During this period of support they have continued long-term program of investigating the shapes of surfaces in mathematical models for crystals (including polycrystalline materials), both in equilibrium and in growth. The accomplishments included the completion of seven papers, all of which have either appeared in print or are in press, and working on five more, three of which have since been finished and accepted for publication. Also completed one videotape that will soon be published. Four papers that had previously been written appeared in print during the period of this grant. In addition, one AWM Special Session was organized and one week long workshop at the Geometry Center, and initiated and edited the proceedings of both (the second after this grant expired). These proceedings are highly innovative in that they include videotapes. The PI gave a large number of invited talks at a variety of meetings.
RUTGERS - THE STATE UNIVERSITY

FINAL REPORT FOR

AFOSR-91-0010

PROFESSOR JEAN E. TAYLOR

PERIOD OF PERFORMANCE

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Final Technical Report
for the period October 1 1990 - January 31 1992
Jean E. Taylor

During this period of support I continued my long-term program of investigating the shapes of surfaces in mathematical models for crystals (including polycrystalline materials), both in equilibrium and in growth. My accomplishments included the completion of seven papers, all of which have either appeared in print or are in press, and working on five more, three of which have since been finished and accepted for publication. I also completed one videotape which has been published and did part of the work which has since resulted in another videotape that will soon be published. Four papers that I had previously written appeared in print during the period of this grant. In addition I organized one AMS Special Session and one week-long workshop at The Geometry Center, and initiated and edited the proceedings of both (the second after this grant expired). These proceedings are highly innovative, in that they include videotapes. I also gave a large number of invited talks at a variety of meetings.

The surface energy of the interface of a crystal with some other given material, such as another crystal, or its melt or vapor or some other matrix, is a function of the oriented normal direction n of the interface. If this surface energy per unit area (i.e., surface tension) \( \gamma \) is sufficiently anisotropic, then the Wulff shape, which is the equilibrium shape of a single crystal surrounded by the other material, is a polyhedron; this is the crystalline case by definition, although not all physical crystals have surface tensions with completely faceted Wulff shapes. There are many other situations besides that of a single crystal in equilibrium in which surface energy plays a role: grain boundaries in a polycrystalline solid, analogs of minimal surfaces and soap films on wire frames, and various types of crystal growth and dissolution.

In growth problems, another factor is the mobility \( M \) (also a function of the unit normal n), which is the ratio of the normal velocity to the force driving it to move (assuming a linear response to the driving force). The driving force can include both surface energy reduction and bulk energy reduction, due to a phase change; I have considered cases where the bulk energy part is zero, is constant, depends only on position and time, depends on the local shape of the surface, and depends on a diffusion field (like temperature or concentration).

My research accomplishments during this year included:

1. Writing three papers (one being the definitive research paper, the other two being relatively short expository papers about the results) and finishing a videotape on the motion of polycrystalline interfaces in 2-d in the crystalline case. Here the normal velocity of a segment \( S_i \) is of the form

\[
-M(n(S_i))(\Omega + \text{wmc}(S_i)),
\]

where \( n(S_i) \) is the oriented unit normal of \( S_i \), \( \Omega \) is a constant, and \( \text{wmc} \) stands for "weighted mean curvature." \( \text{wmc} \) is defined to be the rate of decrease in surface energy with volume under deformations consisting of changing the distance of \( S_i \) from the origin while keeping
its same orientation and adjacencies to other segments. For a line segment in a crystalline polygonal curve in the plane, its turns out to be just the length of the segment on the boundary of the Wulff shape with the same normal, divided by the length of the segment in the polygonal curve, times 1, -1, or 0 (depending on whether the adjacent line segments both bend up from the given segment, both bend down, or bend in opposite ways). A major question, which I had solved the previous year, was how to handle fixed boundaries and triple junctions. A second potential problem, that of changing topology due to portions of curves meeting and annihilating, was fairly easily solved and programmed.

The papers and videos referred to above are:

(i) Jean E. Taylor, Motion of Curves by Crystalline Curvature, Including Triple Junctions and Boundary Points, to appear in the Proceedings of the AMS Summer Institute on Differential Geometry, held in July 1990. This is the definitive paper.

(ii) Jean E. Taylor, Motion by Crystalline Curvature, in Computing Optimal Geometries (Jean E. Taylor, ed.), AMS Selected Lectures in Mathematics, 1991, 63-65 plus 7 1/2 minute video. (This publication has both a written and a video component).


2. Writing two large overview papers, to be published in the July 1992 issue of \textit{Acta Metallurgica}. The first paper, joint with John Cahn and Carol Handwerker, surveys nine different mathematical methods for trying to solve the problem of geometric crystal growth, outlining the methods and giving the circumstances in which each performs best. It also surveys all computational methods of which we are aware. My work on this paper involved considerable effort to understand the various methods, such as viscosity solutions of Hamilton-Jacobi equations, with which I was not previously familiar, and to make them intelligible to Cahn and Handwerker in particular and materials scientists in general. The companion paper is a survey of the different ways in which mean curvature and weighted mean curvature can be represented and interpreted, with the emphasis on the non-isotropic cases. John Cahn wrote of it as follows: "This is a difficult paper, and you may want to obtain some help from a mathematician, but it is the clearest exposition of the principles that I know." Full references are:


3. Working out one of the major features of how surfaces move by crystalline curvature, and continuing the preparation of a computer program to do it. In the period since the expiration of the grant, I have worked out what I believe is the remaining major part, programmed it, and made a video and a short paper about it for publication. The detailed paper with proofs is still in the formative stages.


(ii) Jean E. Taylor, Motion of Surfaces by Crystalline Curvature, in preparation.
4. Helping to devise a new theoretical variational approach to motion by mean curvature or weighted mean curvature, and establishing rigorously the connection between the crystalline method and the completely variational method. Much of the work and part of the writeup was done during the grant period.

   (i) Fred Almgren, Jean E. Taylor, and Lihe Wang, *Curvature Driven Flows*, to appear in SIAM Journal of Control and Optimization. This is the major paper.


5. Supervising my graduate student Andrew Roosen in his work applying the crystalline method to dendritic crystal growth and Ostwald ripening by coupling a diffusion field into the driving force. This work has been proceeding in spectacular fashion, and Roosen has obtained a postdoc position at NIST to work with Cahn after he finishes his Ph.D. I wrote one joint paper on this with Roosen, and he has published one additional paper since then.

   (i) Andrew Roosen and Jean E. Taylor, *Simulation of crystal growth with faceted interfaces*, in Interface Dynamics and Growth, MRS Symposia Proc. Ser. Vol 237, to appear (12 pages). This paper is a fairly complete description of the algorithm used and a brief description of the theoretical ideas behind it, together with 4 pages of pictures of the output of the program.

   (ii) Andrew Roosen, *Simulation of two-dimensional faceted crystal growth in a single diffusion field*, in Computational Crystal Growers Workshop (Jean E. Taylor, ed.), Selected Lectures in Mathematics, Amer. Math. Soc. (1992), 3 pages plus 6 minute video. In press. This is a short expository summary of the above approach, together with a video showing the results of the program under varying conditions leading to dendritic crystal growth or dense branching. It also shows an application to Ostwald ripening with 2000 initial crystals.

6) Finishing the paper *Destabilization of the Tetrahedral Point Junction by Positive Triple Junction Line Energy*, with Frank Morgan. This paper points out that the standard tetrahedral point junction, where four regions meet at a point, is no longer energy-minimising when a junction line energy is included in the total energy along with surface area. Rather, a surface with a line segment along which four surfaces meet is shown to have less total energy. An estimate is made for the length that such a four-fold junction line might be expected have, based on estimates for line junction energy that are given by dislocation energies; this distance is of the order of several atomic dimensions and might therefore be seen in experiments. Brakke’s computer program *evolver* was used to compute the figures for the paper and to get better estimates for some of the numbers.


7) Writing the paper *The Motion of Multiple-Phase Junctions under Prescribed Phase-Boundary Velocities*. This paper has still not been totally completed, since I have not put it at a very high priority, but it should be finished soon. It shows that the motion of triple junctions can in general uniquely defined, using Huygen’s principle of least time,
for three arbitrary normal velocity functions and three arbitrary half lines meeting at a point. This motion can be found by the appropriate use of characteristics, with something like "refraction" of the characteristics when the growth is first through one phase and then another. There are important exceptions: situations where there is no solution, and situations where for certain initial configurations, there is non-uniqueness (although once growth has started using any of the possibilities, it is then unique for all subsequent time). One accomplishment during this grant period was that I found and fixed a problem with part of my description of the least time formulation in this multiple-phase case.

Jean E. Taylor, The Motion of Multiple-Phase Junctions under Prescribed Phase-Boundary Velocities, (nearly finished) preprint.

8) Organizing the AMS Special Session on Computing Optimal Geometries with Fred Almgren and Al Marden (held at the AMS meeting in San Francisco, January 1991), and initiating and editing the proceedings of that session as the AMS publication Computing Optimal Geometries, in the series Selected Lectures in Mathematics. A novel feature of this proceedings is that it is a 70 page book together with a 90 minute videotape. The book contains 16 papers and the videotape contains 14 videos.

9) Organizing the Computational Crystal Growthers Workshop, held at the Geometry Center Feb. 24-28, 1992. I conceived of and did much of the organisational work during the period of this grant; since then, I have organized a proceedings quite similar to the Computing Optimal Geometries proceedings (it is now in press).

10) I gave a large number of invited talks at a large number of conferences and universities. These include

Frontiers of Science, Irvine, CA Nov. 1990
Materials Research Society fall meeting, Dec. 1990
Mathematical Sciences Research Institute, Berkeley, Jan 1991
AMS winter meeting (1 special session), San Francisco Jan 1991
The Metallurgical Society winter meeting, New Orleans Feb. 1991
Australia: 5 talks under 5 auspices in 3 cites, including an invited hour address at the Australian Math Society annual meeting, June-July 1991
Regional Geometry Institute, South Hadley July 1991
Institute for Theoretical Physics, Aspen, August 1991
AMS regional meeting (2 special sessions), Philadelphia Oct. 1991
U Mass GANG seminar Sept. 1991
Williams College Math Colloquium Sept. 1991
Materials Research Society fall meeting, Boston, December 1991
This grant provided major portions of my support at all of the non-mathematics meetings above.

11) The four papers which I had previously written but which appeared in print during the grant period are:


ii) Jean E. Taylor, Zonohedra and Generalized Zonohedra,
Amer. Math Monthly 99 (1992), 100-111.


Also, a video for which I was one of the authors was published during this grant period, as the video portion of: