CRYSTALLINE GEOMETRIC CRYSTAL GROWTH

by Jean E. Taylor

Department of Mathematics, Rutgers University, New Brunswick, NJ 08903

taylor@math.rutgers.edu

In geometric crystal growth, the normal velocity of the interface is the product of the mobility of the interface in that normal direction with the force driving the crystal to grow. This force is often a constant Ω, representing the decrease in free energy per unit volume due to the crystal growing, plus the "weighted mean curvature," representing the change in surface energy per unit volume swept out by the growth. A survey of nine mathematical formulations of such motion is in preparation [TCH].

This paper is a progress report on the "crystalline" formulation, in which the surface free energy γ is so highly anisotropic that the equilibrium crystal shape

$$W = \{\mathbf{x} : \mathbf{x} \cdot \mathbf{n} \leq \gamma(\mathbf{n}) \text{ for every unit vector } \mathbf{n}\}$$

is a polyhedron, with its set of normals equal to a specified finite set $\mathcal{N}$. It was first introduced in [T1] and was discussed in [T2].

Crystalline geometric crystal growth is studied for three reasons: (1) sometimes physical problems require it, (2) it ought to be useful as a natural polyhedral approximation to more smooth motions, and (3) it has an interesting formulation and theory of its own, in which curvature is not defined at points but on line or plane segments. Results have been proved which sometimes parallel the results for motion by mean curvature and which sometimes are strikingly different [T3]. Also, a computer program has been written which computes this motion, for immersed as well as embedded and multiple-grain-junction curves in the plane (with and without fixed boundaries), and another program is under development for surfaces. These programs are illustrated in the a videotape which is part of [T4]. (A very early version of this program was demonstrated in [T2].) A related program for the motion of curves in 2-d was developed by Roberts and is described in [R].

In the crystalline formulation, the partial differential equation for geometric crystal growth becomes a system of ordinary differential equations for the distances of the flat segments $\{S_i\}$ of the surface from some fixed origin:

$$ds_i/dt = -M(\mathbf{n}_i)\,(\Omega + wmc\,(i))\,.$$

Here $wmc(i)$ stands for the analog of the weighted mean curvature for the ith plane segment, namely the rate of increase in surface energy with volume under deformations consisting of changing the distance of a single plane. For surfaces in 3-space, one computes

$$wmc(i) = \sum_{j \neq i} \frac{\delta_{ij} f_{ij} l_{ij}}{area(S_i)},$$

where l_{ij} is the length of the intersection of segment S_i and S_j (and is thus 0 if those segments are not adjacent in the interface), δ_{ij} is 1 or -1, depending on whether the type of the $S_i - S_j$ edge is *regular* (like that in W) or *inverse* (like that in the central inversion of W) [TC], and f_{ij} is a factor determined by the normals and γ,

$$f_{ij} = (\gamma(\mathbf{n}_j) - \mathbf{n}_i \cdot \mathbf{n}_j \gamma(\mathbf{n}_i))\,/\sqrt{1 - (\mathbf{n}_i \cdot \mathbf{n}_j)^2}.$$

(In 2-d, $area(S_i)$ is replaced by $length(S_i)$ and the l_{ij} are simply omitted.) For directions not in $\mathcal{N}$ to be interpreted consistently as varifolds, the mobility M must be determined by its values on $\mathcal{N}$ via $M(a\mathbf{n}_1 + b\mathbf{n}_2 + c\mathbf{n}_3) = aM(\mathbf{n}_1) + bM(\mathbf{n}_2) + cM(\mathbf{n}_3)$, assuming facets with orientations $\mathbf{n}_1$, $\mathbf{n}_2$, and $\mathbf{n}_3$ meet at a corner of W and a, b, and c are nonnegative numbers.

A major issue is to determine when additional facets must be added to those in the initial surface or to the surface at later stages of its motion. This issue has been completely settled for curves in the plane and partially settled for surfaces in three-space. Insertions of such facets is required in particular when corners are "too sharp" and when there are fixed boundaries.

To extend the definition of the motion to the case where there are junctions of three or more curves (there is a parallel formulation for surfaces in 3-d), one recasts the problem

as a variational problem: given a network at some particular time, if we let h_i be the rate at which facet S_i is to move (so that $ds_i/dt = h_i$) and let l_i be the length of facet S_i, then the variational problem, to first order, is to maximize the decrease in total free energy,

$$-\sum_i(\Omega l_i h_i + \sigma_i \Lambda(\mathbf{n}_i)h_i),$$

subject to

$$\sum_i(h_i/M(\mathbf{n}_i))h_i l_i = constant.$$

This constraint says that the integral of the driving force over the region swept out by the motion is a prescribed constant. (If no motion can decrease the total free energy, then the variational formulation is abandoned and one simply sets $h_i = 0$ for all i.) For triple junctions, one adds the constraint that the three segments continue to meet (e.g., if segments 1, 2, 3 form a triple junction, then there exists a point $\mathbf{p}$ such that $\mathbf{n}_i \cdot \mathbf{p} = h_i$ for $i = 1, 2, 3$); the formula for computing the net change in surface free energy also now depends on the new intersection point $\mathbf{p}$. Because it may be advantageous to add a new infinitessimal line segment at a triple junction, one has to do the maximization over all possible such additions of line segments; the best addition may well be a segment which is a varifold, having a normal which is not in $\mathcal{N}$, but the correct varifold solution can be closely approximated by using small segments of alternating good orientations. It should be, and is, the case that this variational approach gives the same result when $\gamma = 0$ as does the use of characteristics or the least time formulation [T5].

Both the theory and the computer program have been fairly extensively developed in the 2-dimensional case; the full three dimensional case is only partially investigated and programmed at this point. The way in which the motion for an arbitrary γ and M can be approximated by this type of polyhedral motion is also to be investigated.

This work was supported in part by NSF, AFOSR, and the Geometry Supercomputer Project

References

[R] Stephen Roberts, *A line element algorithm for curve flow problems in the plane*, research report CMA-R58-89, Centre for Math. Analysis, ANU.

[T1] Jean E. Taylor, *Constructions and Conjectures in Crystalline Nondifferential Geometry*, Proceedings of the conference on Differential Geometry, Rio de Janeiro, 1988, Pittman Publishing Ltd., to appear.

[T2] Jean E. Taylor, *Crystals, in Equilibrium and Otherwise*, videotape of AMS-MAA joint lecture, Boulder CO 1989, American Mathematical Society, Providence (1990).

[T3] Jean E. Taylor, *Motion of Curves by Crystalline Curvature, Including Triple Junctions and Boundary Points,*, to appear in Proceedings of Symposia in Pure Mathematics (1990 AMS Summer Institute on Differential Geometry); also available as Research Report GCG 26 from the Geometry Center, 1200 Washington Ave S, Minneapolis, MN 55415.

[T4] Jean E. Taylor, *Motion by Crystalline Curvature*, in *Computing Optimal Geometries*, Selected Lectures in Mathematics, American Mathematical Society (1991), 63-65 plus video clip number 14, 1:31:11-1:38.

[T5] Jean E. Taylor, *The Motion of Multiple-Phase Junctions under Prescribed Phase-Boundary Velocities,* preprint.

[TC] Jean E. Taylor and John W. Cahn, *Catalog of saddle shaped surfaces in crystals,* Acta Metall. 34 (1986), 1-12.

[TCH] Jean E. Taylor, John W. Cahn, and Carol A. Handwerker, *Geometric Models of Crystal Growth,* in preparation.