Journal of Statistical Physics, Vol. 95, Nos. 5/6, 1999

A Variational Approach to Crystalline Triple-Junction Motion

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Received August 4, 1998

A variational description is given for curves with triple junctions for the motion with normal velocity $v = M(C + \kappa_\Phi)$, where κ_Φ stands for the crystalline curvature as determined by the curves and by the crystalline (polygonal Wulff shape) surface free energy functions Φ for each interface, C is constant on each interface, and M is a compatible normal-dependent mobility function for each interface. This variational formulation is based on the idea that the motion should be gradient flow, in the L^2 inner product, for the sum of the surface free energy and the bulk free energy. If the surface free energy functions Φ are identically zero, the motion is that given by Taylor (1995). If the surface free energy functions are positive and crystalline, then the motion is that given by Taylor (1993). Finally, if the surface free energy functions are written as $\Phi = \varepsilon\Phi_0$, then the limiting motion as $\varepsilon \downarrow 0$ is in general different from the motion for $\varepsilon = 0$ [and hence different from that given by Taylor (1993); the limiting motion is presumably that given by Reitich and Mete Soner (1996)].

KEY WORDS: Motion by weighted mean curvature; geometric crystal growth; triple-junction motion; L^2 gradient flow; crystalline surface energy; mobility; grain growth; polycrystalline evolution; variational.

1. INTRODUCTION

This paper provides a variational formulation for geometric crystal growth of polycrystals. It primarily considers polyhedral curves in R^2 meeting at triple junctions; these curves form the boundaries of regions (which are not necessarily connected or simply connected). To be precise and more general, a polycrystal configuration consists of a finite number N of closed regions $\{K_\alpha\}_{\alpha = 1, \ldots, N}$ with rectifiable boundaries having finite surface area,

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0022-4715/99/0600-1221$16.00/0

such that each region is the closure of an open set, their union is all of R^d, and each pair of regions intersects only along the portion of their boundaries that they have in common (the *interface* between those regions). The words "volume" and "surface area" will continue to be used when $d=2$, although speaking of area in the 2-dimensional plane and length of curves respectively.

Let $S_{\alpha\beta}$ denote the interface between K_α and K_β, oriented as part of the boundary of K_α (positively oriented). Thus $S_{\beta\alpha}$ is $S_{\alpha\beta}$ with the opposite orientation. Also $S_{\alpha\beta}$ might well be empty for a given pair α, β. If $\mathbf{x}$ is in $S_{\alpha\beta}$, let $\mathbf{n}_{\alpha\beta}(\mathbf{x})$ be the oriented normal to $S_{\alpha\beta}$ at $\mathbf{x}$; it thus points from region α into region β.

We will consider a class of motions driven by surface free energy changes and/or bulk free energy changes. For each α, let $\mathscr{B}_\alpha$ be the bulk free energy per unit volume of the phase of K_α. We assume for convenience (and without loss of generality) that the regions are indexed so that $\mathscr{B}_\alpha \leqslant \mathscr{B}_\beta$ if $\alpha < \beta$. The surface free energy per unit area for an interface $S_{\alpha\beta}$ is a function $\Phi_{\alpha\beta}$ from R^d to R which is either positive on unit vectors $\mathbf{n}$ and satisfies $\Phi_{\alpha\beta}(r\mathbf{n}) = r\Phi_{\alpha\beta}(\mathbf{n})$ for all $\mathbf{n}$ and all $r \geqslant 0$, or else is zero on all vectors in R^d. For geometric crystal growth, as reviewed in [TCH], the normal velocity $v(\mathbf{x})$ at a point $\mathbf{x}$ in $S_{\alpha\beta}$ is given by

$$v(\mathbf{x}) = M_{\alpha\beta}(\mathbf{n}_{\alpha\beta}(\mathbf{x}))(C_{\alpha\beta} + \kappa_{\Phi_{\alpha\beta}}(S_{\alpha\beta}, \mathbf{x}))$$

Here $M_{\alpha\beta}$ is a mobility function (assumed to be positive), $C_{\alpha\beta} = \mathscr{B}_\beta - \mathscr{B}_\alpha$, and $\kappa_{\Phi_{\alpha\beta}}(S_{\alpha\beta}, \mathbf{x})$ is the weighted mean curvature of $S_{\alpha\beta}$ at $\mathbf{x}$. For further assumptions made on the Φ and M and the definition of $\kappa_{\Phi_{\alpha\beta}}(S_{\alpha\beta}, x)$ and other terms, see Section 2 below. For a discussion of how surface free energies arise thermodynamically, see [TC].

Motion by crystalline curvature of polygonal curves separating two regions was defined, analyzed and programmed in [T1], and was independently defined and analyzed in [AG]. In [T1] a statement was also given of a variational approach to determine geometric crystal growth for crystalline curves with triple junctions and boundary points; this variational approach involved only "surface" integrals, and it was given in principle rather than worked out explicitly. Computer programs to implement the principle, as illustrated for example in the video part of [T3], looked for, the minimizers using random insertion of extra segments and computational minimization. Section 3 of this paper makes this formulation explicit, identifying the precise class of situations where it can be applied and solving for the exact minimizing position motion of the triple junction at each time step.

In [ATW], a general means of finding motion by weighted mean curvature of surfaces separating two regions was given which involved

constructing approximating flows at discrete times and then proving that the approximating flows had a convergent subsequence as the time step decreased toward zero. Given an initial crystal position $K = K(0)$ (precisely, the d-dimensional positively-oriented integral current of multiplicity 1 everywhere that is determined by K) and a time step Δt, for each nonnegative integer n the new approximating crystal position at time $(n+1)\,\Delta t$, was found from $K_n = K(n\,\Delta t)$ by setting $K((n+1)\,\Delta t)$ equal to the minimizer, over all possible new crystal positions K, of an "energy"

$$\mathscr{E}_{ATW}(K, K_n, \Delta t) = \int_{\mathbf{x} \in \partial K} \Phi(\mathbf{n}_{\partial K}(\mathbf{x}))\, d\mathscr{H}^{d-1}\mathbf{x} + \frac{1}{\Delta t} \int_{\mathbf{x} \in K \sim K_n \cup K_n \sim K} \operatorname{dist}(\mathbf{x}, \partial K_n)\, d\mathscr{L}^d \mathbf{x}$$

In [AT] it was shown that the crystalline motion of [T1] was the same as the motion obtained by the volume-integral variational framework of [ATW]. Roosen [R] proposed, and Yip [Y] proved, that one could extend this formulation to the case where the mobility M depends on the normal direction of the interface by replacing the last term by

$$\frac{1}{\Delta t} \int_{\mathbf{x} \in K \sim K_n \cup K_n \sim K} \inf_{\mathbf{y} \in \partial K_n} M^*(\mathbf{x} - \mathbf{y})\, d\mathscr{L}^d \mathbf{x}$$

Here M^* is the dual norm to M, defined by $M^*(\mathbf{p}) = \sup_{\mathbf{q} \neq 0} (\mathbf{p} \cdot \mathbf{q}/M(\mathbf{q}))$. When the interface ∂K_n is planar, with normal $\mathbf{n}$, then $\inf_{\mathbf{y} \in \partial K_n} M^*(\mathbf{x} - \mathbf{y})$ is just $\operatorname{dist}(\mathbf{x}, \partial K_n)/M(\mathbf{n})$.

It is conjectured here that the appropriate analog to [ATW] for the polycrystalline case is the following: Given $\Delta t > 0$, an "old" polycrystal configuration $\{L_\alpha\}$ with interfaces $\{T_{\alpha\beta}\}$, and a "new" polycrystal configuration $\{K_\alpha\}$ with interfaces $\{S_{\alpha\beta}\}$, define

$$\mathscr{E}(\{K_\alpha\}, \{L_\alpha\}, \Delta t) = S_v + B_v + I_v$$

where S_v is the surface free energy change:

$$S_v = \sum_{1 \leqslant \alpha < \beta \leqslant N} \left(\int_{\mathbf{x} \in S_{\alpha\beta}} \Phi_{\alpha\beta}(\mathbf{n}_{S_{\alpha\beta}}(\mathbf{x}))\, dA\,\mathbf{x} - \int_{\mathbf{x} \in T_{\alpha\beta}} \Phi_{\alpha\beta}(\mathbf{n}_{T_{\alpha\beta}}(\mathbf{x}))\, dA\,\mathbf{x} \right)$$

B_v is the bulk free energy change:

$$B_v = \sum_\alpha \mathscr{B}_\alpha(\text{volume}(K_\alpha \sim l_\alpha) - \text{volume}(L_\alpha \sim K_\alpha))$$

and I_v is the "penalty" term corresponding to the integral of M^*:

$$I_v = \frac{1}{\Delta t} \sum_{\alpha < \beta} \int_{\mathbf{x} \in \mathscr{R}_{\alpha\beta}} \inf_{\mathbf{y} \in T_{\alpha\beta}} M^*_{\alpha\beta}(\mathbf{x} - \mathbf{y})\, dV$$

where $\{\mathscr{R}_{\alpha\beta}\}$ is a set of regions such that there exits a collection of $(d-1)$-dimensional rectifiable sets Q_i and a set of numbers $\{\delta_{i,\alpha\beta}\}$, each from the set $\{1, -1, 0\}$, with the boundary of $\mathscr{R}_{\alpha\beta}$ equal to $S_{\alpha\beta} - T_{\alpha\beta} + \sum_i \delta_{i,\alpha\beta} Q_i$ and with each i having $\delta_{i,\alpha\beta}$ nonzero for precisely three pairs $\alpha\beta$, $\beta\gamma$, $\gamma\alpha$ with $\alpha < \beta < \gamma$. A more general condition would have to be devised in case force-balanced quadrijunctions needed to be considered. The crystalline version presented in this paper, the $\mathscr{E}_c$ of Section 4, uses essentially this approach, but assumes that all the Q_i are straight line segments, $\delta_{i,\alpha\beta}$ is nonzero only for two values of i for each connected component of $S_{\alpha\beta}$, and all the $S_{\alpha\beta}$ are of a particular polygonal form.

Note that any given point $\mathbf{x}$ might be in several different $\mathscr{R}_{\alpha\beta}$, thereby allowing for several changes of phase for a point during the time step Δt. Caraballo [C] extended the [ATW] formulation and some of the analysis to some polycrystalline cases, but he only considered the case where all $C_\alpha\beta = 0$ and he used a different version of I_v. His version of I_v did not account for several changes of phase and does not extend correctly to general geometric motions with bulk free energies, but it was adequate since the exact form of the volume integral is relatively unimportant when the $C_{\alpha\beta}$ are all zero.

As in [ATW], motion over time Δt should be the minimizer of $\mathscr{E}$ over all such $K_{\alpha\beta}$ and $\mathscr{R}_{\alpha\beta}$, using for $\{L_\alpha\}$ the minimizer for the previous time step (or, at time 0, the given initial data). In both [C] and [ATW], it is important that ALL comparison surfaces be considered, but in the crystalline case outlined here only a particular limited class of polygonal comparisons is considered. It is conjectured, but not proven here, that minimizing $\mathscr{E}_c$ within this class is sufficient to give the same motion as would be obtained by minimizing $\mathscr{E}$ over all polycrystal configurations. (For motion by crystalline curves without triple junctions, this equivalence was proved in [AT], as stated above.) Also, future efforts will have to deal with the evolution through collisions of interfaces and triple junctions.

Because this volume-integral variational formulation is a direct consequence of the idea that the motion should be gradient flow, in the L^2 inner product, for the sum of the surface free energy and the bulk free energy, the motion it produces is a "natural" one. The motion that occurs when the surface free energies are zero is in general different from the limiting motion as those energies approach zero (i.e., using $\varepsilon\Phi$ as the surface free energy and letting ε go to zero). Furthermore, only these two varieties of motion

of triple junctions occur; there is no family of motions interpolating between them in this L^2 formulation. However, the physically correct motion is probably the limit motion rather than the zero-energy motion, whenever it is physically possible for there to be a surface free energy, even if that energy is usually neglected and thus by default set equal to zero.

The "surface" integral formulation yields Euler's method for solving the system of ordinary differential equations which give the desired motion, and the motion obtained by using finite time steps converges to the limit motion as the time step goes to zero. The system of ordinary differential equations has no particular stiffness until a segment with non-zero weighted mean curvature goes to zero length. The volume integral formulation is essentially an implicit method for solving the system, as the Euler-Lagrange equations involve the weighted mean curvature of the moved interfaces rather than the initial ones.

It is sometimes argued that triple junctions should have their own mobility, and thus be able to have the surface energy at the junction not be in force balance. Whether or not such mobilities exist, it is useful to see what results follow from the simpler assumption that there are no such separate mobilities.

There is a significant literature on motions of this type. See [TCH] for a survey as of 1992. Many authors listed in that bibliography continue to work on such problems. There have been particular advances in the diffuse interface approach [NC].

2. DEFINITIONS

Throughout this section, we specialize to the crystalline case in R^2. As the purpose of this paper is to lay out the variational framework, in many cases we make more restrictive assumptions than are absolutely necessary on the $\Phi_{\alpha\beta}$ and $M_{\alpha\beta}$.

Definition 2.1. A surface free energy function $\Phi_{\alpha\beta}$ is either identically zero on all vectors in R^2 or is positive on all unit vectors and satisfies $\Phi(r\mathbf{n}) = r\Phi(\mathbf{n})$ for all $r \geqslant 0$. We further assume that Φ_{ab} is convex (i.e., that $\Phi(a\mathbf{n}_1 + b\mathbf{n}_2) \leqslant a\Phi(\mathbf{n}_1) + b\Phi(\mathbf{n}_2)$). (Otherwise, we would have to use varifolds—infinitesimal corrugations—with the same underlying sets.) Except for the facet that we do not assume evenness, $\Phi_{\alpha\beta}$ is thus a norm on R^d. Each $\Phi_{\alpha\beta}$ has a Wulff shape $W_{\Phi_{\alpha\beta}} = \{\mathbf{x}: \mathbf{x}\cdot\mathbf{n} \leqslant \Phi_{\alpha\beta}(\mathbf{n})\}$. We assume that $\Phi_{\alpha\beta}$ is *crystalline*, i.e., that $W_{\Phi_{\alpha\beta}}$ is a polygon in R^2 (or just a point if $\Phi_{\alpha\beta} \equiv 0$). In order to avoid the necessity of considering infinitesimal layers, we require $\Phi_{\alpha_i\alpha_j}(\mathbf{n}) + \Phi_{\alpha_j\alpha_k}(\mathbf{n}) \geqslant \Phi_{\alpha_i\alpha_k}(\mathbf{n})$, for every triple of distinct indices i, j, k and every unit vector $\mathbf{n}$.

Definition 2.2. A mobility function $M_{\alpha\beta}$ is a function such that $M_{\alpha\beta}(r\mathbf{n}) = rM_{\alpha\beta}(\mathbf{n})$ for all $r \geqslant 0$ and $M_{\alpha\beta}$ is positive on unit vectors. We require that the mobility shape $W_{M_{\alpha\beta}} = \{\mathbf{x}: \mathbf{x} \cdot \mathbf{n} \leqslant M_{\alpha\beta}(\mathbf{n})\}$ have the same normal directions that $W_{\alpha\beta}$ has (if $\Phi_{\alpha\beta}$ is identically zero, we require that $W_{M_{\alpha\beta}}$ be a polygon). We further assume that $M_{\alpha\beta}$ is convex. To avoid the necessity of considering infinitesimal layers, we require that for every unit vector $\mathbf{n}$ and $\alpha < \beta < \gamma$, if $M_{\beta\gamma}(\mathbf{n})\, C_{\beta\gamma} < M_{\alpha\beta}(\mathbf{n})\, C_{\alpha\beta}$, then $M_{\alpha\gamma}(\mathbf{n})\, C_{\alpha\gamma} \geqslant M_{\beta\gamma}(\mathbf{n})\, C_{\beta\gamma}$. (Recall that we assumed the phases were indexed so that $\mathscr{B}_\alpha \leqslant \mathscr{B}_\beta$ if $\alpha < \beta$.)

Definition 2.3. Given a Φ with a polygonal Wulff shape W_Φ, an oriented polygonal curve S is *admissible* for Φ if the set of normals to S is contained in the set of normals to W_Φ and adjacent segments of S have adjacent normals in W_Φ. All interfaces in Section 3 are required to be admissible. S is defined to be *almost admissible* for Φ if S is polygonal and, when a normal direction $\mathbf{n}$ of S is not a normal of W_Φ, then $\mathbf{n}$ and the normals of the adjacent segments in S must all be normals of supporting planes at the same corner of W_Φ. An interface $S_{\alpha\beta}$ in Section 4 has to be almost admissible provided $\Phi_{\alpha\beta}$ is not identically zero.

Definition 2.4. We will often denote a given segment of S by S_i (or T_i) and its normal by $\mathbf{n}_i$; we then abbreviate $\Phi_{\alpha\beta}(\mathbf{n}_i)$ by Φ_i and $M_{\alpha\beta}(\mathbf{n}_i)$ by M_i. We use the notation "$i+$" to denote the immediately following segment to S_i (as determined by the orientation of $S_{\alpha\beta}$), and "$i-$" to denote the immediately preceding segment (if any). Thus segment S_{i+} follows segment S_i, and its normal direction is $\mathbf{n}_{i+}$.

Definition 2.5. For an admissible curve S in the $\alpha\beta$ interface, if the i_+ (resp., i_-) end of S_i is not at a triple junction, then we define δ_{i+} (resp., δ_{i-}) to be 1 if the final (resp., initial) end of the ith segment is regular (locally bounds a convex positively-oriented region; the normals of two adjacent segments in the curve are in the same order on the Wulff shape as on the curve) and -1 if it is inverse (locally bounds a concave positively-oriented region). We also define

$$f_{i_\pm} = (\Phi_{i\pm} - \Phi_i \mathbf{n}_i \cdot \mathbf{n}_{i\pm}) / \sqrt{1 - (\mathbf{n}_i \cdot \mathbf{n}_{i\pm})^2}$$

$$f_{M,\, i_\pm} = (M_{i\pm} - M_i \mathbf{n}_i \cdot \mathbf{n}_{i\pm}) / \sqrt{1 - (\mathbf{n}_i \cdot \mathbf{n}_{i\pm})^2}$$

Definition 2.6. If neither end of S_i is at a triple junction, then its weighted mean curvature $\kappa_\Phi(S_i)$ is defined to be the initial rate of decrease of surface energy with "volume" (here 2-dimensional area) swept out under

a deformation which consists of shifting the position of the whole segment, added or removing bits of the segment and adjoining segments to maintain a connected polygonal curve. One computes

$$\kappa_{\Phi}(S_i) = -(\delta_{i+} f_{i+} + \delta_{i-} f_{i-})/\ell_{S_i}$$

where ℓ_{S_i} is the length of edge S_i. Since the length Λ_i of the facet with normal $\mathbf{n}_i$ of W_{Φ} is $f_{i+} + f_{i-}$, it is also true that

$$\kappa_{\Phi}(S_i) = \sigma_{S_i} \Lambda_i / \ell_{S_i}$$

where $\sigma_{S_i} = (\delta_{i+} + \delta_{i-})/2$. See [T4] for further information.

Definition 2.7. A vector ξ is a ξ-vector for an oriented line segment T if ξ is in the subgradient of $\Phi_{\alpha\beta}$ at $\mathbf{n}(T)$. Since we have assumed $\Phi_{\alpha\beta}$ is convex, any such ξ is a point on $W_{\Phi_{\alpha\beta}}$ for which $\mathbf{n}(T)$ is a normal (or, is a corner of $W_{\Phi_{\alpha\beta}}$, if $\mathbf{n}(T)$ is not a normal of a facet of $W_{\Phi_{\alpha\beta}}$). See [HC].

Definition 2.8. A configuration of three segments with a common initial endpoint is *force-balanced* if there is a ξ vector for each segment such that the sum of those three ξ vectors is zero. If the segments are not oriented to have a common initial point, then the condition is that they be force-balanced if the curves were given such an orientation (if $\mathbf{n}$ is changed to $-\mathbf{n}$, then obviously one also changes $\alpha\beta$ to $\beta\alpha$).

Definition 2.9. A polycrystal configuration is *admissible* for $\{\Phi_{\alpha\beta}\}$ and $\{M_{\alpha\beta}\}$ as above if each interface is required to be admissible for its $\Phi_{\alpha\beta}$ and M_{ab}, and the admissible curves meet three at a time at force-balanced triple junctions. It is *almost admissible* if the interfaces are merely almost admissible.

3. SURFACE-INTEGRAL FORMULATIONS

3a. Heuristics

The "energy" $\mathscr{E}_{ATW}$ described in the Introduction was adopted in [ATW] in order to handle singularities, including places where the normal is undefined. Since $\int_0^h x\,dx = h^2/2$, a related formulation involving only "surface" integrals for an admissible crystalline curve with segments

$\{T_i\}_{i\in\mathscr{I}}$ would be to minimize, just among other crystalline curves $\{S_i\}_{i\in\mathscr{I}}$ with $\mathbf{n}_{S_i}=\mathbf{n}_{T_i}=\mathbf{n}_i$ for each i, the energy

$$\sum_i \Phi(\mathbf{n}_{S_i}(x))\,\ell_{S_i}-\sum_i \Phi(\mathbf{n}_{T_i}(x))\,\ell_{T_i}+\frac{1}{2\,\Delta t}\sum_i \operatorname{dist}^2(S_i,\,T_i)\,\ell_{T_i}$$

$$=\sum_i \sigma_i \Lambda_i z_i+\frac{1}{2\,\Delta t}\sum_i z_i^2\ell_{T_i}$$

where $z_i=\mathbf{n}_i\cdot(\mathbf{y}-\mathbf{x})$ for any $\mathbf{x}\in T_i$ and $\mathbf{y}\in S_i$. Minimization leads to $z_i=-(\sigma_i\Lambda_i/\ell_i)\,\Delta t$.

Our objective is to extend these formulations, for crystalline curves, to general geometric motion ($v=M(C+\kappa_\Phi)$) with triple junctions. Suppose $\{T_i\}_{i\in\mathscr{I}}$ are the segments of the interfaces of an admissible polycrystal configuration. Abbreviate $M_i=M_{\alpha\beta}(\mathbf{n}_i)$ and $\Phi_i=\Phi_{\alpha\beta}(\mathbf{n}_i)$, where $\alpha\beta$ is the interface of which T_i is a part. Suppose $\{S_i\}_{i\in\mathscr{I}'}$ also form admissible curves that are interfaces of regions, with these curves meeting three at a time at triple points, and $\mathbf{n}_{S_i}=\mathbf{n}_{T_i}$ for each $i\in\mathscr{I}$, whereas each segment in $\{S_i\}_{i\in\mathscr{I}'\sim\mathscr{I}}$ is short (of order Δt) and has one endpoint at a triple junction.

Definition.

$$\mathscr{F}_c(\{S_i\}_{i\in\mathscr{I}'},\,\{T_i\}_{i\in\mathscr{I}},\,\Delta t)$$

$$=\sum_{i\in\mathscr{I}'}\Phi(\mathbf{n}_i(x))\,\ell_{S_i}-\sum_{i\in\mathscr{I}}\Phi(\mathbf{n}_i(x))\,\ell_{T_i}+\sum_{i\in\mathscr{I}}-C_i z_i\ell_{T_i}+\frac{1}{2\,\Delta t}\sum_{i\in\mathscr{I}}\frac{z_i^2}{M_i}\,\ell_{T_i}$$

The "surface-integral formulation" of the variational problem is to minimize (as stated in [T1]) the quantity $\mathscr{F}_c$ over all such $\{S_i\}$ and $\{Z_i\}$. This minimization gives

$$\frac{z_i}{\Delta t}\approx M_i(C_i+\kappa_{\Phi_{\alpha\beta}}(S_i))$$

for each $i\in\mathscr{I}$ such that T_i has no endpoint at a triple junction; it also preserves the idea of L^2 gradient flow where there are triple junctions.

The biggest question is: when do additional line segments $\{S_i\}_{i\in\mathscr{I}'\sim\mathscr{I}}$ have to be added and what directions do they have? The basic answer, for curves, as shown in [T1] is: only at triple junctions and then only if adding them further decreases the total energy $\mathscr{F}$. We show below that at most one segment needs to be added at each triple junction if the $\{T_i\}$ configuration is almost admissible and initially force-balanced at each triple junction; furthermore, the possible direction of any such added segment is completely determined by the starting configuration $\{T_i\}$.

3b. Octagonal Specific Example, with All $C = 0$ and $\Phi > 0$

Here is one specific example of how to determine exactly how to move a triple junction, assuming both W_Φ and W_M are the same regular octagon for all interfaces (which are assumed to be admissible) and assuming all bulk driving forces C are zero, so motion is just motion by weighed mean curvature. All force-balanced triple junctions for this situation are shown in Fig. 1.

Assume the triple junction has all initial points at the origin. Suppose the three segments have normals $(-1/\sqrt{2}, -1/\sqrt{2})$, $(0, 1)$, and $(1, 0)$. See Fig. 2. Denote the lengths of these segments by l_s (for sloped), l_h, (for horizontal) and l_v (for vertical) respectively. Finally, assume that the values of δ at the terminal ends, $\delta_{s+}, \delta_{h+}, \delta_{v+}$, equal $+1$, $+1$, and -1 respectively. (Because all three Wulff shapes are octagons and all curves are admissible, the angle between normals at these final endpoints is each 45 degrees.)

Lemma 3.1. Under these assumptions, if Δt is small enough, then two, and only two, types of positions of the triple junction can possibly be minimizing; which one in fact minimizes depends on the values of the ℓ's (specifically, the sign of $\ell_v(3-2\sqrt{2}) - \ell_s(3\sqrt{2}-4)/2$). The positions are:

(1) move the triple point to position (x, y) with $x \geqslant -y \geqslant 0$, and move all three initial segments so that they meet at this point (see Fig. 2(a)), or

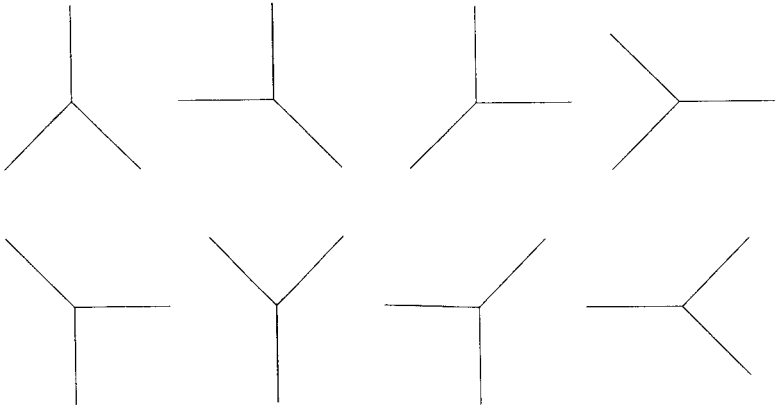

Fig. 1. The complete set of force-balanced crystalline triple junctions is shown, when the Wulff shape for each of the three interfaces is the same regular octagon.

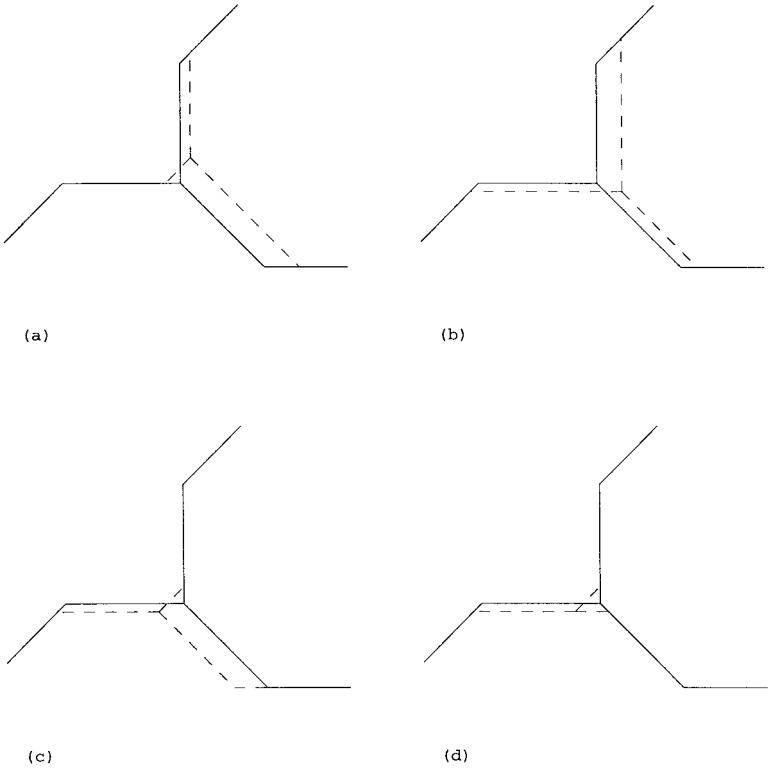

Fig. 2. The dotted lines in (a) and (b) indicate the types of configurations that might possibly be minimizing, given the solid-line configuration as the initial condition. Configuration (c) cannot be minimizing, as can be seen by considering configuration (d), which has the same surface free energy and a non-force-balanced triple junction.

(2) move the triple point to position (x, y) with x and y both greater than or equal to zero, move the vertical and sloped segments so that they meet at this point, add a small segment of slope 1 from the triple point down to the x axis, and leaving the horizontal segment at height zero, extend or shorten it to meet that small segment; finally, adjust the segments at the final endpoints and their adjacent segments to maintain connectivity (see Fig. 2(b)).

Proof. There are six regions of the plane defined by the lines containing the three segments. The triple junction could be inside the closure of any of those six regions. Consider placing the triple junction (x, y) in one of the six, subject to having each $|(x, y) \cdot \mathbf{n}_i| \leqslant 2A_i \Delta t/\ell_i$. Once the position of the triple junction is given, each of the three interfaces which minimizes

$\mathscr{F}$ is easily determined; it will be a straight line segment to the adjacent segment if the triple junction is on the same side of segment i as the adjacent segment, but will be a short segment down to the original line of T_i if the triple point is on the opposite side from the adjacent segment (since no surface energy change is made by putting it anywhere except at T_i, and there is a cost in putting it elsewhere due to the $z_i^2 l_i$ term). Now, again with (x, y) fixed determine whether the configuration formed by the three independently minimizing interfaces at (x, y) is force-balanced; if it is not, then the whole cannot be minimizing. Finally, the constraint $|(x, y) \cdot \mathbf{n}_i| \leqslant 2\Lambda_i \Delta t/\ell_i$ is in fact not a constraint, since moving the triple junction farther than that cannot decrease energy: no edge will be computed to move further than $\Lambda_i \Delta t/\ell_i$. One runs through the six possibilities and sees that only two allow force-balance. See Fig. 1(c-d) for an example of a non-force-balanced choice of (x, y).

In case 2, (and writing $L_s = l_s/2$), is

$$\mathscr{F} = -(\sqrt{2}-1)\, x - (3-2\sqrt{2})\, y + (1/(2\Delta t))(x^2 l_v + (x+y)^2 L_s)$$

and it is minimized by

$$x/\Delta t = ((3\sqrt{2}-4)\, L_s)/(l_v L_s)$$
$$y/\Delta t = (l_v(3-2\sqrt{2}) - L_s(3\sqrt{2}-4))/(l_v L_s)$$

For this configuration, y is required to be nonnegative; if it is computed to be negative, then case 2 cannot occur.

In case 1, the net energy change is

$$-(\sqrt{2}-1)\, x - (3-2\sqrt{2})\, y + (1/(2\Delta t))(x^2 l_v + y^2 l_h + (x+y)^2 L_s)$$

and it is minimized by

$$x/\Delta t = ((\sqrt{2}-1)\, l_h + (3\sqrt{2}-4)\, L_s)/d$$
$$y/\Delta t = (l_v(3-2\sqrt{2}) - L_s(3\sqrt{2}-4))/d$$

where $d = l_v l_h + l_v L_s + l_h L_s$, Now we require $x \geqslant -y > 0$. The transition from case 1 to case 2 is continuous: the values of x are equal when $y = 0$, $x > -y$ always, and either one condition is true or the other is (with both being true only when $y = 0$).

The system for doing the motion of the curves is now to move each curve by the appropriate z_i, and then to repeat the minimization. If no segment was added the first time, then the configuration is the same as it was, except for the lengths being slightly different; when the energy is minimized again starting from the new polycrystal configuration, it will likely

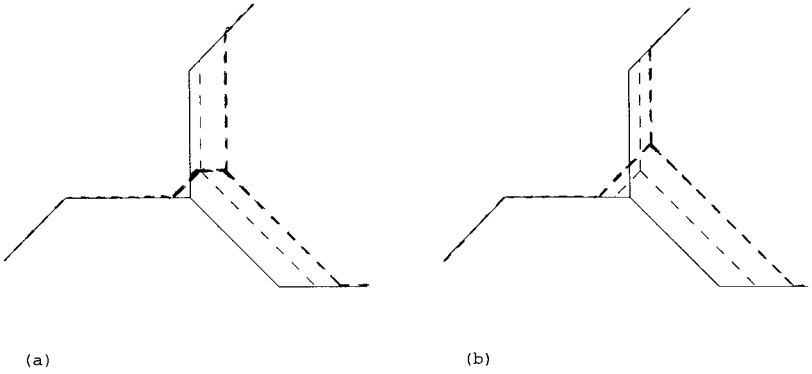

Fig. 3. Here are the two types of configurations, shown in darker dashed lines, that could be minimizing for the second time step, if the first time step produced the configuration indicated by the lighly dashed lines.

(but not necessarily) again result in not adding a segment. But if a segment was added, then one starts from the configuration of Fig. 2(b), where there are now two possibilities *a priori*. In one case, a new segment is added, this time of normal (0, 1), as in Fig. 3(a). In the other case, no new segment is added but all three segments move which meet at the triple junction (one of them being the small segment added at the previous time step), as in Fig. 3(b).

In the latter case, the most likely scenario is that in successive time steps, the three segments keep moving, with no new segments added. In the former case, the new configuration after this second time step is the same as the original configuration, and the most likely result of the third time-step minimization process is to produce yet another small segment, of the same direction as that introduced in the first time-step minimization. Thus in this case, new segments of alternating direction are produced at each time step. This results in an approximation to a varifold being created along the path of the triple junction. The limit motion, as the time step Δt goes down to zero, is actually a varifold.

3c. The General Surface-Integral Formula, for Nonzero Φ

We rewrite the "energy difference" $\mathscr{F}_c$ defined above, and derive a condition which we call COND, depending only on the surface energy functions $\{\Phi_{\alpha\beta}\}$ for the three interfaces and the variables $\{g_i\}$ defined below. If COND does not hold, then this surface-integral formulation gives

a unique motion for time step Δt for the triple junction. Otherwise, the volume formulation of Section 4 must be used. COND is a condition on the three Φ which holds with probability zero for three arbitrary Wulff shapes for the interfaces; in particular, it never holds when all three Wulff shapes are the same regular octagon. Nevertheless, it does hold when all the Φ are identically zero, and also in the particular case when all three Wulff shapes are the same regular hexagon, with choices of the variables $\{g_i\}$ appropriate to the segments.

Without loss of generality, assume that a force-balanced triple junction is initially at the origin, and that segments T_1, T_2, T_3 have their initial points at that triple junction, but none of their terminal endpoints are at triple points.[2] Denote $\mathbf{n}_i = (c_i, s_i)$ and $\cos\theta_{i+} = \mathbf{n}_i \cdot \mathbf{n}_{i+}$, where $\mathbf{n}_{i+}$ is the normal of the segment just beyond segment i in its interface.

In the following, (x, y) are the coordinates of the new triple junction position, z_i is the distance that segment i is to be moved in the direction of its oriented normal, and each $g_i = 0, -1$ or $+1$. Setting a particular $g_i = 0$ corresponds to adding no segment to the interface of S_i at the triple point, whereas setting $g_i = \pm 1$ corresponds to adding a new small segment between the triple point (x, y) and the ith edge, so that g_i becomes δ_{i-} for S_i. As for all admissible curves, there are two possible orientations (from the appropriate Wulff shape) for such a new segment on the interface of S_i, one making a regular (convex) intersection with S_i and one making an inverse (concave) intersection. In the first case, set $g_i = 1$ and $\mathbf{n}_{ia}$ the normal preceding $\mathbf{n}_i$ in the appropriate Wulff shape, and in the second set $g_i = -1$ and $\mathbf{n}_{ia}$ the normal following $\mathbf{n}_i$. (Again, "preceding" and "following" are determined by orienting the boundary of the Wulff shape as the boundary of the positively oriented Wulff shape, by the right hand rule.) One imposes the requirements that $z_i = xc_i + ys_i$ for any i such that $g_i = 0$, and $g_i(z_i - (xc_i + ys_i)) > 0$ for each i with $g_i \neq 0$. Let Φ_i be the surface energy per unit length of segment T_i, and similarly for Φ_{ia} and Φ_{i+}. If $g_i \neq 0$, define $f_{i-} = (\Phi_{ia} - \Phi_i \mathbf{n}_i \cdot \mathbf{n}_{ia})/(\sqrt{1 - (\mathbf{n}_i \cdot \mathbf{n}_{ia})^2})$.

The formula for $\mathscr{F}_c$ (assuming the triple junction is force-balanced) becomes

$$\mathscr{F}_c(\{z_i\}, \{T_i\}, \{g_i\}, \Delta t) = S_s + B_s + I_s$$

[2] If there are in fact triple points at both ends of a segment, the changes to make in what follows are obvious: one just gets equations coupling the positions of the two triple point positions if the g's at both ends are zero, whereas if one or both g's are nonzero, then there are just constraints on the values of z_i from both ends.

where

$$S_s = \sum_{i=1}^{3} (z_i \delta_{i+} f_{i+} + \Phi_i(xs_i - yc_i) + g_i(z_i - (c_i x + s_i y)) f_{i-}) + \text{rest of interfaces}$$

$$B_s = -\sum_{i=1}^{3} z_i C_i l_i + \text{rest}$$

$$I_s = \frac{1}{2\Delta t} \sum_{i=1}^{3} l_i z_i^2 / M_i + \text{rest}$$

and we require, as stated previously, that $z_i = xc_i + ys_i$ for any i such that $g_i = 0$, and $g_i(z_i - (xc_i + ys_i)) > 0$ for each i with $g_i \neq 0$.

Definition 3.1. Assume the triple junction is force-balanced. In the notation above, condition COND holds if for one or more values of $k = 1, 2, 3$ and for some nonzero choices of $\{g_i\}_{i \neq k}$,

$$\Phi_k = s_k \sum_{i \neq k} g_i c_i (f_{i-} - \Phi_i s_i) - c_k \sum_{i \neq k} (g_i s_i f_{i-} + \Phi_i c_i)$$

or if $\mathbf{n}_i = -\mathbf{n}_j$ for some $1 \leqslant i < j \leqslant 3$. In particular, COND holds whenever all the Φ_i are zero. Observe that COND holds at the extremes of force balance.

Theorem 3.2. If COND does not hold, then unique minimizers exist, and they have at most one g_i nonzero. The minimization of $\mathscr{F}_c$ at successive time steps is the same as that described in [T1] for triple junction motion.

Proof. In [T1], precisely the same variational scheme is described, choosing among the various possibilities for setting one g_i nonzero, but without the explicit formulas given below for computing x and y and whether any g_i is nonzero.

Abbreviating

$$a_{11} = \sum_{i=1}^{3} (1 - g_i^2) c_i^2 \frac{l_i}{M_i}, \qquad a_{12} = a_{21} = \sum_{i=1}^{3} (1 - g_i^2) s_i c_i \frac{l_i}{M_i}$$

$$a_{22} = \sum_{i=1}^{3} (1 - g_i^2) s_i^2 \frac{l_i}{M_i}$$

$$a = \sum_{i=1}^{3} ((1 - g_i^2) c_i (C_i l_i - \delta_{i+} f_{i+}) + g_i c_i f_{i-} - \Phi_i s_i)$$

$$b = \sum_{i=1}^{3} ((1 - g_i^2) s_i (C_i l_i - \delta_{i+} f_{i+}) + g_i s_i f_{i-} + \Phi_i c_i)$$

we compute that $(\partial \mathscr{F}_c/\partial x) = (1/\Delta t)(a_{11}x + a_{12}y) - a$ and $(\partial \mathscr{F}_c/\partial y) = (1/\Delta t)(a_{21}x + a_{22}y) - b$. Thus any critical point with this choice of $\{g_i\}$ will have

$$z_i = \begin{cases} \Delta t M_i \left(C_i - \dfrac{(\delta_{i+} + g_i)\,\Lambda_i}{2l_i} \right) & \text{if} \quad g_i \neq 0 \\ xc_i + ys_i & \text{if} \quad g_i = 0 \end{cases}$$

where x and y satisfy

$$a_{11}x + a_{12}y = a\,\Delta t, \qquad a_{21}x + a_{22}y = b\,\Delta t$$

Let $d = a_{11}a_{22} - a_{12}^2$. Observe that d can be rewritten as $\sum (l_i l_j / M_i M_j)(c_i s_j - c_j s_i)^2$ where the sum is over all $i > j$ such that g_i and g_j are zero. In particular, $d > 0$ if at most one of the g_i is nonzero (since COND not holding ensures that $\mathbf{n}_j \neq \mathbf{n}_k$) and $d = 0$ if two or more g_i are nonzero.

Suppose two of the g_i are nonzero and the third (say g_3) is zero. In this case, $d = 0$; the equations for x and y are consistent if and only if $as_3 = bc_3$. Since the terms involving $C_i l_i$ cancel, this statement reduces precisely to condition COND and thereby violates a hypothesis of the theorem.

Suppose all three g_i are nonzero. Then there is an interior critical point in the open triangle of possible values of x and y determined by the signs of the g_i only if $a = b = 0$. But then in fact COND holds, a contradiction again.

Suppose one g_i is non-zero and the rest zero. Then $d > 0$ and there is a unique solution for x and y by simple linear algebra; Provided it satisfies the constraint $g_i(z_i - (xc_i + ys_i)) > 0$, $\mathscr{F}_c$ has a local minimum (since $a_{11} > 0$) at x, y. Since all $g_i = 0$ is an endpoint of such configurations, the existence of any local minimum with a $g_i \neq 0$ implies that the configuration with all $g_i = 0$ cannot also be a minimum. On the other hand, if none of the constraints holds for any g_i nonzero, then the unique minimum must be at the (x, y) determined by setting all $g_i = 0$.

We now show that there can be at most one of these local minima with a g_i nonzero, and therefore that if it exists, it is the unique global minimizer. A given position (x, y) can be at a minimizer of $\mathscr{F}_c$ only if for each i, $g_i = 0$ if $0 \leqslant \delta_{i+}(C_i \Delta t - 1/M_i(x, y) \cdot \mathbf{n}_i) \leqslant (\Lambda_i / l_i)$, $g_i = -\delta_{i+}$ if $0 > \delta_{i+}(C_i \Delta t - 1/M_i(x, y) \cdot \mathbf{n}_i)$ and $g_i = \delta_{i+}$ if $\delta_{i+}(C_i \Delta t - 1/M_i(x, y) \cdot \mathbf{n}_i) > (\Lambda_i \Delta t / l_i)$. If there are two positions (x'', y'') and (x', y') satisfying the inequalities above, one with, say, $g_1 \neq 0$ and $g_2 = 0 = g_3$, and the other with $g_2 \neq 0$ and $g_1 = 0 = g_3$, then there is a one-parameter family of (x, y) also satisfying the inequalities which interpolates between these two configurations and which has both $g_1 \neq 0$ and $g_2 \neq 0$. But since COND does not

hold, the minimum of $\mathscr{F}_c$ occurs uniquely at just one of the endpoints, contradicting the possibility of there being local minima at each end.

One sees that the condition cannot hold for both $g_i = 1$ and $g_i = -1$ for the same i, since both holding would imply that with f^* the value of f_{i-} corresponding to $g_i = -1$ and f^{**} the value of f_{i-} corresponding to $g_i = 1$, $f^* + f^{**} < 0$. But in fact $f^* + f^{**} = \Lambda_1 > 0$, so this is a contradiction. (The computation can be done most easily by assuming, without loss of generality, that $i = 1$, $\mathbf{n}_i = (0, 1)$, and $\delta_{i+} = 1$, and then solving for (x, y) in each case. Under these-assumptions, one in fact computes that $f^* + f^{**} < -(\Lambda_1 \Delta t/l_1)((d/a_{11}) < 0.)$

Therefore the constraint can hold only for at most one i and one choice of a g_i.

Comment 3.3. The minimization of $\mathscr{F}_c$, when COND does not hold, under this positive-Φ assumption, implies force-balance. Therefore one can determine from the initial triple junction normals (before actually computing any x, y, z_i) just which g_i need to be considered. However, for computer calculations it is probably better just to search for the minimum among all seven possibilities and check that the resulting x, y, $\{z_i\}$ satisfy the constraints (and that COND does not hold).

Theorem 3.4. If COND does not hold and if the bulk driving forces are written as $\varepsilon C_{\alpha\beta}$, then the limiting motion obtained by minimizing $\mathscr{F}_c$ as ε approaches zero is the same as that with ε equal to zero.

Proof. Determine which g_i, if any, should be nonzero when $\varepsilon = 0$. Then the distance the segments move varies continuously with ε, and the criterion that that g_i should be nonzero (or that no g_i should be nonzero) remains true for small ε.

4. THE VARIATIONAL APPROACH USING THE VOLUME FORMULATION $\mathscr{E}_C$ AS THE ENERGY

The family of variations we will consider consist of interfaces derived from the original interfaces by moving their segments parallel to themselves and by adding extra segments at triple junctions; maintaining continuity of the interfaces by extending or truncating segments as necessary. The variational problems at each triple junction are independent of those at the other triple junctions provided there is no segment with triple junctions at both ends; therefore we will consider only the situation around one particular triple junction. (The extension to the case of segments with triple junctions at both ends should be obvious.) We will assume the triple point

is initially at the origin, with each interface oriented outward from that triple junction (i.e., so that the triple junction is the initial point of each interface). Again, we do not consider here the case where any triple junctions come together during the time step of the minimization, nor where there are any other topological changes.

Thus we assume we have segments T_i, $i=1, 2, 3$ with initial endpoints at the origin. We do not require that the normals $\mathbf{n}_i$ be normals of their appropriate Wulff shapes (or mobility shapes W_M).

The variables in this volume-integral formulation are (x, y), $\{z_i\}_{i=1,2,3}$, $\{n_i\}_{i=1,2,3}$, $\{z_{i1},..., z_{in_i}\}_{i=1,2,3}$, as well as $\{g_i\}_{i=1,2,3}$ and $\mathbf{n}_e$ (a possible special orientation for an added segment). For each $i=1, 2, 3$, we move T_i a distance z_i in its normal direction to create a new long segment S_i, extending or contracting it and its neighbor at its terminal end to maintain connectedness, and at the initial end we add segments S_{ij}, $j=1,..., n_i$, with normals $\mathbf{n}_{ij}$ and at distances z_{ij} from the origin. Various constraints on these variables will be described. In particular, all segments must be such that each interface forms a continuous embedded polygonal curve, and each pair of distinct interfaces intersects only at (x, y).

Number the added segments sequentially backward so that S_{i1} is adjacent to S_i and S_{in_i} has (x, y) as initial endpoint. Let $\mathbf{n}_{ij}$ be the normal of S_{ij} for $i=1, 2, 3$ and $j=1,..., n_i$. For ease of notation, let $\mathbf{n}_{i0}=\mathbf{n}_i$, $z_{i0}=z_i$, and let $(x_{in_i}, y_{in_i})=(x, y)$. Define (x_{ij}, y_{ij}) to be the intersection point satisfying the equations $\mathbf{n}_{ij+1}\cdot(x_{ij}, y_{ij})=z_{ij+1}$, $\mathbf{n}_{ij}\cdot(x_{ij}, y_{ij})=z_{ij}$ for $j=0,..., n_i-1$. Require $z_{in_i}=\mathbf{n}_{in_i}\cdot(x, y)$. One of the normals $\mathbf{n}_{in_i}$, $i=1, 2, 3$ might be the variable $\mathbf{n}_e$. Apart from that one possible exception, the normal directions $\mathbf{n}_{in_i},..., \mathbf{n}_{i0}$ are required to be exactly the normals of W_{M_i} in counterclockwise order if $g_i=1$, and in clockwise order if $g_i=-1$. If $\mathbf{n}_i$ is not a normal of W_{M_i}, then $\mathbf{n}_i$ must be the normal of a supporting plane of W_{M_i} at the corner for which a plane with normal $\mathbf{n}_{i1}$ is also a support plane.

Define three long thin trapezoids R_i and three sequences of triangles $\Delta_{i1},..., \Delta_{in_i}$ as follows. The trapezoids R_i have have T_i and S_i as their parallel sides; the vertices at one end are $(0, 0)$ and (x_{i0}, y_{i0}), and the vertices at the other end are the original intersection point of segments S_i and S_{i+} and the intersection of T_i with the extension or truncation of S_{i+}. For $j=1,..., n_i$, Δ_{ij} has vertices (x_{ij-1}, y_{ij-1}), $(0, 0)$, and (x_{ij}, y_{ij}), with that order specifying the orientation of the triangle. The triangles and/or trapezoids of one interface may overlap those of another.

Definition 4.1. We define the energy change $\mathscr{E}_c$ to consist of three parts,

$$\mathscr{E}_c = S_v + B_v + I_v$$

where S_v is the total surface energy of the new configuration minus that of the old,

$$B_v = -\sum_i C_i \left(\text{Sign}(z_i)\ \text{Area}(R_i) + \sum_{j=1,\ldots,n_i} \text{Sign}(z_{ij})\ \text{Area}(\Delta_{ij}) \right)$$

$$I_v = \frac{1}{\Delta t} \sum_i \left(\int_{\mathbf{x} \in R_i} \frac{|\mathbf{x} \cdot \mathbf{n}_i|}{M_i(\mathbf{n}_i)}\, dA + \sum_{j=1}^{n_i} \int_{\mathbf{x} \in \Delta_{ij}} \frac{|\mathbf{x} \cdot \mathbf{n}_{ij}|}{M_i(\mathbf{n}_{ij})}\, dA \right)$$

except that if $\mathbf{n}_{in_i}$ is $\mathbf{n}_e$ then the integrand over Δ_{in_i} should be the more precise $M_i^*(\mathbf{x})$ (which will turn out to be $(|\mathbf{x} \cdot \mathbf{n}_{in_i}|)/(M_i(\mathbf{n}_{in_i}))$ for the minimizer).

$\mathscr{E}_c$ should be minimized over all choices of $x, y, z_i, g_i, n_i, z_{i1}, \ldots, z_{in_i}$, and $\mathbf{n}_e$. In the case that there are only two phases, this is a reasonable crystalline analog to the approach of [ATW], as extended by Yip [Y], in the sense that [AT] proved that the motion of [T1] is the same as that of [ATW]. In the polycrystalline case, this formulation explicitly accounts for the effects of changing phase twice, via overlap of trapezoids and triangles. For example, $\mathbf{x}$ may initially be in K_γ but change to be in K_β and then K_α in the course of time Δt.

Theorem 4.2. Minimizers for $\mathscr{E}_c$ exist.

Proof. There is at least one configuration with a set of distances satisfying all the hypotheses, including that each pair of distinct interfaces intersects only at (x, y), namely that of a construction of a "consistent motion" as in [T2]. (The fact that the C_i arise from differences in bulk free energy densities $\mathscr{B}_\alpha$ guarantees that not all C_i have the same sign unless all are zero, and therefore that the only-one-intersection condition can be enforced.) Because each $W_{M_{\alpha\beta}}$ is a polygon, there are a finite number of different configurations to consider (each use of an extra normal $\mathbf{n}_e$ being considered to be a different configuration, but with different values of $\mathbf{n}_e$ considered to be the same configuration). The values of $\mathscr{E}_c$ become infinite as any of the variable distances become unbounded, and the open constraints on the distances correspond to transitions to other allowable configurations, with a continuous change in $\mathscr{E}_c$. Therefore minimizers exist.

Theorem 4.3. Minimizers of $\mathscr{E}_c$ need not be unique, at least if all Φ are identically zero.

Proof. A simple crystalline example has for each interface Φ identically zero and W_M equal to the square $\{(x, y): |x| \leqslant 1, |y| \leqslant 1\}$, $C_1 = 1 = -C_2$, $C_3 = 0$, and $\mathbf{n}_1 = (0, 1)$, $\mathbf{n}_2 = (-1, 0)$, and $\mathbf{n}_3 = (-1, 1)/\sqrt{2}$. The

origin is the initial point of each of the three segments. Then the new triple junction position can be any point (x, y) with $|x| \leqslant \Delta t$, $y = \Delta t$ or $|y| \leqslant \Delta t$, $x = \Delta t$. All have exactly the same value of $\mathscr{E}_c$. This situation was previously observed in [T2].

There are also situations where several configurations satisfy the construction of [T2], and all are local minimizers of $\mathscr{E}_c$, but only one is a global minimizer. One such example has everything as above, except that W_{M_2} is that square rotated by 45° and $\mathbf{n}_2 = (-1/\sqrt{2}, -1/\sqrt{2})$. There are now three different points at which the triple junction could be placed, satisfying the construction. Two of these have the same value for $\mathscr{E}_c$, but the symmetric one in the middle has a slightly higher value, as somewhat less matter gets converted to one of the preferred phases. The absolute minimum in this example in fact splits off two crystals: all three intersection points become triple junctions, and the origin becomes a point where four crystals meet, alternating between two phases. A more extreme version of the same phenomenon occurs if $\mathbf{n}_2 = (-1, 1)/\sqrt{2}$ (and $\mathbf{n}_3$ is some convex combination of $\mathbf{n}_1$ and $\mathbf{n}_2$). Then there are five different possible positions for the triple point, three of them with one value for $\mathscr{E}_c$ and two with a slightly higher value, and the smallest value for $\mathscr{E}_c$ being obtainable by having all five be triple junctions, thereby splitting off four new crystals, so that six crystals meet at the origin.

Proposition 4.4. (1) If the surface energies are nonzero and the initial configuration is force-balanced, then at most one segment needs to be added to each interface at any time step.

(2) If additionally COND does not hold, then at most one interface needs to have a segment added at any minimization step.

(3) Under the assumptions of (1) and (2), in time intervals where no further singularities develop in solving the limiting system of ordinary differential equations determined by the minimizing $\mathscr{F}_c$, the motion derived from doing successive minimizations of $\mathscr{E}_c$ over time step Δt, and then taking the limit as Δt goes to zero, is the same as obtaining by the limit of motions minimizing $\mathscr{F}_c$ as detailed in Section 3c.

Proof. It is straightforward to compute the derivatives of $\mathscr{E}_c$ with respect to x, y, z_i, and any z_{ij}, $j = 1,..., n_i - 1$. For each segment with no endpoint at the new position of the triple junction, the Euler-Lagrange equation is (up to order $(\Delta t)^2$) that $z = M\,\Delta t(C - (\delta_+ f_+ + \delta_- f_-)/\ell)$, where ℓ is the length of the moved segment rather than its initial length. Therefore, as in the surface integral formulation, there can be at most one non-zero g_i, and force-balance of the original plus force-balance at the minimum implies that at most one segment has been added on that inter-

face. The equations for the z_i with $g_i = 0$ are, except for terms of order $(\Delta t)^2$, the same as they were in the minimization of the surface-integral formulation. When a minimizer for $\mathscr{E}_c$ uses an added segment S with normal $\mathbf{n}_e$, the surface formulation $\mathscr{F}_c$ produces segments of alternating direction approximating S, with the position of the triple junction after two time steps approximating that from obtained by two time steps of minimizing $\mathscr{F}_c$ to within $(\Delta t)^2$.

Theorem 4.5. With all Φ identically zero, a motion resulting from minimizing $\mathscr{E}_c$ gives a "consistent motion" of [T2], one obtained by use of characteristics.

Note. This theorem does not say anything about any limit as the Φ approach zero; for that situation, see the following theorem.

Proof. Assuming one is at a minimum of $\mathscr{E}_c$, varying z_{ij} will not change $\mathscr{E}_c$ to first order. This automatically implies that $0 = -C_i l_{ij} + (1/\Delta t)\, z_{ij} l_{ij}$. Alternatively, one can set to zero the derivative of $\mathscr{E}_c$ with respect to z_{ij}, for j between 1 and $n_i - 1$ inclusive. For example, in the case where $g_i = 1$, observe

$$
\begin{aligned}
B_v = -\sum_{i=1}^{3} C_i \Bigg(z_i \Bigg(l_i + \frac{\delta_{i+}}{2} \frac{z_{i+} - z_i \mathbf{n}_i \cdot \mathbf{n}_{i+}}{\sqrt{1 - (\mathbf{n}_i \cdot \mathbf{n}_{i+})^2}} + \frac{g_i}{2} \frac{z_{i1} - z_i \mathbf{n}_i \cdot \mathbf{n}_{i1}}{\sqrt{1 - (\mathbf{n}_i \cdot \mathbf{n}_{i1})^2}} \Bigg) \\
+ \sum_{j=1}^{n_i - 1} z_{ij} \Bigg(\frac{g_i}{2} \frac{z_{ij-1} - z_{ij} \mathbf{n}_{ij-1} \cdot \mathbf{n}_{ij}}{\sqrt{1 - (\mathbf{n}_{ij-1} \cdot \mathbf{n}_{ij})^2}} + \frac{g_i}{2} \frac{z_{ij+1} - z_{ij} \mathbf{n}_{ij+1} \cdot \mathbf{n}_{ij}}{\sqrt{1 - (\mathbf{n}_{ij+1} \cdot \mathbf{n}_{ij})^2}} \Bigg) \\
+ z_{in_i} \Bigg(\frac{g_i}{2} \frac{z_{in_i - 1} - z_{in_i} \mathbf{n}_{in_i - 1} \cdot \mathbf{n}_{in_i}}{\sqrt{1 - (\mathbf{n}_{in_i - 1} \cdot \mathbf{n}_{in_i})^2}} + \frac{1}{2} (xs_{in_i} - yc_{in_i}) \Bigg) \Bigg)
\end{aligned}
$$

Thus one obtains

$$
\begin{aligned}
& C_i \Bigg(\frac{z_{ij-1} - z_{ij} \mathbf{n}_{ij-1} \cdot \mathbf{n}_{ij}}{\sqrt{1 - (\mathbf{n}_{ij-1} \cdot \mathbf{n}_{ij})^2}} + \frac{z_{ij+1} - z_{ij} \mathbf{n}_{ij+1} \cdot \mathbf{n}_{ij}}{\sqrt{1 - (\mathbf{n}_{ij+1} \cdot \mathbf{n}_{ij})^2}} \Bigg) \\
& = \frac{z_{ij}}{M_i(\mathbf{n}_{ij})\, \Delta t} \Bigg(\frac{z_{ij-1}(2/3 + 1/3(z_{ij-1} M_i(\mathbf{n}_{ij}))/(z_{ij} M_i(\mathbf{n}_{ij-1}))) - z_{ij} \mathbf{n}_{ij-1} \cdot \mathbf{n}_{ij}}{\sqrt{1 - (\mathbf{n}_{ij-1} \cdot \mathbf{n}_{ij})^2}} \\
& \quad + \frac{z_{il}(2/3 + 1/3(z_{ij+1} M_i(\mathbf{n}_{ij}))/(z_{ij} M_i(\mathbf{n}_{ij+1}))) - z_{ij} \mathbf{n}_{ij+1} \cdot \mathbf{n}_{ij}}{\sqrt{1 - (\mathbf{n}_{ij+1} \cdot \mathbf{n}_{ij})^2}} \Bigg)
\end{aligned}
$$

The derivative with respect to z_i is similar, except that there is an additional term l_i inside the big parentheses on each side of the equation; this term is of order 1 whereas the other terms are of order Δt. Therefore, up

to a correction of order Δt, $z_i/\Delta t = M_i(\mathbf{n}_i)\, C_i$ for the long segments. Observe that if $z_i/\Delta t = M_i(\mathbf{n}_i)\, C_i$ we can obtain the solution to the system of equations by setting $z_{ik}/\Delta t = M_i(\mathbf{n}_{ik})\, C_i$ for each k, since then $z_{il} M_i(\mathbf{n}_{ik})/(z_{ik} M_i(\mathbf{n}_{il})) = 1$ for each pair k, l.

At the triple junction, the two interfaces which do not use $\mathbf{n}_e$ determine (x, y), if one uses z_{ij} as above. The variable thus becomes $\mathbf{n}_e$, which determines its z, together with g_i and n_i. The determination of the optimal $\mathbf{n}_e$ reduces to a single-interface problem having nothing to do with triple junctions. One computes that the single tangent segment used in the tangent construction of [T2] produces the value of $\mathbf{n}_e$ that occurs in the minimizer and satisfies $M^*(\mathbf{x}) = \mathbf{x} \cdot \mathbf{n}_e / M(\mathbf{n}_e)$ for every $\mathbf{x}$ in Δ_{in_i}; also $z = \Delta t M_i(\mathbf{n}_e)\, C_i$.

Theorem 4.6. If one writes $\Phi = \varepsilon \Phi_0$ and determines a motion as a limit for time step Δt going to zero, and then takes a limit of these motions as ε goes down to zero, then the result need not be the same as any motion obtained with $\varepsilon = 0$. In fact, the discontinuity as a function of ε is explained by the fact that for any $\varepsilon > 0$, $\min\{\sqrt{(1/\Delta t)\, \varepsilon / C^3}, k\}$ is k for small enough Δt, whereas the minimum is always zero when $\varepsilon = 0$. Here C is a measure of the constants C_i and k is a measure of the distance between the position of the triple junction under the assumption that $\varepsilon = 0$, and the position of the triple junction at force balance, given the same local boundary data as for the $\varepsilon = 0$ case.

Proof. We assume the same initial surface as in the example of Section 3, and the same regular octagon for all W_M and W_Φ. We further assume $C_1 = 0$, $C_2 = C$, $C_3 = -C$. When $\varepsilon = 0$, the minimizer of $\mathscr{E}_c$ (and thus the motion of [T2]) adds segments of normal $\mathbf{n}_{2t} = (1/\sqrt{2})(1, -1)$, $\mathbf{n}_{3t} = (1/\sqrt{2})(-1, 1)$ at distances $z_{2t} = C\, \Delta t$, $z_{3t} = -C\, \Delta t$, and moves segments 2 and 3 the same distances, respectively. Now consider putting a small "tent" further out along interface 1, adding another segment, this time of normal $\mathbf{n}_2 = (1, 0)$ to interface 2 and one of normal $\mathbf{n}_3 = (0, 1)$ to interface 3, at distances so that the triple point is now at $(C\, \Delta t/\sqrt{2})$ $(1 + d, -(1 + d))$. We minimize the volume-form of the energy and see that it occurs at $d = \min\{\sqrt{2} - 1, \sqrt{\varepsilon}\, C^{-3/2} (\Delta t)^{-1}\}$. Thus when $\varepsilon = 0$, the minimum is at $d = 0$, whereas for any positive ε, once Δt is small enough the minimum is at $d = \sqrt{2} - 1$ (the corner is fully pushed out and the two segments of normal $\mathbf{n}_2$ are merged, as are those of normal $\mathbf{n}_3$; this is the minimizer for $\mathscr{F}_c$).

Although it is a specific computation, this example embodies the central issue and explains the discontinuity. It is relatively easy to work out other particular cases of the limit motions and compare them to the $\varepsilon = 0$ motion.

5. CONJECTURES

Conjecture 5.1. A minimizer for $\mathscr{E}_c$ is conjectured to be a minimizer for $\mathscr{E}$, at least to within $o(\Delta t)$.

Conjecture 5.2. For each positive integer n, obtain an approximate motion by setting $\Delta t = 2^{-n}$ and doing a sequence of minimizations of $\mathscr{E}$ [resp., $\mathscr{E}_c$], using a minimizer at time $m\,\Delta t$ as the "old" polycrystal to determine the "new" polycrystal at time $(m+1)\,\Delta t$. Then for some subsequence n_k, we conjecture that there is a Hölder estimate relating the approximate motions derived from minimizing $\mathscr{E}$ [resp., $\mathscr{E}$], and therefore a limit motion as n_k goes to infinity. Furthermore, the motions derived from minimizing $\mathscr{E}$ are conjectured to be the same as those from minimizing $\mathscr{E}_c$, just as crystalline motion of curves as described in [T1] gave the same motion as that of [ATW], as proved in [AT].

Conjecture 5.3. A limit motion derived from minimizing $\mathscr{E}$ as ε goes to zero (which by Theorem 4.6 is not necessarily the same as with $\varepsilon = 0$) is conjectured to be the one which Reitich and Soner [RS] get as their viscosity solution when the surface energy is identically zero.

Possible outline of a proof: One might take the examples in their paper, make crystalline approximations to them, use appropriate energies Φ, and show that the limit as ε goes to zero is the same as their motion. The $\varepsilon = 0$ motion is clearly different from theirs, by the example of Theorem 4.6.

Conjecture 5.4. The following is a possible different version of the term I_v in $\mathscr{E}$ for general dimensions d.

If we focus on partitioning up R^d as in [C] rather than on sets such as $\mathscr{R}_{\alpha\beta}$ as in Section 4, then we need to allow several different regions to sweep over a given point within time Δt. We might set

$$I_v = \frac{1}{\Delta t} \sum_j \sum_{\alpha \leqslant \beta} \int_{\mathbf{x} \in (K_\alpha \sim L_\alpha) \cap L_\beta} \sum_{i=1,\,J} \tau_{\alpha_{j(i-1)}\alpha_{j(i)}}(\mathbf{x})\, dV$$

where for any (α, β), $\tau_{\alpha\beta}(\mathbf{x}) = \inf_{\mathbf{y} \in \mathbb{L}_\alpha \cap \mathbb{L}_\beta} M^*_{\alpha\beta}(\mathbf{x} - \mathbf{y})$ and the sum is over the longest increasing sequence $j(0) = \alpha, \ldots, j(J) = \beta$ such that for any integer $0 < i < J$,

$$\frac{1}{C_{\alpha_{j(i-1)}\alpha_{j(i+1)}}} \tau_{\alpha_{j(i-1)}\alpha_{j(i+1)}}(\mathbf{x}) > \frac{1}{C_{\alpha_{j(i-1)}\alpha_{j(i)}}} \tau_{\alpha_{j(i-1)}\alpha_{j(i)}}(\mathbf{x}) > \frac{1}{C_{\alpha_{j(i)}\alpha_{j(i+1)}}} \tau_{\alpha_{j(i)}\alpha_{j(i+1)}}(\mathbf{x})$$

The author knows of no case where $J > 2$ for triple junctions. The terms in the inequality represent the time required for an interface to advance purely due to bulk driving forces. The sequence of j's is increasing because we assumed $\mathscr{B}_\alpha < \mathscr{B}_\beta$ if $\alpha < \beta$. If no sequence satisfies that condition, in particular if the C's are all zero, then $J = 1$. Observe that points that change from one crystal to another twice within the time step Δt make a contribution both times to I_v, as they should. It is not known whether this approach has any particular virtues.

ACKNOWLEDGMENTS

Partial support for this work was provided by the National Science Foundation. The author appreciates the comments of Diana Dismus-Campbell and the referee. And the author especially appreciates the many years of vigorous intellectual exchange with John Cahn, to whom this volume is dedicated.

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