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SUPPLEMENTARY NOTES
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This is the final technical report on ARO contract DAAH04-95-1-0100, which began March 1, 1995 and ended June 30, 1998. This project's scientific focus was at the frontier where mathematics meets materials science. Physically, it was concerned with issues such as the effective behavior of composites and the formation of microstructure due to coherent phase transformation. Mathematically, it brought to bear a variety of tools including homogenization, the calculus of variations, and nonlinear partial differential equations. Specific accomplishments include: (a) improved understanding of how symmetry and texture determine the recoverable strain of a shape-memory polycrystal; (b) fresh insight concerning twinning and hysteresis in shape-memory materials; (c) progress on fundamental aspects of crystal and polycrystal plasticity; (d) a new approach to pattern formation in certain magnetic materials; and (e) improved models of heterogenous materials including piezoceramic composites and polymer dispersed liquid crystals.
MATHEMATICAL PROBLEMS IN MICROMECHANICS AND COMPOSITE MATERIALS

Final Technical Report for ARO Contract DAAH04-95-1-0100

Principal Investigator: Robert V. Kohn
Co-Principal Investigator: Marco Avellaneda
Courant Institute, New York University

ABSTRACT

This is the final technical report on ARO contract DAAH04-95-1-0100, which began March 1, 1995 and ended June 30, 1998. This project’s scientific focus was at the frontier where mathematics meets materials science. Physically, it was concerned with issues such as the effective behavior of composites and the formation of microstructure due to coherent phase transformation. Mathematically, it brought to bear a variety of tools including homogenization, the calculus of variations, and nonlinear partial differential equations. Specific accomplishments include: (a) improved understanding of how symmetry and texture determine the recoverable strain of a shape-memory polycrystal; (b) fresh insight concerning twinning and hysteresis in shape-memory materials; (c) progress on fundamental aspects of crystal and polycrystal plasticity; (d) a new approach to pattern formation in certain magnetic materials; and (e) improved models of heterogenous materials including piezoceramic composites and polymer dispersed liquid crystals.
1. Introduction

This is the final technical report on ARO contract DAAH04-95-1-0100, which began March 1, 1995 and ended June 30, 1998. The scientific focus of this project lies at the frontier where mathematics meets materials science. We are concerned with the effective moduli of composites, the formation of microstructure in coherent phase transitions, and random solutions of nonlinear evolution equations. These diverse problems are linked by a common theme: the relationship between microstructure and macroscopic behavior. The relevant mathematical tools include homogenization, the calculus of variations, and stochastic processes.

The scope of this effort is rather broad. One goal is to explore the mechanics of smart materials. Projects in this area include analysis of relaxation effects observed in certain shape-memory alloys (Bhattacharya and Swart, with James – Section 2.2); simulation of the microstructural pathway of a stress-induced phase transformation (Killough, working with Kohn – Section 2.3); and a model for how symmetry and texture determine the recoverable strains of shape-memory polycrystals (Bhattacharya and Kohn – Section 2.4). A second goal is to explore micromagnetics, plasticity, and other types of material behavior involving hysteresis and pattern formation. Projects in this area include an analysis of polycrystal plasticity, when the basic crystal has few slip systems (Kohn and Little – Section 2.5); and an explanation for the branching of magnetic domains in a uniaxial ferromagnet (Choksi and Kohn, with Otto – Section 2.7). A third goal is the improved analysis and design of technologically significant composite materials. Projects in this area include analyses of the dielectric properties of various heterogenous polymer and liquid crystal systems (Levy, with Stroud and Palfy-Muhoray – Section 2.6); and a model for the acoustic response of a composite when the wavelength of the incident radiation is not well-separated from the length scale of the microstructure (Avellaneda, with Berlyand and Clouet – Section 2.1).
The mentoring of postdoctoral scientists is a major part of our activity. This grant provided partial support for postdoctoral researchers Pieter Swart (spring 1995), Tom Little (1995-6), Ohad Levy (1995-6 and 1996-7), Rustum Choksi (1995-6 and 1996-7), and Tim Schulze (spring 1998). About 80% of our budget was spent on postdoc salary, fringe benefits, and associated overhead. Our postdocs have done very well in the job market: Swart has been a Staff Scientist at Los Alamos National Laboratory since 1995; Tom Little took a postdoctoral position at the University of Minnesota (1996-7) followed by an NSF Industrial Postdoctoral Fellowship at Columbia University and Morgan Stanley (1997-8); Ohad Levy took a postdoctoral position at the Levich Institute of CCNY-CUNY (1997-8); Rustum Choksi took a tenure-track Assistant Professorship at Simon Fraser University (1997-8). Tim Schulze is still at NYU, supported by a grant from NSF for one more year.

We are also active in the training of students. We supervised the thesis research of Reade Ryan (PhD, July 1996), Weimin Jin (PhD, August 1997) and Matt Killough (PhD, August 1998). This contract did not provide academic year support for these students, but it did provide summer support for Ryan and Jin, and Ryan received academic-year support from an ARO-sponsored AASERT contract.

For an interdisciplinary effort such as ours to succeed, contact with scientists in the relevant application areas is of paramount importance. Therefore we often attend and sometimes organize conferences at the interface between mathematics and mechanics. For example, in 1997 Kohn co-organized, with Steve Cowin of City College, a Workshop on Tissue Adaptation and Structural Optimization (NYU, 1/97); he chaired the organizing committee for the Second SIAM Conference on Mathematical Aspects of Materials Science (Philadelphia, 5/97); he was an invited speaker at the 78th Statistical Mechanics Meeting (Rutgers, 5/97); he served on the Research Advisory Board of the ARO MURI on Control and Design of Smart Structures (Harvard, 8/97); and he attended a meeting on Multiscale Materials Prediction – Fundamentals and Industrial Applications (MIT, 9/97).

2 Major Research Accomplishments

2.1 Piezoelectric composites


The work of Avellaneda, Berlyand, and Clouet addresses the scattering and transmission of an acoustic wave by a composite medium consisting of a periodic array of rods embedded in a homogeneous matrix. The motivation for this problem lies in the analysis and design of piezoelectric composites for use as acoustic transducers. Let $\lambda$ be the wavelength of the incident radiation, and $d$ the length scale of the composite. The limit $d \ll \lambda$ is standard: effective medium theory can be used, i.e. the composite can be treated as a homogeneous effective medium. In applications, however, it is often important to consider corrections due to nonzero $d/\lambda$. This is the "transitional" regime, when frequency dependent effects are no
longer negligible (as in the quasistatic case) but \( d/\lambda \) is small, so that the incident frequency is below the "cross-talk" regime in which the rods interact strongly \( (d \sim \lambda) \). The work of Avellaneda et al. determines the acoustic properties of the composite in the transitional regime, by means of an expansion in powers of \( \epsilon = d/\lambda \). Each term in the expansion is determined by solving a sort of "cell problem." The first few terms determine the essential frequency-dependence of the composite's impedance and reflection coefficients.

The article by Avellaneda and Swart reports work done under our previous ARO grant; its content was included in the final report on that grant.

2.2 Relaxation effects in shape-memory alloys


This work represents the first serious attempt to model the relaxation effects observed in certain shape memory materials in the martensitic phase. In these alloys, a twinned specimen can easily be detwinned by loading. If the loads are released soon after detwinning, the specimen spontaneously returns to the twinned configuration. If the loads are held for some time, however, the specimen remains detwinned even after loads are released. This behavior gives rise to a wide variety of effects, including changes in the hysteresis loops with cycling. There is some controversy as to its origin, which may be due to transient shuffle-twinning or possibly to short-range ordering. The work of Bhattacharya, James, and Swart develops a simple model based on the presence of a slowly-relaxing bulk-energy effect. Numerical simulations show good qualitative agreement with the experimental data. Experiments are proposed which would further test the model and shed light on the physical mechanisms of relaxation.

2.3 Stress-induced twinning and pattern formation


Hysteresis in shape-memory materials is associated with locally-stable microstructures and transitions between them. Recent experiments by Chu and James observed the stress-induced phase transformation from one variant of CuAlNi martensite to another. They observed striking and remarkably systematic microstructural patterns which form the pathway for this transformation.
The work of James, Kohn, and Shield explains how general features of the observed patterns – e.g. the structure of the approximate interfaces – is consistent with a model based on energy minimization.

The Ph.D. research of Killough, advised by Kohn, takes a different, more dynamic and computational approach to the same problem. Killough's simulations are based on a Landau theory (with strain-gradient terms) and viscoelastodynamics (without inertial effects). They capture many qualitative features of the observed patterns, including the nucleation and splitting of needles. These simulations have diffuse phase interfaces; Killough’s approach can be viewed as a sort of phase-field model, with strain as the order parameter. It is natural to inquire about the associated sharp-interface dynamics. The answer is surprisingly classical: the normal velocity of a twin boundary is a specific function of the orientation and "driving force." Recent work by Abeyaratne, Chu, and James proposed that the experimentally observed patterns represented local minima of (elastic + surface) energy. Killough's simulations call this into question, since his patterns are similar to those observed experimentally but they are transient rather than stationary.

2.4 Shape-memory polycrystals


The work of Bhattacharya and Kohn is the culmination of a project begun in 1991, when Bhattacharya came to NYU as an ARO-supported postdoc. This work addresses the effective behavior of polycrystals made from a shape-memory material. The overall goal is to explain how the symmetry of the underlying phase transformation and the texture of the polycrystal combine to determine the recoverable strain of the polycrystal. There is an elementary “Taylor estimate,” analogous to the one introduced by G.I. Taylor in the theory of polycrystal plasticity. The paper in Acta Materialia explores this estimate
and its consequences; the one in *Archive for Rational Mechanics and Analysis* explores the accuracy of the Taylor estimate by using techniques from nonlinear homogenization. One practical conclusion is that even in NiTi, the most common shape-memory material, favorable texture is crucial for good shape-memory behavior. This is documented in the recent paper by Bhattacharya, Kohn, and Shu (and in other recent work by Bhattacharya and Shu).

The paper with S. Kozlov addresses a special class of nonlinear homogenization problems in the plane. The microstructure is a sort of checkerboard polycrystal, and the energy of the basic crystal is degenerate in one direction. The main results are a pair of matching upper and lower bounds for the homogenized energy. This example shows that certain estimates proved by Bhattacharya and Kohn are nearly sharp. It can also be understood as an example in nonlinear effective conductivity, involving a checkerboard polycrystal made from a highly anisotropic nonlinear conductor. As current traverses the polycrystal, it follows a complicated path with logarithmic spirals centered at certain corners which form hotspots.

The work of Bhattacharya and Kohn uses geometrically linear elasticity. Shape-memory materials sometimes recover as much as 10% strain, so the effects of geometric nonlinearity may well be significant. The current work by Kohn and Niethammer provides the first extension of (some of) this work to the geometrically nonlinear setting. Bhattacharya and Kohn considered the recoverable strain of a 2D polycrystal, when the basic crystal has just two variants of martensite; their conclusion was that for polycrystals with sufficient symmetry there can be no recoverable strain. The result in the analogous nonlinear setting is different: there is always some recoverable strain, however its magnitude at most of order $\varepsilon^{3/2}$, where $\varepsilon$ is the transformation strain.

### 2.5 Polycrystal plasticity


This work addresses the yield stress of a (rigid, perfectly plastic) polycrystal in terms of its texture and the yield properties of the basic crystal. That is a classical problem – the first extensive discussion was given by G.I. Taylor in the 1930’s – however it is still not well understood. Kohn and Little concentrate on the case when the basic crystal has a highly eccentric yield set. The elementary Sachs (constant-stress) and Taylor (constant-strain) bounds are very far apart in this case, so it is natural to ask whether they can be improved, and which one describes the “typical” behavior. Kohn and Little show, for antiplane shear and plane stress versions of this problem, that the Bishop-Hill-Taylor cannot be improved while the Sachs bound cannot. Their methods combine nonlinear homogenization, compensated compactness, and the “linear comparison method” for bounding the behavior of nonlinear composites. Examples suggest that the generic behavior is closer to that of the Sachs bound than that of the Bishop-Hill-Taylor bound.

### 2.6 Linear and nonlinear composites

- W. Macevoy Jr. and M. Avellaneda, “Electroosmotic coupling: incorporating larger
surface effects with a new length scale," *J. Colloid and Interface Science* 188 (1997) 139–149.


The work of Macevoy and Avellaneda addresses electroosmosis, the phenomenon whereby an applied current produces flow in a porous medium. Microscopically one is concerned with a porous medium such as sandstone, whose pore space is filled with a fluid containing ions such as salt water. The governing equations are Stokes flow in the fluid, Coulomb's equation for the electric potential, and a diffusion equation for the ions. Macroscopically one expects a law of the form

\[
J_e = L_{11} \nabla \phi + L_{12} \nabla p \\
J_f = L_{12} \nabla \phi + L_{22} \nabla p
\]

relating the electric current \(J_e\), the fluid current \(J_f\), the electric field \(\nabla \phi\), and the pressure gradient \(\nabla p\). If \(L_{12} = 0\) this reduces to Ohm's law and Darcy's law. The coefficient \(L_{12}\) is responsible for electroosmosis; it is nonzero when the microscopic model includes a surface charge. Crucial physical parameters are the ion number density and the pore size. After nondimensionalization these determine the reduced surface charge \(\rho_s\) and the Debye parameter \(\delta\). The work of Macevoy and Avellaneda considers the regime \(\delta \ll 1\) and \(\delta \rho_s \sim 1\). It gives geometry-independent estimates for \(L_{12}\), extending work done earlier by Helmholtz, Smoluchowski, Fixman, and others.

Ohad Levy’s work with Bergman and Kohn addresses some issues involving physically nonlinear behavior of composite materials. The paper with Bergman summarizes part of Levy’s thesis work, concerning optical bistability. The paper with Kohn explores the
implications of duality for nonlinear two-dimensional systems. This work extends the well-known results of Keller and Dykhne concerning linear composites. It focuses on three main types on nonlinear behavior: (i) the weakly nonlinear regime; (ii) power-law behavior; and (iii) dielectric breakdown. Besides making the consequences of duality explicit in each setting, this work gives restrictions on the critical exponents and scaling functions of "dual pairs" of random nonlinear composites near a percolation threshold.

Levy's work with Stroud and Palfy-Muhoray models the dielectric and optical response of some technologically significant heterogeneous media. The project with Palfy-Muhoray concerns optical response of polymer dispersed liquid crystals (PDLC's) - droplets of liquid crystal dispersed in a polymer matrix. The focus here is on nematic droplets in an isotropic polymer matrix. These materials are being considered for a number of applications, including switchable windows and active matrix projection displays. The foundation of these applications is the fact that the dielectric properties of a PDLC can be changed by an externally applied electric field. Levy and Palfy-Muhoray have given the first satisfactory theoretical model for this effect. They use a Maxwell Garnett type mean field theory to represent the dielectric response of a PDLC in terms of the orientation distribution function of the droplets. The response of the PDLC is a nonlinear function of the applied field, because the applied field influences the orientation of each droplet, changing the orientation distribution function.

2.7 Magnetic materials


The work of Choksi, Kohn, and Otto addresses some static and dynamic problems of micromagnetics. The micromagnetic energy involves a competition between "bulk" and "surface" energy, often leading to complex patterns of domains and walls. It is fruitful to do a sort of asymptotic analysis, treating the surface energy as a small parameter. The paper by Kohn and Otto surveys the power and utility of this viewpoint. In particular, it provides an expository summary of Otto's proposed effective equation for dynamics of a ferrofluid in a Hele-Shaw cell under an applied transverse field.

The papers with Choksi apply micromagnetics to analyze the structure of magnetic domains in a uniaxial ferromagnet. This work focusses on the (physically relevant) case when the wall energy is small. Its thesis is that the observed branching of magnetic domains is a feature of any domain pattern with relatively small energy. This is demonstrated by identifying the scaling law of the minimum energy, i.e. by proving a pair of matching upper and lower bounds. Furthermore it is shown that a domain pattern achieving this scaling law must have average width of order $L^{2/3}$, where $L$ is the length of the magnet in the easy direction. Finally, the authors argue that branching is required by considering the
constrained variational problem in which branching is prohibited and the domain structure is invariant in the easy direction; its scaling law is different. The earlier paper by Choksi and Kohn addressed a 2D version of this problem. The extension to 3D, achieved in the later paper with Otto, required introduction of an entirely new technique, based on an interpolation lemma linking $L^2$, $L^\infty$, $BV$, and $H^{-1}$.

2.8 Defect energy


The Ph.D. thesis of Weimin Jin, advised by Kohn, addresses the singularly perturbed variational problem $\min_{\Omega} (|\nabla u|^2 - 1)^2 + \epsilon^2|\nabla \nabla u|^2 \quad dx \; dy$ subject to $u = 0$ and $\partial u / \partial n = 1$ at $\partial \Omega$, in the limit as $\epsilon \to 0$. This problem arose recently in work by Gioia and Ortiz on blistering of compressed thin films. It is the simplest example of a singularly perturbed variational problem whose order parameter is a gradient field, and whose $\epsilon = 0$ limit prefers a continuum of states. Jin has obtained new results concerning the asymptotic energy, and the form of minimizers. A paper based on this work is being prepared for publication.

The work by Choksi, Del Piero, Fonseca, and Owen addresses the theory of "structured deformations." This developing framework permits simultaneous discussion of deformation on two different length scales, macroscopic and microscopic. The new paper by Choksi et al. clarifies the functional analytic foundation of the theory of structured deformations. It also applies this framework to some specific phenomena from crystal plasticity and cohesive fracture: yield, hysteresis, and the associated dissipation in plastic yield are shown to arise from instabilities at the microlevel; also, the dichotomy between brittle vs. ductile fracture is clarified. Some detail concerning the latter point: when the undeformed length of a bar is larger than a certain critical value, the model predicts that small extension induces no crack while large extension induces a single crack of a known size (brittle failure). When the undeformed length of a bar is smaller than the critical value, the model predicts that small extension induces no crack while large extension induces a single crack whose size increases gradually from zero with the amount of extension (ductile failure).

2.9 PDE's modeling turbulent behavior


The 1996 paper by Avellaneda is a survey of his work with Majda and others, using methods from homogenization and probability to derive rigorous results on turbulent advection and anomalous diffusion.

The work of Avellaneda and Vergassola addresses the large-time, large-scale behavior of turbulent transport, when the underlying velocity field is not incompressible. The relevant PDE is \( T_t + \nabla \cdot (uT) - D \Delta T = 0 \), where \( u = u(x,t) \) is a specified random velocity field with mean value 0. When \( u \) is incompressible the effective equation is diffusive. In general, however, transport can be much faster due to the presence of a linear term in the effective equation ("ballistic transport").

The work of Apelian, Holmes, and Avellaneda reports analytical and numerical results concerning the streamlines of a specific class of random velocity fields. Conclusions are drawn concerning the statistical topography of the flow, and concerning the turbulent diffusion associated with it.

### 2.10 Thin film growth


Kohn’s work with Choksi and Otto addressed the structure of domains in a setting where energy minimization is paramount. The work of Schulze and Kohn addresses the structure of domains in a very different setting – spiral growth of thin films – where the behavior is dominated by kinetic effects. A convenient model system is the growth of c-axis YBCO high-temperature-superconductor films on MgO substrates. Experimentalists have observed that the grain size coarsens as a function of distance from the substrate. Schulze and Kohn conjecture that this coarsening is the result of a geometrical competition between the grains, whereby the faster-growing spirals gradually dominate. Their paper formulates this idea, and demonstrates its consequences analytically and numerically, for the simplest possible model in which corrections due to surface diffusion and curvature are ignored.

### 3 Students

We directed the work of three PhD students in areas associated with this project.

**Reade Ryan** completed his Ph.D. in July, 1996 under the direction of Marco Avellaneda. His thesis was entitled “Large Deviation Analysis of Gaussian Fields and the Statistics of Burgers’ Turbulence.” He is currently an Assistant Professor in the Mathematics Department at Columbia University.

**Weimin Jin** completed in Ph.D. in August, 1997 under the direction of Robert Kohn. His thesis was entitled “Singular Perturbation and the Energy of Folds”. He is currently an Assistant Professor in the Mathematics Department at Indiana University.
Matthew Killough will complete his Ph.D. thesis in August, 1998 under the direction of Robert Kohn. His thesis is entitled "A Diffuse Interface Approach to the Development of Microstructure in Martensite." He will begin an Assistant Professorship in the Mathematics Department at University of Minnesota in September, 1998.

4 Publications

In refereed journals:


Book chapters and conference proceedings:


Articles in advanced stages of preparation:
1. M. Avellaneda, L. Berlyand, and J.-F. Clouet, “Frequency dependent acoustics of composites with interfaces”


3. R.V. Kohn and B. Niethammer, “Geometrically nonlinear shape memory polycrystals made from a two-variant material”
