DOE/ER/25015 --- T4

COMPUTATION AND GRAPHICS
IN MATHEMATICAL RESEARCH

Progress Report
for Period September 15, 1992-September 15, 1993

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June 1993

Prepared for
THE U.S. DEPARTMENT OF ENERGY
AGREEMENT NO. DE-FG02-86ER25015

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Progress Report and Description of Current Research

1 Grain Boundaries and Dislocations in Compound Polymers

We describe here our current collaboration with polymer physicists. This is primarily an effort to understand, and ultimately predict, the phase-interface structures for certain classes of compound polymers. A secondary goal is to develop a unified methodology. Previous results appear in [1, 2, 3, 5, 7].

The method of working combines three modes of scientific investigation: theoretical mathematics; transmission electron microscopy; computer simulation and visualization. Here, we will concentrate on one aspect of this work: the study of the structure of grain boundaries in diblocks that form lamellar morphologies. These grain boundaries have yet to be systematically investigated.

The identification and classification of phase interface structures continues, however. Here we give one example of current work. In Figure 1 there is a reproduction of an electron microscope image of a slice of a polymer blend (two diblocks and one homopolymer). We suspect that the surface interface is one in the three parameter family of genus one doubly-periodic surfaces discovered by Karcher and Rosenberg-Meeks several years ago. At this time, simulations are being done to verify this conjecture and to determine which surfaces in the family are the best match. At the same time, extended micrograph imaging is being done to provide data for a tilt series comparison.

In the boundary situation under study, grain boundaries form when regions of different lamellar orientation come into contact, the supposition being that these regions grow by nucleation. There is, a priori, no preferred orientation to the sheets forming the lamellae. The samples under consideration have been annealed as static films, and it is experimentally observed that the grain boundaries remain localized. Our aim here is to identify and classify the morphology of the boundaries.

Theoretical explanations of the localization phenomena justify the use of minimal surfaces as models [4, 9]. Physically, the narrow interfacial surfaces between microphases (with chemical junctions between unlike phases in a region of about $20\text{\AA}$) are not, of course, true surfaces in the mathematical sense. However the energy at the interface is proportional to the surface area, leading to equilibrium configurations corresponding to surfaces that are

A new minimal surface?!
 This is a blend of 2 different but are homoclinic

Figure 1

Singly-periodic
embedded
minimal surface
with one
helicoidal end
and genus one
quotient.

Figure 2

critical points for the area functional. (These are precisely the surfaces with zero mean curvature, or *minimal surfaces*.)

In previous work, [16] it is argued that Scherk's doubly-periodic surface was a reasonable model for a twist-boundary, where the twist angle was $\pi/2$. This surface of Scherk lies in a one-parameter family of surfaces, which model twist boundaries with angles between 0 and $\pi/2$. These interfaces have been observed experimentally and have been compared with mathematical models that can be computed directly. For relatively large angles, the agreement between theory and observation is good. The limit of such a twist boundary as the angle goes to zero, with appropriate scaling, can be considered as a model for a "fault," or *dislocation*. Hoffman and Wohlgemuth had shown that, appropriately normalized, the Scherk family converges to a helicoid as the twist angle goes to zero. This theoretical result meshes well with observed phenomena, at least to first order. This work, in the paper [8] by Hoffman and collaborators, was recently accepted for publication in the journal "Macromolecules." The letter of acceptance from the journal contained the prediction that it would become a seminal and highly quoted paper in the field.

New models for dislocations

Hoffman and Karcher [12] have constructed a family of singly-periodic examples that can be considered to be the desingularization of $2k+1$ coaxial helicoids, $k \geq 1$. Each of these surfaces is deformable through a smooth 1-parameter family. The defect core postulated to exist in lamellar phases, seems to be one of the surfaces in the family with $k = 1$. The fit to both data and theory is much better than the assumption of several coexisting helicoidal defects, or of a deformation of a twisted Scherk tower.

New models for twist boundaries: embedded minimal surfaces of finite type

Building on a discovery of Fusheng Wei [19], then a postdoctoral student at GANG, Karcher [18] discovered an embedded doubly-periodic minimal surface that desingularizes the meeting of two families of parallel halfplanes. This is the first new example of such a surface since those of Scherk, which were found in the 1830's. The idea is simple: replace every other saddle in the Scherk example by a tube. To do this, it is necessary to have different thickness for the phases in the lamellar structure, and the ratio of these thicknesses is rigidly determined, as is the diameter of the tube. This gives the surface a distinctive signature. We will use numerical methods to model TEM experiments for comparisons with real samples.

Hoffman, Karcher and Wei have discovered that this surface sits in a one-parameter family, each with its own distinguished signature. These surfaces have the amazing property that they limit to a singly-periodic surface which is asymptotic to the helicoid and has genus-one in the quotient. See image 2, taken from [11].

This newly-discovered surface is now being investigated as a model for dislocations [13]. Mathematically, this example is more difficult than Scherk's classical surface. Both surfaces exhibit a twist boundary with angle $\pi/2$. A detailed paper on this surface (more than 50

Figure 3

pages) is completed and in galley form [14] to be published this year. More work is currently being done by Hoffman and collaborators on the subject of complete embedded minimal surfaces of finite topology but infinite total curvature. In particular the end behavior has never been investigated. (There was no real reason to do so before the discovery of this example.). See Image 3. This involves not only classical analysis and computer simulation, but also the investigation of the infinite genus Riemann surfaces of "algebroid" functions.

2 Boundary value problems for hypersurfaces constant Gaussian curvature

Given a disjoint collection $\Gamma = (\Gamma_1, \dots, \Gamma_m)$ of smooth Jordan curves in R^3 , a fundamental question is to decide if there exist surfaces of constant Gauss curvature K (K -surfaces) with boundary Γ . More generally we consider $\Gamma \subset R^{n+1}$ with each Γ_i a closed, codimension-2 embedded submanifold, and seek a K -hypersurface of constant Gauss-Kronecker curvature K . Of course, the range of allowable K depends on Γ . An elementary necessary condition for $\Gamma \subset R^3$ to span a surface S of positive Gauss curvature $K(S) > 0$ is that each Γ_i have no inflection points. In particular, a single planar Jordan curve bounded by S must be strictly convex and S must meet the plane transversally.

Thus far, the known existence results find K -hypersurfaces as graphs over a smooth domain $\Omega \subset R^n$ using the theory of Monge-Ampère equations. In 1984 in a fundamental paper, Caffarelli, Nirenberg and Spruck [6] proved that if Ω is strictly convex and ϕ is a C^∞ function on $\partial\Omega$, then $\Gamma = \text{graph } \phi$ bounds a K -hypersurface M for $K > 0$ sufficiently small. Moreover, M is a graph over Ω . This result was extended recently by Hoffman, Rosenberg and Spruck [15] who considered domains $\Omega \subset R^n$ with boundary components $\partial\Omega = (\gamma_1, \dots, \gamma_m)$ where each γ_i is strictly convex or concave with respect to Ω . Assuming there is a C^∞ strictly locally convex graph $M = \text{graph } u(x)$, $x \in \bar{\Omega}$ with $K(M) > K$, then there is a K -graph $x_{n+1} = u(x)$ with $u = \underline{u}$ on $\partial\Omega$. This last result was motivated by the geometric problem $\Gamma = (C_1, C_2)$ where C_1, C_2 are strictly convex curves in parallel planes. In the special case that there is a translation which rigidly moves one of the curves inside the other, the theorem implies there is a K -graph (with respect to the translation direction) for K sufficiently small.

The work of Hoffman, Rosenberg and Spruck was continued by Spruck and his Ph.D student Guan who again used Monge-Ampère equations to find K -hypersurfaces but in a much more geometric setting. Their approach was motivated by the problem of finding K -hypersurfaces spanning "strictly extreme" Γ :

$$(2.1) \quad \begin{cases} \text{Let } M \text{ be a smooth strictly convex closed hypersurface in } R^{n+1} \text{ and} \\ \text{let } D \text{ be a smooth subdomain of } M \text{ with } \partial D = \Gamma = (\Gamma_1, \dots, \Gamma_m). \\ \text{For } 0 < K < K(M) = \inf_{P \in M} K(P) \text{ find a } K\text{-hypersurface spanning } \Gamma. \end{cases}$$

The idea is to represent M as a radial graph over a domain Ω on the unit sphere $S^n \subset R^{n+1}$ (with respect to a suitable choice of origin) and to deform M to a K -graph over Ω . For $0 < K < K(M)$, M serves as a strict subsolution for the resulting problem and the deformation takes place inside M . Thus we arrive at the following formulation of our boundary value problem on S^n :

Let Ω be a smooth domain on $S^n \subset R^{n+1}$. We seek a smooth strictly locally convex hypersurface which can be represented as

$$(2.2) \quad X(x) = \rho(x)x, \quad \rho > 0, \quad x \in \Omega,$$

with Gauss curvature

$$(2.3) \quad K[X(x)] = \psi(x), \quad x \in \Omega,$$

and boundary value

$$(2.4) \quad X(x) = \phi(x)x \quad \text{on } \partial\Omega,$$

where $\psi \in C^\infty(\bar{\Omega})$, $\phi \in C^\infty(\partial\Omega)$, $\psi, \phi > 0$.

We assume that

$$(2.5) \quad \Omega \text{ does not contain any hemisphere,}$$

and that there exists a smooth, strictly locally convex, radial graph $\bar{X}(x) = \bar{\rho}(x)x$ over Ω satisfying

$$(2.6) \quad \begin{aligned} K[\bar{X}(x)] &\geq \psi(x) + \delta_0 && \text{in } \Omega, \\ \bar{\rho} &= \phi && \text{on } \partial\Omega, \end{aligned}$$

for some $\delta_0 > 0$.

The main result of Guan and Spruck [10] may be stated as follows.

Theorem 2.1. *Under conditions (2.5)-(2.6), there exists a smooth strictly locally convex radial graph $X(x) = \rho(x)x$ with $\rho \leq \bar{\rho}$ which satisfies (2.3)-(2.4). Moreover any such solution satisfies the a priori estimate*

$$(2.7) \quad \|\rho\|_{C^{2,\alpha}(\bar{\Omega})} \leq C, \quad \rho \geq c_0 > 0, \quad \kappa_i \geq \epsilon_0 \quad (i = 1, \dots, n),$$

where the κ_i are the principal curvatures of X and C, c_0, ϵ_0 are uniform constants.

As an immediate corollary of this result we can solve Problem (2.1):

Corollary 2.2. *Let M be strictly convex hypersurface in R^{n+1} , and let $\Gamma = (\Gamma_1, \dots, \Gamma_m)$ be strictly extreme, that is, $\Gamma = \partial D$ for a smooth subdomain $D \subset M$. Then for $0 < K < K(M)$, Γ bounds an embedded K -hypersurface which is contained inside M .*

By using a modification of this result suggested by our colleague Robert Kusner, one can construct smooth embedded K -surfaces of any genus! In particular, one verifies the existence of the K -surface of genus 2 suggested in [15, Remark 2].

One of the surprising and important features of Theorem 2.1 with respect to the theory of Monge-Ampère equations is that there are no geometric assumptions on $\partial\Omega$. That is, all of the analytic and geometric obstructions to proving existence are now embodied in the assumption of the existence of a strict subsolution of (2.6). This has led us to a careful reexamination of the local regularity estimates of [6, 15]. In particular, it is worthwhile to state a global result which contains an optimal smooth existence result for graphs over domains in R^n of prescribed Gauss curvature.

Theorem 2.3. *Let $\Omega \subset R^n$ be a smooth bounded domain with boundary components $\partial\Omega = (\gamma_1, \dots, \gamma_m)$. Assume there is a smooth strictly locally convex function $\underline{u}$ in $\bar{\Omega}$ satisfying*

$$(2.8) \quad \begin{aligned} \det(\underline{u}_{ij}) &\geq \psi(x, \underline{u}, \nabla \underline{u}) + \delta_0 \text{ in } \Omega \\ \underline{u} &= \phi \text{ on } \partial\Omega \end{aligned}$$

where ϕ, ψ are smooth, $\psi > 0$ and $\psi^\pm(x, u, p)$ is convex in p . Then there is a smooth locally convex solution $u \in C^\infty(\bar{\Omega})$ to the Monge-Ampère boundary value problem:

$$(2.9) \quad \begin{aligned} \det(u_{ij}) &= \psi(x, u, \nabla u) \text{ in } \Omega, \\ u &= \phi \text{ on } \partial\Omega. \end{aligned}$$

If $\psi_u \geq 0$ the solution is unique.

The choice $\psi(x, u, p) = K(x, u)(1 + |p|^2)^{\frac{n+1}{2}}$, $K(x, u) > 0$ corresponds to prescribing the curvature function $K(x, u)$.

Many of these results have been extended to large classes of fully nonlinear equations in the Ph.D thesis of Bo Guan. In particular, Guan has shown that the existence of a strict subsolution is the essential obstruction to proving existence in domains of arbitrary geometry. This work has been continued by Rosenberg and Spruck (On the existence of convex hypersurfaces of constant Gauss curvature in hyperbolic space), Nate Whitaker (U.Mass) and Frank Baginski are pursuing computations of surfaces of constant Gauss curvature based on methods and algorithms contained in the papers above.

3 Discrete Computational Geometry

Kusner and co-workers have completed a series of experiments minimizing discrete versions of $W = \int H^2 dA$ and the results are summed up best in Hsu, Kusner and Sullivan [17]. In particular, they have discovered experimentally, and are now trying to construct analytically many new minimal surfaces in S^3 as well as W -stable surfaces. In addition to edge curvature and the original discrete mean curvature described in [17], they have defined and used a third notion, "normal curvature", which avoids most of the pathology of sharp edges or corners and works for non-convex surfaces of any genus. Normal curvature also allows us to discretize and minimize energy integrands like $(H - H_0)^2$. This gives a way of

approximating surfaces with constant mean curvature H_0 , which are unstable for energies proportional to area, but absolute minima for $\int (H - H_0)^2$. Brakke and Kusner have recently considered replacing the constant H_0 by functions of the position X and normal N . They expect that this will give experimental evidence for high genus solutions to both the self-similar and translating mean curvature flows.

Kusner has begun to investigate another conformally invariant energy functional for embedded submanifolds. In joint work with Denus Kim [Torus knots extremizing the conformal energy, to appear in *Experimental Mathematics*] they found the first nontrivial examples of knots that are critical for the nonlocal energy recently introduced by O'Hara and studied by Freedman-He-Wang. They found critical links with more than component.

Kusner generalized this conformally invariant energy to Riemann surfaces. Recently, he and Sullivan have found a nice way to define the energy in any dimension [A conformally invariant, nonlocal energy for embedded submanifolds, in preparation]. They can prove that the round sphere S^k is the unique minimizer among k -manifolds in R^n , and that there are many critical points in general. The regularity theory of finite energy and minimizers is now being worked out. The hope is that for simple situations, like embedded 2-spheres in R^3 , we shall be able to prove that the only critical point is round. This may be applicable to proving the Smale conjecture.

(a)

(b)

Computing higher-genus
Willmore surfaces

References

- [1] D. Anderson, C. Henke, D. Hoffman, and E. L. Thomas. Periodic area-minimizing surfaces in block copolymers. *Nature*, 334(6184):598-601, 1988. August 18 issue.
- [2] D. Anderson and E. L. Thomas. Microdomain morphology of star copolymers in the strong-segregation limit. *Macromolecules*, 21:3221-3230, 1988.
- [3] D. M. Anderson, J. Bellare, J. T. Hoffman, D. Hoffman, and E. L. Thomas. Algorithms for the computer simulation of 2D projections from structures determined by dividing surfaces. to appear in the *Journal of Colloid and Interface Science*.
- [4] D. M. Anderson, H. T. Davis, J. C. C. Nitsche, and L. E. Scriven. Periodic surfaces of prescribed mean curvature. *Advances in Chem. Phys.*
- [5] D. M. Anderson, D. C. Martin, and E. L. Thomas. Maximum entropy data restoration using both real and Fourier space analysis. *Acta Crystallographica*, A45, pages 686-698, 1989.
- [6] L. A. Caffarelli, L. Nirenberg, and J. Spruck. The Dirichlet Problem for Nonlinear Second-Order Elliptic Equations I. Monge-Ampere Equations. *Comm. on Pure and Applied Math*, 37:369-402, 1984.
- [7] M. Callahan, D. Hoffman, and J. Hoffman. Computer graphics tools for the study of minimal surfaces. *Communications of the ACM*, 31(6):648-661, 1988.
- [8] S. Gido, J. Gunther, D. Hoffman, and E. L. Thomas. Block copolymer grain boundary morphology I. Lamellar twist boundary. to appear in *Macromolecules*.
- [9] S. Gido and E. L. Thomas. Block copolymer grain boundary morphology II. preprint.
- [10] Bo Guan and J. Spruck. Boundary value problems on S^n for surface of constant Gauss curvature. to appear in *Annals of Math*.
- [11] D. Hoffman. Comment utiliser un ordinateur pour trouver de nouvelles surfaces minimales et des bulles de savon. In *Surfaces minimales et solutions de problèmes variationnels*. Société Mathématique de France, 1993. Journée Annuelle du 5 juin, 1993.
- [12] D. Hoffman and H. Karcher. Singly periodic minimal surfaces derived from crystallographic examples. in preparation.
- [13] D. Hoffman, H. Karcher, and F. Wei. Adding handles to the helicoid. to appear in *Bull. A.M.S.*, 1993.

- [14] D. Hoffman, H. Karcher, and F. Wei. The genus-one helicoid, and the surfaces that led to its discovery. to appear in the Palais Festival Volume, Publish or Perish Press, 1993.
- [15] D. Hoffman, H. Rosenberg, and J. Spruck. Boundary Value Problems for Surfaces of constant Gauss curvature. *Comm. on Pure and Applied Math.*, XLV:1051-1062, 1992.
- [16] D. Hoffman and M. Wohlgemuth. Limiting behavior of classical periodic minimal surfaces. In preparation.
- [17] L. Hsu, R. Kusner, and J. Sullivan. Minimizing the squared-mean curvature integral for surfaces in spaceforms. *Experimental Math.*, 1(3):191-207, 1992.
- [18] H. Karcher. Comparison theorems for minimal surfaces. preprint.
- [19] F. Wei. *The existence and topology of properly embedded minimal surfaces in $\mathbb{R}^3$* . PhD thesis, University of Massachusetts at Amherst, 1991.

List of Visitors

The following is a list of speakers and visitors who participated in the GANG Geometry Seminars or worked on projects with GANG members since August 1992:

Professor Nicholas Korevaar, University of Utah and IAS

Professor Franz Pedit, Emory University

Pascal Romon, École Normale Supérieure, Paris, France

Martin Traizet, École Normale Supérieure, France

Meinhard Wohlgemuth, Universität Bonn, Germany

Eric Boix, École Normale Supérieure, Paris, France

Professor Remi Langevin, Université de Dijon, France

Michael Callahan, Harvard University

Professor Chuu-lian Terng, Northeastern University

Professor Richard Palais, Brandeis University

Dr. Charles S. Peskin, Courant Institute of Mathematical Sciences, New York

Dr. Bruce Kleiner, Institute for Advanced Study, Princeton

Helio Lopes, FUC, Rio de Janeiro, Brazil

Professor Geovan Tavares, FUC, Rio de Janeiro, Brazil

Professor Wenmao Yang, Wuhan University, PRC

Professor Bruce Kleiner, Institute for Advanced Study, Princeton

Professor Ulrich Pinkall, Universität Berlin

Matthias Heil, Universität Berlin

Professor Carolyn Gordon, Dartmouth College

Professor Richard Schoen, Stanford University and the IAS, Princeton

Professor Henry Wente, University of Toledo

Konrad Polthier, Universität Bonn

Professor Nick Firoozye, Universität Bonn

Professor Steven Krantz, Washington Univ., St. Louis

Professor Frank Baginski, George Washington Univ., Washington, DC