0$. Setting $s = (V/B)^{1/3}s_2$, where V is the wave speed, the problem to be satisfied by Ψ could be formulated as:

$$\begin{cases} \Psi_{sss} = \sin \Psi, & s \in (-\infty, 0) \cup (0, \infty), \\ \Psi(0^+) = \Psi(0^-) + 2 \arcsin(m/2), \\ \Psi_s(0^+) = \Psi_s(0^-), \\ \Psi_{ss}(0^+) = \Psi_{ss}(0^-), \\ \Psi(\pm\infty) = 0. \end{cases} \quad (9)$$

Based on this formulation and using a shooting argument, the following could be proven:

Theorem [31]. For all $m \in [0, 2)$, there exists a traveling wave solution to the coupled exterior surface and grain boundary problem (9) for the quarter loop geometry. For $0 < m \ll 1$, there exists a traveling wave solution which can be described via graphs of functions.

For all $0 \leq m < 2$, given a solution Ψ to (9), Φ can be prescribed in term of Ψ , and the wave speed is given by $V = B(\lambda/H)^3$ where λ is the unique real solution to the following algebraic equation

$$\lambda^3 + \lambda^2 \Psi_{ss}(0^+) - \frac{\mathcal{A}H^2}{B} \left[\frac{\pi}{2} - \frac{1}{2}(\Psi(0^+) + \Psi(0^-)) \right] = 0. \quad (10)$$

The existence of nonclassical (not graphs of functions) traveling wave solutions could be demonstrated numerically for $m \in (0, 2)$ sufficiently large. For the case of classical traveling wave solutions for $0 < m \ll 1$ sufficiently small, spectral stability of the 2D traveling wave solution in 3D was demonstrated numerically by Beck, Pan and Wetton [8]. Further stability results are possible [28].

8 Estimating the Reduced Mobility

The equation for motion by mean curvature, (2), contains a kinetic parameter, $\mathcal{A}$, the reduced mobility. In the context of evolution of microstructure, it is not so obvious how to estimate this parameter. Shvindlerman and colleagues developed a methodology for estimating $\mathcal{A}$ based on the half-loop geometry [2, 5]. The half-loop geometry

refers to a bi-crystal with bamboo structure, consisting of a layer with finite height and with infinite lateral extent, containing two crystals. One crystal is embedded within the other, and the grain boundary which separates them is U-shaped, with ends which are asymptotically parallel. They analyzed grain boundaries in the laboratory fitting the description above, which appeared to move with constant speed. Neglecting the effects of the exterior surface and assuming the grain boundary within its interior to move by mean curvature motion, they looked for traveling wave solutions with this shape. Such mean curvature motion solutions, which they referred to as U-shape solutions, were already known to exist [35] and can be prescribed explicitly by $Y_{\pm}(x - V_0 t)$, where

$$V_0 = \frac{A\pi}{4Q}, \quad Y_{\pm}(x) = \pm \left(Q - \frac{2Q}{\pi} \arcsin(e^{-\frac{\pi}{2Q}x}) \right), \quad x \in \mathbb{R}^+, \quad (11)$$

and $2Q$ is the asymptotic width of the embedded crystal, far from the “nose” of the U-shaped profile. Later in the mathematical literature, these solutions came to known as grim reaper solutions [1]. These solutions could be used to estimate the reduced mobility $\mathcal{A}$, using the formula for V_0 in (11), [2, 5, 44].

Based on our remarks up to now, it is clear that if the exterior surfaces evolve by surface diffusion, then they should have some effect of the motion, and hence in the process of estimation or measurement of $\mathcal{A}$. Anna Zigelman set out to estimate this effect in her MSc and PhD theses [43, 52, 53]. To simplify the analysis, she considered the effect of surface diffusion only in the neighborhood of the thermal groove. She derived equations for the leading order corrections to the shape of the exterior surface, the grain boundary profile, the shape of the thermal groove, as well as to the traveling wave velocity, by formal asymptotic analysis based on the assumption that $0 < m \ll 1$ in two distinguished limits:

$$(i) \quad L/Q = m^{1/3}, \quad (ii) \quad L/Q = O(1). \quad (12)$$

Limit (i) can be considered as a thin film (thin specimen) limit [43, 52], while limit (ii) corresponds better to the conditions of Shvindlerman’s original experiments [52]. In both cases, the exterior surface could be shown at leading order to satisfy a fourth order parabolic problem which decouples from the remainder of the system describing the motion. The leading order perturbation to the shape of the thermal groove is described by a second order parabolic equation with force which depends on the angle of inclination of the exterior surface along the thermal groove, as well as on V_1 , the perturbation to the velocity, V_0 at the nose of the profile. After some analysis [52, 53], V_1 , the perturbation to the velocity, could be prescribed as

$$V_1(t) = \frac{d}{dt}(r * B)(t), \quad r(t) = \mathcal{L}^{-1} \left[\frac{1}{\omega \mathcal{L}[G](\omega)} \right](t), \quad (13)$$

where $\mathcal{L}$, $\mathcal{L}^{-1}$ denote, respectively, the Laplace transform and its inverse, $*$ denotes the convolution operator, $B(t)$ depends on the inclination of the exterior surface along

the thermal groove, the shape of the thermal groove, and on an appropriately defined heat kernel, and $\mathcal{G}$ is a weighted integral of the heat kernel.

In the experiments the motion was viewed from above, and measurements were made not of V_n and κ , but rather of $(V_n)_{\text{effective}}$, the projection of the normal velocity at the nose on the plane of observation, and $\kappa_{\text{effective}}$, the curvature at the nose of the projection of the groove root on the plane of observation. The measurements utilized the formula

$$(V_n)_{\text{effective}} = A_{\text{effective}} \kappa_{\text{effective}}, \quad (14)$$

and our results can be used to correct to the reduced mobility measurements by noting that

$$\frac{A_{\text{effective}}}{A} = \frac{(V_n)_{\text{effective}}}{V_n} \cdot \frac{\kappa}{\kappa_{\text{effective}}}, \quad (15)$$

where V_n , κ can be approximated via their zeroth order description and the leading order corrections.

9 Parametric Surfaces

Vadim Derkach developed and implemented a numerical code in his MSc and PhD Theses [15, 16, 18, 19] based on parametric surfaces, staggered grids, and finite differences designed to follow the evolution of certain special geometries containing a small number of grains, with the goal of gaining insight into various known physical phenomena such as pitting, grain annihilation, dewetting, and void formation (Figure 1). The small systems studied numerically by Vadim modeled thin or even nano-thin polycrystalline films with the bamboo structure mentioned earlier. Here “thin” and “nano-thin” refers to material layers ranging in thickness from a fraction of nanometer to several microns, and typically solid thin films are polycrystalline. They are highly important in many technological applications, such as electronic semiconductors, microchips, computer memory, optical coatings, and much more. Thermal grooving, pitting and hole formation influences thin film stability and robustness, and wetting/dewetting phenomena can lead to total film degradation. Let us now describe the numerical framework which was developed for studying small thin polycrystalline systems, which was later adapted for studying more specifically wetting and dewetting dynamics. Vadim’s MSc Thesis [15, 18] treated the special five and three-grain systems portrayed in Fig. 2, which led the way to the study in his PhD Thesis [16] of three-grain systems bounded within a triangular domain, which upon reflection could yield a “tiling” of the plane with a thin material layer. In these three-grain triangle systems, the initial film height was approximately uniform, see Fig. 3, and projections of the initial resultant tilings are portrayed in Figs. 4–5.

Let us now consider these three-grain systems in the triangular domains in some detail. Looking at Fig. 3, we see that they contain three exterior surfaces, three-grain boundaries, three triple junctions along the exterior surface which develop into

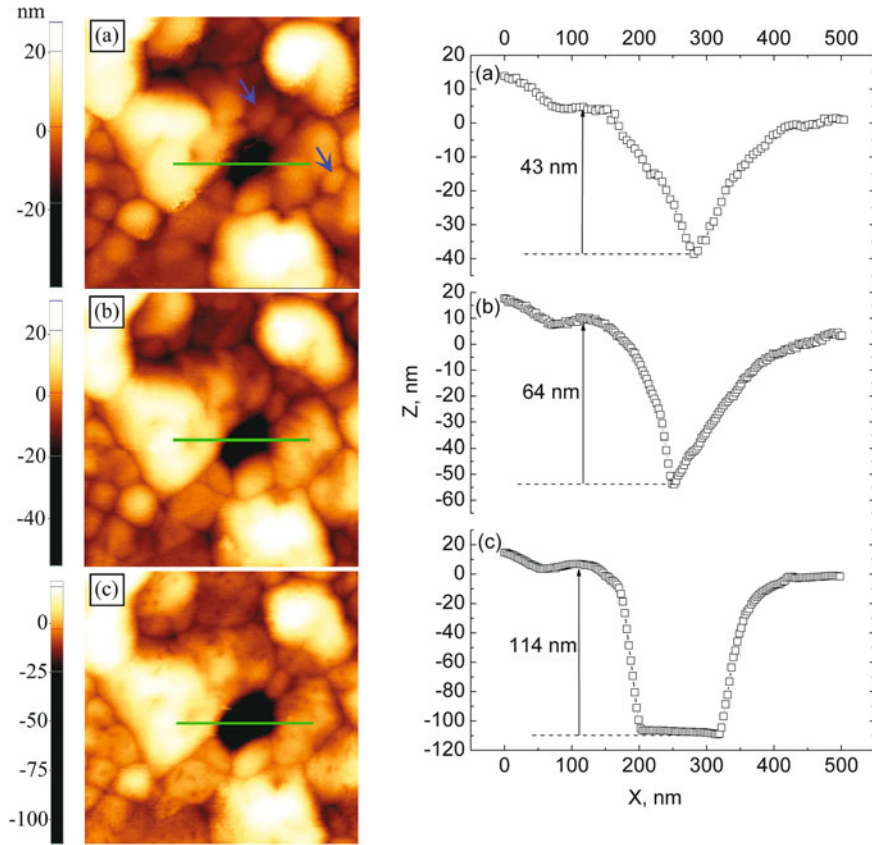


Fig. 1 (a–c). AFM images of a Cu thin film on sapphire substrate after the first (a), second (b), and third (c) consecutive anneal for 10 min at 300°C. The lateral dimensions of the image are $1 \times 1 \mu\text{m}^2$, and the color code labeled “nm” indicates the film height. A small grain visible in (a), sinks after the second anneal, leading to hole formation after the third anneal. Grains which disappeared after the second anneal without hole formation are marked in (a) by arrows which are blue in the online version. (d–f). The line topography profiles taken along the respective lines in (a–c). From Derkach, Novick-Cohen, Vilenkin and Rabkin [18], reproduced with permission

thermal grooves, as well as one internal triple junction line. There is a quadruple junction where the four triple junction lines meet. The triangular domain is bounded on three sides by vertical planes, as well as by a “mid-plane” located below at $z = 0$.

It is possible to prescribe a problem formulation for the evolution of these three-grain systems in accordance with the Mullins’ framework discussed earlier. Namely, the exterior surfaces are assumed to evolve by surface diffusion, and the grain boundaries are assumed to evolve by mean curvature motion. Along the thermal grooves, the conditions imposed include: (i) persistence, (ii) balance of mechanical force (angle conditions), (iii) continuity of the chemical potential, (iv) balance of mass flux. Along the internal triple junction line, (I) persistence and (II) angle conditions

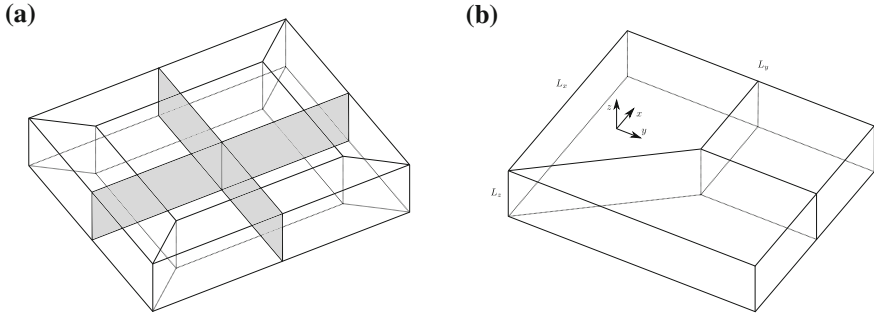
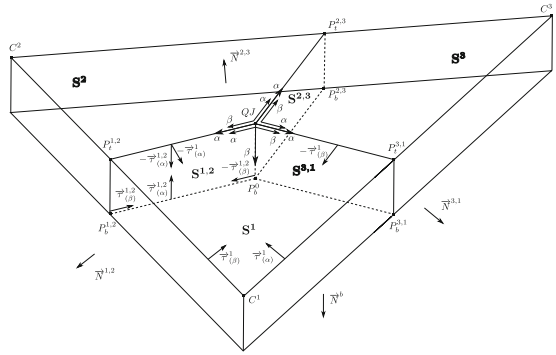


Fig. 2 Sketch of 5-grain and 3-grain geometries, see [19]

Fig. 3 Three grains in a triangular domain



are imposed. Symmetry is imposed with respect to the three planes bounding the triangular domain along its sides as well as with respect to the “mid-plane” at $z = 0$. At the corners of the domain and at the intersection of the evolving surfaces with the bounding planes, conditions can be imposed in accordance with (i)–(iv), (I)–(II), and symmetry.

The six evolving surfaces can be described by extending the parametric representation for a regular evolving curve in R^2 given in (1) to the parametric representation of a regular evolving surface in R^3 by setting $\mathcal{S}(t) := \{X(\alpha, \beta, t) : [0, 1]^2 \times [0, T] \rightarrow R^3\}$, where

$$X(\alpha, \beta, t) = (x(\alpha, \beta, t), y(\alpha, \beta, t), z(\alpha, \beta, t)), \quad 0 \leq \alpha, \beta \leq 1, \quad t \in [0, T]. \quad (16)$$

The coordinate orientations for the various surfaces are indicated in Fig. 3. The normal velocity V_n of X is given by $V_n = \langle X_t, \vec{n} \rangle$, where $\vec{n}$, the unit normal to X , may be expressed as $\vec{n} = \frac{X_\alpha \times X_\beta}{\|X_\alpha \times X_\beta\|}$. The mean curvature of X is given by

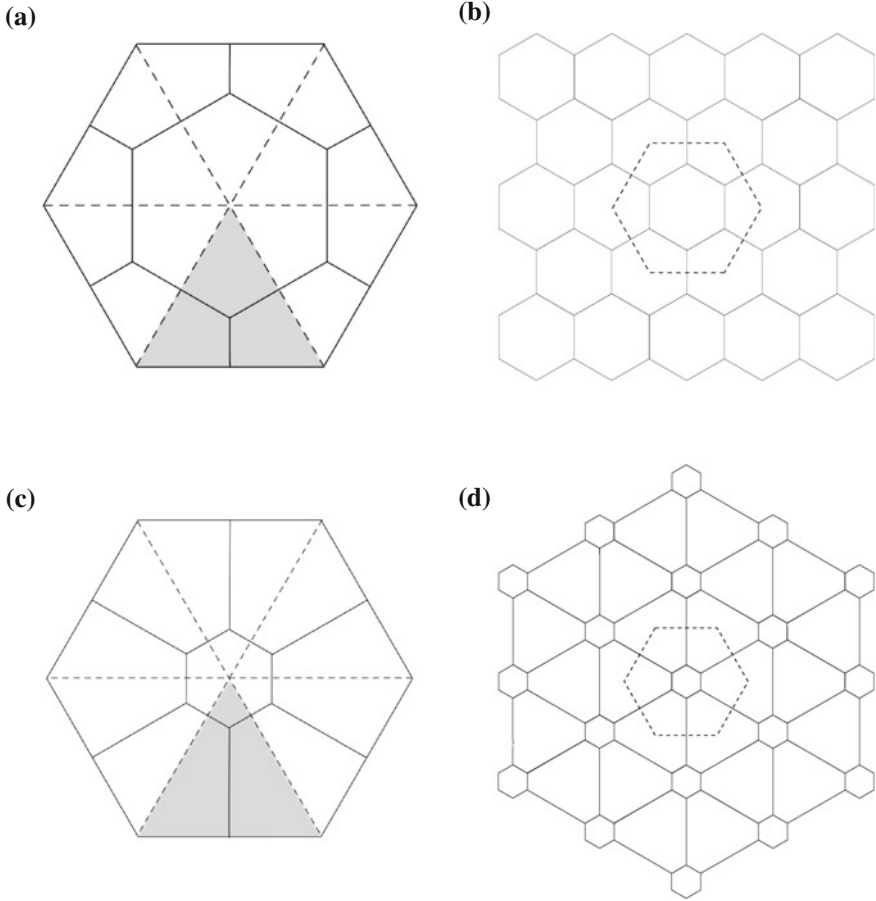


Fig. 4 The x - y projection of the three-grain system shown in the grey equilateral triangular domain in (a) can be extended by reflection to yield the hexagonal tiling of R^2 portrayed in (b). The x - y projection of the three-grain system shown in the grey equilateral triangular domain in (c) can be extended by reflection to yield the tiling of R^2 portrayed in (d) comprised of hexagons and truncated triangles

$$H = \frac{\langle \langle X_\beta, X_\beta \rangle X_{\alpha\alpha} - 2 \langle X_\alpha, X_\beta \rangle X_{\alpha\beta} + \langle X_\alpha, X_\alpha \rangle X_{\beta\beta}, \vec{n} \rangle}{2 \left[\langle X_\alpha, X_\alpha \rangle \langle X_\beta, X_\beta \rangle - \langle X_\alpha, X_\beta \rangle^2 \right]}. \quad (17)$$

Rather than specifying tangential velocities, we impose the conditions

$$\langle X_\alpha, X_{\alpha\alpha} \rangle = 0, \quad \langle X_\beta, X_{\beta\beta} \rangle = 0, \quad (18)$$

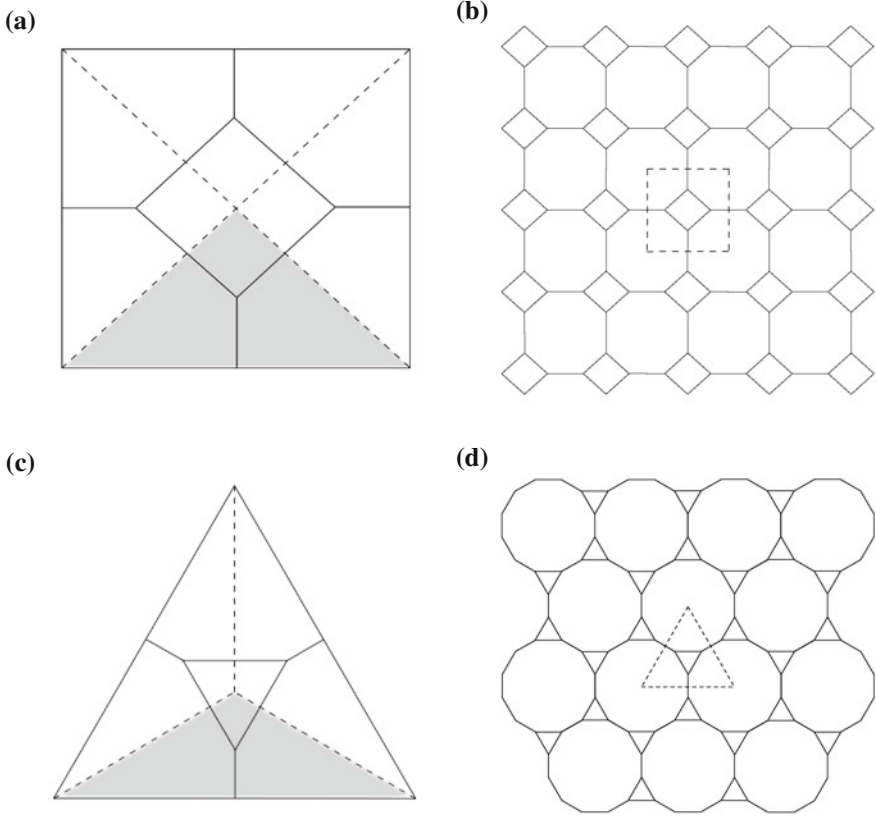
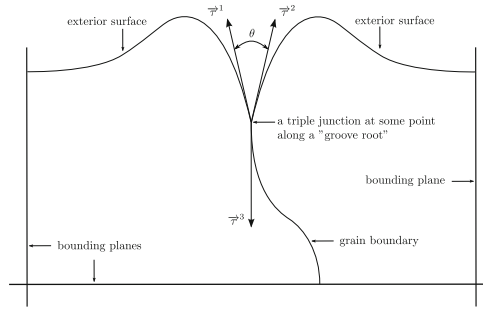


Fig. 5 The x - y projection of the three-grain system shown in the grey equilateral triangular domain with angles $\pi/4$, $\pi/2$, $\pi/4$ in (a) can be extended by reflection to yield the tiling of R^2 portrayed in (b) comprised of hexagons and truncated triangles. The x - y projection of the three-grain system shown in the grey equilateral triangular domain with angles $\pi/6$, $2/3\pi$, $\pi/6$ in (c), yields upon reflection a truncated square tiling and a truncated hexagonal tiling, respectively, of R^2 , portrayed in (d)

which guarantees uniform grid spacing in sense that $\|X_\alpha\|_\alpha = \|X_\beta\|_\beta = 0$; a similar approach was used in [42] for the coupled evolution of three curves in the plane. Let X^1 , X^2 , X^3 denote two exterior surfaces and a grain boundary which couple along a thermal groove. Along the thermal groove (i) persistence can be expressed as $X^1 = X^2 = X^3$, and (ii) balance of mechanical forces in the plane orthogonal to the thermal groove implies that $\vec{\tau}^1 + \vec{\tau}^2 + m\vec{\tau}^3 = 0$, where for $i = 1, 2, 3$, $\vec{\tau}^i$ is an outward unit tangent vector to X^i in the plane orthogonal to the thermal groove, see Fig. 6, and m was defined in (5). The angle θ indicated in Fig. 6 satisfies

$$\theta = \pi - 2 \arcsin(m/2), \quad (19)$$

Fig. 6 The normal cross-section to a thermal groove



and is known as the *dihedral angle*. Moreover, (iii) continuity of the chemical potential can be expressed as $H^1 = H^2$, since the chemical potential can be identified with the mean curvature along the exterior surface, and (iv) balance of mass flux along the exterior surface may be expressed as $\langle \vec{\tau}^1, \nabla_s H^1 \rangle + \langle \vec{\tau}^2, \nabla_s H^2 \rangle = 0$, since along the exterior surface the mass flux is proportional to $\nabla_s H$.

Along the internal triple junction line, letting now X^1, X^2, X^3 denote the three-grain boundaries which couple along the internal triple junction line, (I) persistence may be expressed as $X^1 = X^2 = X^3$, and (II) Young's law may be expressed as $\vec{\tau}^1 + \vec{\tau}^2 + \vec{\tau}^3 = 0$, respectively.

Let Π denote one of the three vertical bounding planes, $\vec{N}$ denote a vector which is normal to Π , and r_0 denote a point on Π . If X denotes an evolving exterior surface which intersects Π , then persistence, symmetry, and zero mass flux through Π may be expressed as $\langle X - r_0, \vec{N} \rangle = 0$, $\langle \vec{n}, \vec{N} \rangle = 0$, and $\langle \vec{N}, \nabla_s H \rangle = 0$, respectively, and if X denotes an evolving grain boundary surface then persistence and symmetry may be expressed as $\langle X - r_0, \vec{N} \rangle = 0$ and $\langle \vec{n}, \vec{N} \rangle = 0$, respectively. Where two exterior surfaces intersect a bounding plane (see $P_t^{1,2}, P_t^{2,3}, P_t^{3,1}$ in Fig. 3) or an exterior surface intersects two bounding planes (see C^1, C^2, C^3 in Fig. 3), conditions are formulated in accordance with persistence, symmetry and zero mass flux. At the intersection of a grain boundary and a bounding plane with the mid-plane (see $P_b^{1,2}, P_b^{2,3}, P_b^{3,1}$ in Fig. 3) or at the intersection of the interior triple junction line with the mid-plane (see P_b^0 in Fig. 3), conditions are formulated in accordance with persistence and symmetry.

To follow the motion of the various coupled surfaces using regular parametric representations, it is necessary to prescribe boundary conditions at the quadruple junction. The condition which we impose is based on the assumptions that (i) Young's law holds along all triple junction lines up to the quadruple junction, and (ii) limiting regularity at the quadruple junction, implying that the triple junction lines become asymptotically straight as the quadruple junction is approached. Assumptions (i)–(ii) imply the unique construction, up to similarity, of a tetrahedron with prescribed angles at the quadruple junction, based on the tangents to the triple junctions lines meeting at the quadruple junction. See Fig. 7.

Assumptions (i)–(ii), together with a bit of trigonometry, imply that

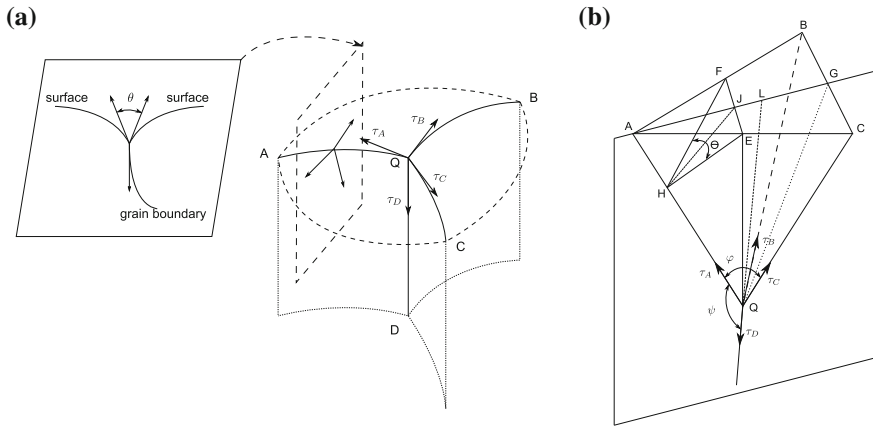


Fig. 7 (a) Sketch of the quadruple junction. Here τ_A, τ_B, τ_C denote tangents to the triple junction lines which meet at the quadruple junction. (b) The tetrahedral construction based on the tangents τ_A, τ_B, τ_C

$$\cos(\varphi) = -\frac{2 - m^2}{4 - m^2}, \quad 0 \leq \varphi \leq \frac{2\pi}{3}, \quad (20)$$

$$\cos(\psi) = -\frac{1}{\sqrt{3}} \frac{m}{\sqrt{4 - m^2}}, \quad \frac{\pi}{2} \leq \psi \leq \pi, \quad (21)$$

where $\varphi = \cos^{-1}(\tau_A \cdot \tau_C)$ and $\psi = \cos^{-1}(\tau_A \cdot \tau_D)$, see Fig. 7b. Recalling from (see (7)) that $m \in [0, 2)$, it follows from (21) that the construction requires that $m \in [0, \sqrt{3}) \subset [0, 2)$. The breakdown of the construction when $m = \sqrt{3}$ can be seen as indicating $m = \sqrt{3}$ as a quadruple junction wetting criterion, Derkach, 2010 [15]. Smith [45] employed a similar construction in 1948 in analyzing the stability of triple junctions in the microstructure in two-phase alloys. Straumal, Kogtenkova and Zięba [47] found a similar criteria in 2007 in the context of wetting of triple junctions by melt. The (F, ϵ, δ) minimal surfaces approach for soap-bubbles (Taylor 1976 [49]) is relevant here also [48].

The problem formulation outlined above yields a PDE system which was solved numerically using finite difference methods to spatially discretize the system. Staggered grids were employed for each evolving α - β surface, using ghost points on each grid to accommodate the boundary conditions. The mean curvatures of the exterior surfaces were defined as additional variables [6]. The resultant DAE (differential and algebraic equation [4]) system was solved using a backward Euler (implicit) method. Newton iterations were used to solve the resultant nonlinear equations at each time step. Partial parallelization was used in calculating the Jacobian matrix and in solving the large system of linear equations which results at each Newton's method iteration. The approach here extends that of Pan and Wetton [42] to three spatial dimensions. For details, see [15, 16, 19].

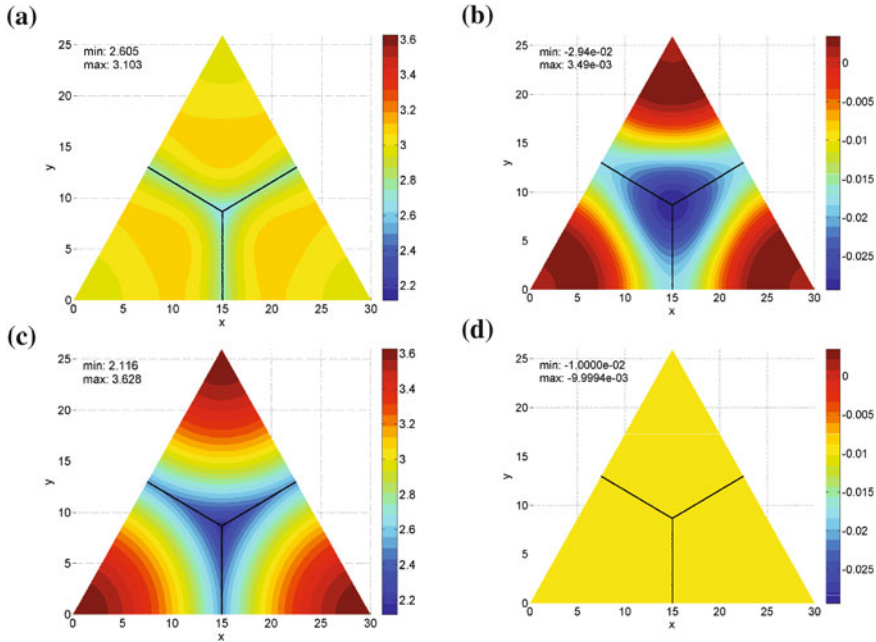


Fig. 8 Here initially the grain volume fractions are equal, $L_C^1 C^2 = 30$, $L_z = 3$, and $m = 0.3$. Exterior surfaces heights at times (a) $t = 50$, (c) $t = 6300$, and mean curvatures at times (b) $t = 50$, (d) $t = 6300$. Threefold symmetry is maintained. The mean curvatures converge to $\approx 10^{-2} = mL_{C^1 C^3}^{-1}$ in accordance with the spherically capped hexagon configuration, despite earlier small slope predictions indicating hole formation at the quadruple junctions, Génin et al. [21]

The algorithm was implemented in [18] where good qualitative agreement with experiment could be seen with regard to physical features such as pitting, grain annihilation, and hole formation. Results from more recent simulations which were undertaken for initial conditions corresponding to the triangular configurations shown in Fig. 4 are portrayed in Figs. 8, 9 and 10. Note that in Fig. 8, where the initial configuration possesses three-fold symmetry, the three fold symmetry is maintained, the grain boundaries remain flat, and the exterior surfaces seem to approach constant mean curvature spherical caps. In Fig. 9, where the initial conditions have reflectional symmetry but not three-fold symmetry and one of the three grains is slightly smaller than the other, the system seems to be evolving towards the limiting spherically capped configuration seen in Fig. 8, indicating some measure of stability for this configuration. In Fig. 10, the initial conditions were similar to those portrayed in Fig. 9, but here the third smaller grain was taken to be smaller than before, and the system no longer seems to be evolving toward the spherically capped configuration.

To gain some comprehension and interpretation of these results, let us consider steady states with threefold symmetry with triangular bounding planes, whose x - y projection yield *hexagonal tilings* upon extension by reflectional symmetry. For

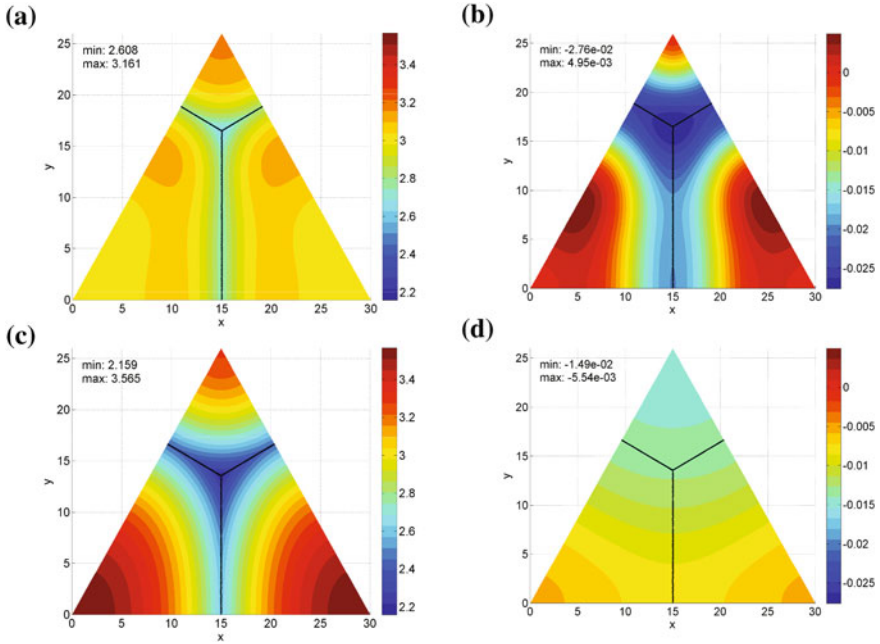


Fig. 9 Here the initial grain volume fractions are given by $\phi_{C^1} = \phi_{C^3} = 0.45$, $\phi_{C^2} = 0.1$, $L_{C^1C^2} = 30$, $L_z = 3$ and $m = 0.3$. Exterior surface heights at times (a) $t = 50$, (c) $t = 2310$, and mean curvatures at times (b) $t = 50$, (d) $t = 2310$. The smaller grain is seen to grow, and the system appears to approach the steady state seen in Fig. 8

these configurations there exist steady states for our dynamic problem formulation if the initial volume is sufficiently large and if the parameter m is sufficiently small. Some details follow below. Further details will appear in [17]. By considering the reflectional extension to hexagons, these configurations can be viewed as spherically capped hexagonal cylinders. Some discussions in these directions were given some 30 years by Finn [20] and Srolovitz and Safran [46].

To understand the restrictions, let us consider some details of the geometry, see Fig. 11. The intersections of the spherical caps with the flat vertical grain boundaries define circular sections, whose maximal height relative to the height of the spheres' centers is given by $z_{\max} = (L_{C^3C^1} \sqrt{4 - m^2}) / (2m)$, and whose minimal height, which is attained at the quadruple junctions, is given by $z_{\min} = (L_{C^3C^1} \sqrt{3 - m^2}) / (\sqrt{3}m)$. In particular, the construction requires $0 < m < \sqrt{3}$, and hence $m = \sqrt{3}$ appears again as a quadruple junction wetting criterion. This restriction may be seen as being sharp by considering the following *nonexistence result*.

Theorem. Given a domain Ω containing a corner with interior angle α . If $\alpha + \theta < \pi$, then there exist no constant mean curvature surfaces defined over Ω which are bounded from below which meet $\partial\Omega$ with contact angle $\theta_c = \frac{1}{2}(\pi - \theta)$.

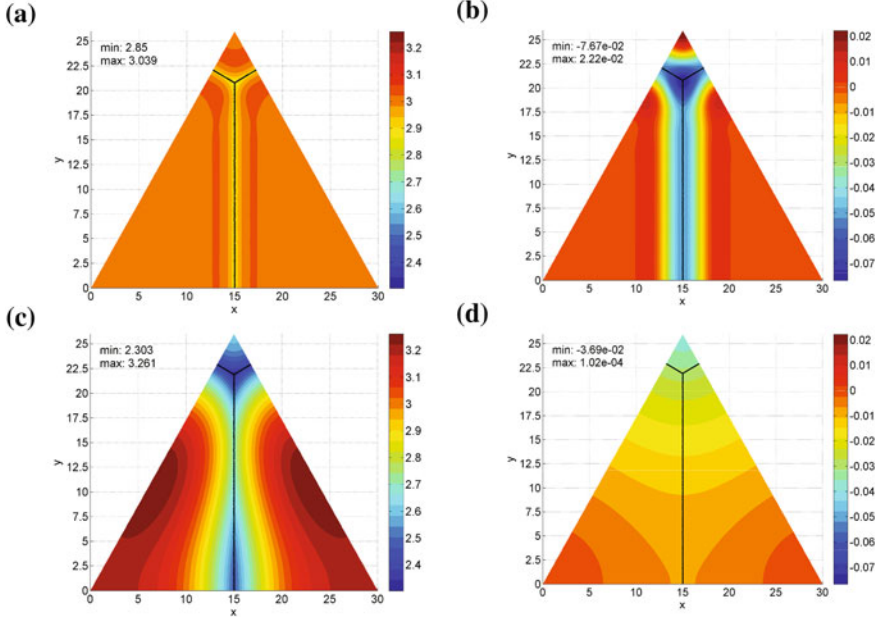


Fig. 10 Here the initial grain volume fractions are given by $\phi_{C^1} = \phi_{C^3} = 0.485$, $\phi_{C^2} = 0.03$, $L_{C^1C^2} = 30$, $L_z = 3$ and $m = 0.3$. Exterior surface heights at times (a) $t = 1$, (c) $t = 703$, and mean curvatures at times (b) $t = 1$, (d) $t = 703$. We observe shrinkage and sinking of the smaller grain. Apparently if initially one grain is much smaller than the others, the steady state seen in Fig. 8 is not approached

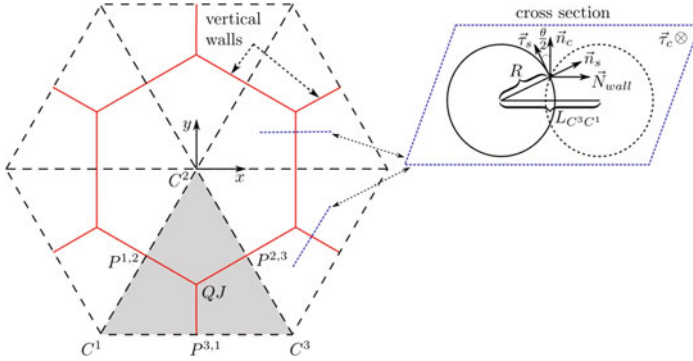


Fig. 11 The x - y projection of the three-grain system shown in the grey equilateral triangle extends by reflection to yield a tiling by hexagonal grains. The exterior surface above each hexagonal grain is a spherical cap. The spherical caps intersect each other with dihedral angle $\theta = \pi - 2 \arcsin(m/2)$ along thermal grooves lying above the sides of the hexagon. Vertical planar grain boundaries surround each grain, intersecting with three fold symmetry along internal triple junction lines which lie above the corners of each hexagon. See Finn, 1985 [20], Srolovitz and Safran, 1986 [46], Derkach, 2016 [16]

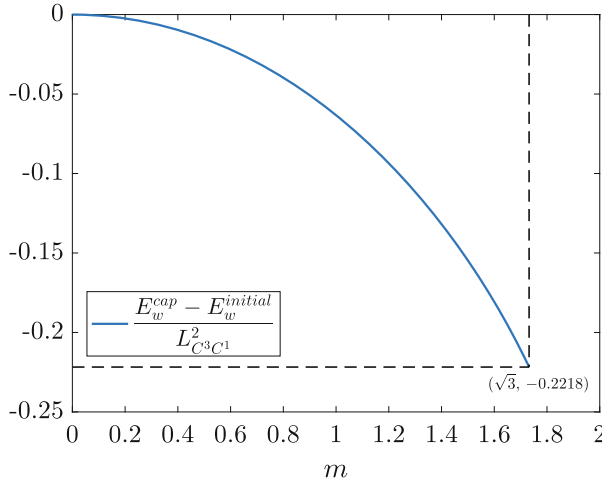


Fig. 12 A plot of $(E_w^{cap} - E_w^{initial})L_{C^3C^1}^{-2}$ for $m \in (0, \sqrt{3})$

Proof. The proof follows from Finn [20, Corollary 5.5] and the definitions given there.

In the context of the equilateral triangular system, $\alpha = \frac{2\pi}{3}$ and it follows from (19) that $\theta = 2 \cos^{-1}(m/2)$. The restriction $\alpha + \theta < \pi$ implies that the nonexistence of solutions which are bounded from below if $m > \sqrt{3}$. The non-boundedness from below can be shown [20] to occur at the vertex of the interior corner. In terms of the geometry of the spherical capped hexagon, this implies that any such steady states for $m \in [\sqrt{3}, 2)$ must necessarily penetrate the film at the quadruple junction.

The results above were concerned with equilibrium capillary surfaces in unbounded cylinder with unbounded mass. In the context of thin films, the film thickness required to guarantee film stability is a technologically critical issue. This leads us to consider volume restrictions for the realization of these configurations. The volume of the spherical cap over the hexagon and above height $z_{\min}$ is given by

$$V^{cap} = L_{C^3C^1}^3 \left[\mathcal{F}(m) - \frac{\sqrt{3-m^2}}{2m} \right],$$

where

$$\mathcal{F}(m) = \frac{3}{2} \int_0^1 \left[\frac{\xi \sqrt{3-m^2\xi^2}}{3m} + \frac{4-m^2\xi^2}{2m^2} \arcsin\left(\frac{m\xi}{\sqrt{3}\sqrt{4-m^2\xi^2}}\right) \right] d\xi.$$

Letting L_z^* denote the height of a flat configuration with equivalent volume, namely the height L_z^* such that $V^{cap} = \frac{\sqrt{3}}{2} L_z^* L_{C^3C^1}^2$, we obtain that realization of the capped hexagon configuration requires that

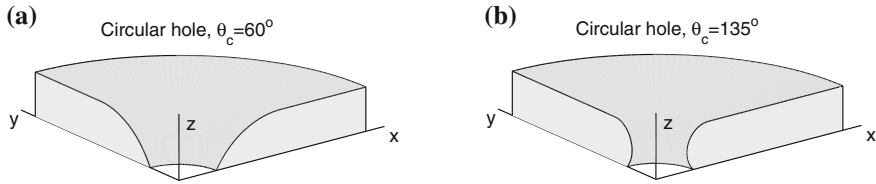


Fig. 13 Sketches of the initial circular 3D-domains which used to model hole growth and hole shrinkage by wetting and dewetting in mono-crystals. (a), (b), circular holes in mono-crystals with contact angles $\theta_c = 60^\circ$ and $\theta_c = 135^\circ$, respectively

$$L_z \geq L_z^* = \frac{2}{\sqrt{3}} \left[\mathcal{F}(m) - \frac{\sqrt{3-m^2}}{2m} \right] L_{C^3C^1}.$$

Note in particular that if $m = 0.3$, then $L_z^* \approx 0.02946 L_{C^3C^1}$.

If the conditions are such that the spherically capped hexagon configuration can be realized, is it energetically preferable relative to say the equivalent volume flat configuration? The relevant energy to consider in this regard is the weighted energy, E_w , (see (6)) which for the capped hexagons is

$$E_w^{cap} = L_{C^3C^1}^2 \mathcal{G}(m) + \sqrt{3} m L_z L_{C^3C^1}, \quad (22)$$

where the function $\mathcal{G}(m)$ may be explicitly prescribed, and which for the equivalent volume flat configuration with flat grain boundaries is given by

$$E_w^{initial} = \frac{\sqrt{3}}{2} L_{C^3C^1}^2 + \sqrt{3} m L_z L_{C^3C^1}. \quad (23)$$

It follows from (22)–(23) that $(E_w^{cap} - E_w^{initial})/L_{C^3C^1}^2$ is a function of m only. This function was calculated numerically using Matlab and is portrayed in Fig. 12; it can be clearly seen in Fig. 12 that $E_w^{cap} \leq E_w^{initial}$ for $m \in (0, \sqrt{3})$.

In the discussions above, weighted energies were compared for configurations with the same volume and where the length, $L_{C^3C^1}$, of side of the bounding triangle was fixed. Note that by virtue of the geometry, $L_{hexagon} = \frac{1}{\sqrt{3}} L_{triangle} = \frac{1}{\sqrt{3}} L_{C^3C^1}$. Let us compare the weighted energies for spherically capped hexagon configurations with the same volume, but allowing now the length of the triangle (hexagon) side to vary. Taking V , the volume of the system, to be fixed, implies that, L_z , the height of the equivalent volume flat triangular system satisfies $L_z = \frac{2}{\sqrt{3}} V L_{C^3C^1}^{-2}$. It then follows from (22) that E_w^{cap} may be expressed as

$$E_w^{cap} = L_{C^3C^1}^2 \mathcal{G}(m) + \frac{2mV}{L_{C^3C^1}}, \quad (24)$$

which attains a minimum at

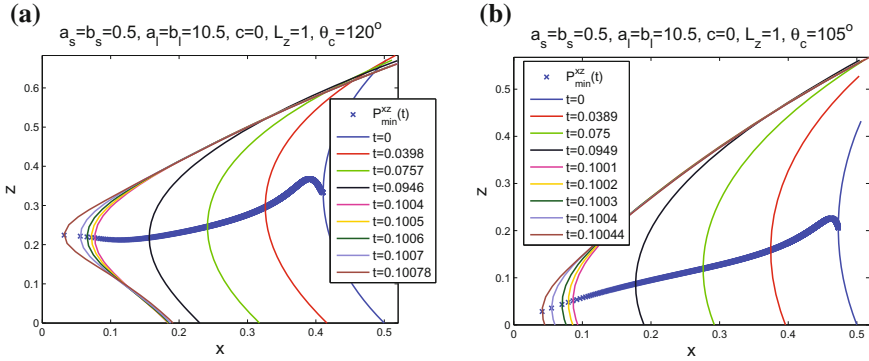


Fig. 14 Diagram showing the void creation in the wetting case when $\theta_c > \frac{\pi}{2}$, where the initial hole radius was 0.5 and the initial film height was $L_z = 1$. Profiles of the free boundary along xz bounding plane for: (a) $\theta_c = 120^\circ$; (b) $\theta_c = 105^\circ$. Evolution in (a) appears to be asymptotically self-similar, see Bernoff, Bertozzi and Witelski [10], whereas what is happening in (b) is less clear

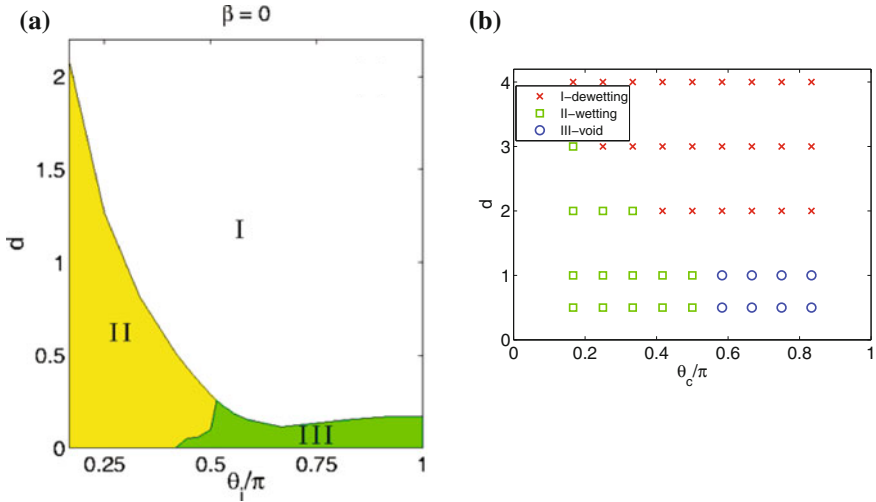


Fig. 15 Diagram indicating the dependence of I) dewetting, II) wetting, III) void creation on the initial hole diameter and on the contact angle θ_c . (a) Results from the simulations of Wang, Jiang, Bao and Srolovitz [50] (reproduced with permission) for holes in 2D films with initial diameter d . Here $\beta = 0$ indicates isotropy is being assumed. (b) Results from our simulations for 3D circular holes with initial diameter d , see Fig. 13. Comparing the 2D results with the 3D results, we conclude that the second curvature appearing in the 3D calculations acts effectively as a drag force, allowing holes with larger initial radius to shrink

$$L_{C^3C^1}^{\min} = \left[\frac{mV}{\mathcal{G}(m)} \right]^{\frac{1}{3}}. \quad (25)$$

We conjecture that (25) is indicative of an energetically preferred length scale for grains with prescribed volume in a bamboo structured system.

Should coarsening be expected to ensue in the spherically capped system? It follows from (22) that the weighted energy per unit area of the capped hexagon system is given by

$$\frac{2}{\sqrt{3}} \frac{E_w^{cap}}{L_{C^3C^1}^2} = \frac{2}{\sqrt{3}} \mathcal{G}(m) + \frac{2mL_z}{L_{C^3C^1}}. \quad (26)$$

Since (26) decreases as $L_{C^3C^1}$ increases, there is an energetic preference for coarsening. However coarsening may be hindered by dynamic considerations such as local energy barriers.

In concluding we remark that while many open questions remain regarding the system of capped hexagons, we see in Figs. 13, 14 and 15 that the algorithmic approach developed for studying systems of grains can be adapted for studying wetting and dewetting phenomena, [16].

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