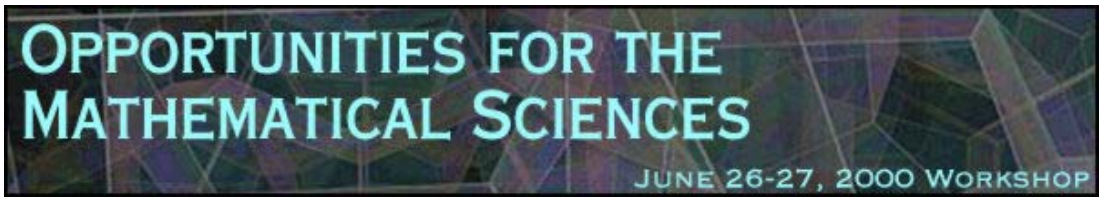

Mathematics in Materials Science

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A vibrant community has developed at the triple point where mathematics meets physics and materials science. The very successful Third SIAM Conference on Mathematical Aspects of Materials Science provides a convenient snapshot of its scope (Philadelphia, May 2000, [http://www.siam.org/meetings/ms00]) .

The boundary between mathematics and materials science is fuzzy, and should remain so. Yet mathematicians have a special role to play, in part because they tend to use different tools and focus on different questions than their materials science colleagues. Their goals naturally include modeling phenomena at the edge of current capabilities or understanding, and developing new tools that advance the scientific frontier. But their goals also include clarifying conclusions through rigorous analysis, and taking advantage of common themes in apparently distinct disciplines. One such theme is the linking of models on different length scales: this grand challenge of materials science has much in common with numerical analysis (especially domain decomposition and adaptive mesh refinement) and homogenization (which provides macroscopic constitutive laws for materials with microstructure).

Here is a highly selective survey of past accomplishments, present directions, and future promise in eight areas.

1. EFFECTIVE MODULI OF COMPOSITES

The analysis of composite materials has a long history. Traditionally, most attention has focused on composites with known or measured microstructure--developing methods for estimating macroscopic behavior such as the effective dielectric constant or Hooke's law. Recently some investigators have addressed what amounts to the opposite problem--finding microstructures with extremal effective behavior, and more generally exploring the range of possible effective behaviors as the microstructure varies. This effort has been remarkably successful, leading to homogenization-based numerical algorithms for optimal design and an impressive array of explicit examples [1,2]. In the process, new methods have been developed for establishing geometry-independent bounds on effective moduli, and for constructing composites with extremal behavior.

The present understanding of bounds and optimal microstructures is most complete for two-component linear composites. Similar progress in other settings--multicomponent composites, polycrystals, and nonlinear material response--will require new ideas. But perhaps the proper immediate goal is less directed: we should seek a deeper understanding of links to the multidimensional calculus of variations. The analysis of effective moduli and coherent phase transformation is driving this field in much the same way that analysis of soap films and minimal surfaces drove development of geometric measure theory a generation ago. One tantalizing development is the recent use of results about quasiconformal mappings to prove new bounds on effective conductivity [3,4].

2. MARTENSITIC PHASE TRANSFORMATION

The mechanical response of a shape-memory material is highly nonlinear, giving rise to a wide range of applications including actuators, eyeglass frames, dental

wire, and medical devices. The special properties of these materials are attributable to their crystalline structure, and in particular to a martensitic phase transformation. The nonlinearity of their response is due to stress-induced changes in microstructure. We need better models for such materials, both to predict and control their behavior and to facilitate the design of new materials.

Recent mathematical work has greatly improved our understanding. A major breakthrough was the realization that the phenomenological "crystallographic theory of martensite" can be deduced from elastic energy minimization [5]. This has led to fresh understanding of various material systems, and quite recently to the design of new thin-film devices and magnetostrictive materials [6,7].

Most manufacturable shape-memory materials are polycrystals rather than single crystals. This raises both analysis and design questions: given a material with known polycrystalline texture, can we model its overall response? And are there special polycrystalline textures with unusually good response? Methods from polycrystal plasticity are relevant, through an analogy between slip systems and twinning systems. However the situation is rather different--shape memory materials have relatively few twinning systems while most metals have many slip systems--so the two subjects are by no means equivalent [8]. One current activity is the development of a novel scheme for simulating random polycrystals [9].

The link between shape memory behavior and elastic energy minimization has driven, over the past ten years, a very productive re-examination of nonconvex problems in the multidimensional calculus of variations. One striking accomplishment was V. Sverak's demonstration that rank-one convexity is different from quasiconvexity [10].

3. AVERAGING, HOMOGENIZATION, AND MEAN FIELD THEORIES

We often wish to describe the essential character of a heterogeneous system. This is commonly done using approximate, ad-hoc, or formal arguments, leaving some doubt about the correctness of the model. Mathematical analysis is valuable for its ability to set the record straight, sometimes leading to unexpected conclusions.

Ostwald ripening provides a convenient example. This surface-energy-driven, volume-preserving evolution of inclusions in a matrix arises in the modeling of phase separation. Forty years ago Lifshitz, Slyozov, and Wagner analyzed the case of well-separated, low-volume-fraction inclusions, deriving an evolution equation for the radius distribution function then finding a similarity solution representing its asymptotic large-time dynamics. Their analysis was widely accepted, however recent work has shown that it is incomplete. In fact the LSW similarity solution is not the only stable one; other asymptotic regimes are possible as well, depending on the details of the initial distribution [11].

An open problem involving averaging is the analysis of length scale effects in plasticity. It has long been known that the hardness of a ductile polycrystal increases as the grain size decreases. The standard explanation involves dislocation pileup at grain boundaries; this may well be right, but we lack understanding of its macroscopic consequences. Recently phenomenological "strain gradient" theories have been proposed and calibrated against various experiments [12]. There remains, however, no derivation of strain-gradient theory from a finer-scale model of mechanical behavior.

A somewhat different question is the analysis of random composites. Attention has traditionally focused on macroscopic effective behavior, and on bounding or estimating this behavior using statistical measurements such as two- or three-point correlation functions [13]. In an unexpected convergence of interests, the image processing community has also been studying random patterns--known to them as textures [14]. But specialists in vision rarely use real-space representations of images; they prefer multiscale or wavelet representations. Might wavelet representation also be useful for analyzing the properties of a composite--for example for predicting the statistics of local fields, given a finite-sizes sample of the microstructure?

4. DEFECTS AND SINGULARLY PERTURBED VARIATIONAL PROBLEMS

Many physical systems have Landau theories, which amount to nonconvex

variational problems regularized by higher-order singular perturbations. Micromagnetics provides an example: there the higher-order term is exchange energy. The analysis of shape memory via elastic energy minimization provides another example: there the singular perturbation is surface energy. The mechanics of thin sheets provides a third example, with bending energy as the singular perturbation.

The metastable states associated with such singularly perturbed energies typically have defects. Magnetic domain walls and elastic twin boundaries are familiar examples. Since these problems have a small parameter, it is natural to do an asymptotic analysis as that parameter tends to zero [15]. There are in fact two distinct tasks, which should be separated: understanding the internal structure of defects, and understanding their spatial distribution. The theory known as Gamma-convergence provides a convenient framework and a powerful set of analogies. The physically relevant examples usually lie beyond the power of the existing theory, however, so examples based on Landau theories are helping drive the subject. Recent studies in this area have addressed, among other topics (a) soft magnetic thin films [16] and (b) delamination and blistering of compressed thin films [17].

5. INTERFACE MOTION

Interface motion laws are central to materials science--and to other areas including differential geometry and image processing. The past ten years' progress in this area has been quite striking.

On the numerical side, a family of "level-set" methods has been developed for tracking the motion of oriented curves in the plane or surfaces in R^3 [18]. The great advantage of these methods is their seamless handling of topological change. The earliest implementations were for local laws of motion, however the current technology also handles nonlocal laws such as those that arise in deposition processes (where shadowing is important), solidification (where interface motion is coupled to a bulk diffusion), and fluid dynamics (where the interface is a free boundary) [21].

On the analytical side, a viscosity-solution-based theory of existence and uniqueness [19,20] has clarified the handling of topological transitions such as pinch-off. It is natural to wonder whether the continuation of the solution is uniquely determined after pinch-off, or whether additional constitutive information might be required at the singular time. The PDE theory shows, in a certain precise sense, that the evolution after pinch-off is usually determined without any need for further information--but it also gives examples where this is not the case [22].

Much remains to be done. The level set and viscosity methods are mainly restricted to two-phase problems and oriented interfaces; the simulation and analysis of multiphase problems is very different and far less well understood. Even in the two-phase setting, our understanding of the analysis lags far behind the numerics. For example, the current generation of level-set-based numerics seems to handle topological transitions for fourth-order problems like "motion by surface diffusion", however there is as yet no corresponding theory of weak solutions.

6. EPITAXIAL GROWTH

Epitaxial growth is the process by which a crystalline film is formed. The fundamental mechanisms were explored by Burton, Cabrera, and Frank almost fifty years ago. However the system-specific details and the mesoscopic consequences of these mechanisms are still poorly understood.

Below the roughening temperature the crystal surface consists of steps and terraces. Atoms land on terraces, diffuse to steps, then get incorporated into the crystal. The attachment of atoms at steps accounts only for horizontal growth; vertical growth requires creation of new steps, for example through nucleation of islands or through the presence of screw dislocations. As details vary--for example attachment and detachment laws, anisotropy, and misfit--these elements combine in various ways to determine the crystalline structure, defects, and roughness of a growing film [23].

Epitaxial growth can be modeled in different ways: molecular dynamics tracks the positions of atoms; kinetic Monte Carlo tracks transitions between specific configurations; step flow laws track the positions of steps; and surface evolution laws track the continuum-scale surface as the solution of a partial differential

equation. All these approaches are valuable; they describe different length and time scales. Molecular dynamics, the smallest-scale tool, is used to determine the statistics of configurational transitions. Monte Carlo is still essentially an atomic scale technique; since little averaging is done within the model, the correspondence between parameters and morphology must be explored through simulation--a laborious procedure due to the very small length scale and time step. Step flow laws do some local averaging, by solving a diffusion equation instead of a random walk on each terrace, and by representing step positions as smooth curves. This is useful, for example, for understanding instabilities and step bunching. Surface evolution laws do much more averaging--though the precise amount is often unclear, since those models are usually obtained phenomenologically rather than by averaging a finer-scale theory.

The tasks of simulating these models efficiently, using them effectively, and linking them with one another are among the grand challenges of materials science. One recent development is a continuum approach to island growth. It tracks the terrace adatom density and the evolving island geometry by deterministic partial differential equations (using the level-set method, which handles topological transitions easily). Atomic-scale stochasticity is kept only where it matters--in the nucleation of new islands. Numerical experiments have shown that this method, properly calibrated, can reproduce the results of kinetic Monte Carlo simulation [24].

7. MICROMAGNETICS

Magnetic storage devices lie at the foundation of modern computing. Their modeling, simulation, analysis, and design raise fundamental questions of physics and mathematics, many still unanswered. Technology is changing the research frontier: as device sizes decrease, issues that seemed academic a few years ago--such as the effects of thermal noise and spatial disorder--are acquiring practical importance.

A distinguishing feature of this topic is the existence of a well-established and benchmarked mathematical model: micromagnetics [25]. This theory, now over fifty years old, describes metastable magnetization patterns as local minima of a suitable energy (composed of "exchange," "anisotropy," and "magnetostatic" terms). Moreover it prescribes the evolution of magnetization via the Landau-Lifshitz-Gilbert equation. Micromagnetics has relatively few constitutive parameters, yet (like fluid dynamics) its solutions can have complex behavior on multiple length scales.

One important direction for mathematical work is numerical micromagnetics. Numerical simulation is widely used already, but existing methods are only adequate for studying extremely small devices. There are basically three difficulties: (a) magnetic domain walls are thin, requiring a small spatial grid for resolution; (b) the evolution equations are stiff, requiring a small time step for stability; and (c) the magnetostatic interactions are long-range, requiring evaluation of a convolution at each time step. The usual way of handling (c) is to use a fast Fourier transform--which however requires a uniform spatial grid. This wastes spatial degrees of freedom on large regions where nothing interesting is happening. Adaptive mesh refinement is a natural alternative, coupled with a version of the fast multipole method [27] for evaluating magnetostatic interactions. Another natural direction is the development of implicit time-stepping schemes, to permit simulation with much larger time steps [26].

A different direction is the role of noise in magnetic switching. The switching of a uniformly-magnetized particle has been considered at great length. However the systems of real interest are not uniformly magnetized: the configuration space is truly infinite-dimensional (magnetization fields) rather than finite-dimensional (constant magnetization), and switching involves nucleation and motion of domain walls. Even without noise, the present understanding of switching in the spatially-distributed setting is very incomplete. As for the role of noise: this is a question of large deviations, for a system described by stochastic PDE's rather than stochastic ODE's. The relevant theory is in its infancy [29]; our current understanding is based mainly on numerical and physical experiments [28].

8. ALGORITHM DEVELOPMENT

Numerical simulation plays a major role in modern materials science. The increasing power of computation is only partly due to the development of bigger and faster computers. It is also due to the development of better algorithms, maximizing the impact of computational resources. A familiar example is the fast Fourier transform, which is routinely used in micromagnetics and many other areas

of condensed matter physics.

A recent development of comparable importance is the invention of fast multipole methods for evaluating long-range interactions of irregularly-placed sources. Problems of this type arise, for example, in analyzing scattering from rough surfaces, in predicting the performance of complex circuit boards, and in evaluating the magnetostatic interactions of irregularly-spaced dipoles. Before fast multipole methods, such computations on a system with N sources took order N^2 steps. The new algorithms reduce this to order N (or sometimes N log N) steps. Thus, a simulation previously limited to 10^4 sources can now be done with 10^8, giving access to whole new range of spatial and temporal scales.

Fast Fourier transform, fast multipole method--what's the next element in this sequence? That's hard to say, but a new scheme for accelerating molecular dynamics could be a serious contender. The importance is clear: molecular dynamics is in many settings the most fundamental model available, being based directly on a description of atomic interactions. However molecular dynamics is currently limited to extremely small time intervals, because the fast vibration times of an atomic scale model require extremely small time steps for accurate integration. This is a serious problem, since our main interest is in transitions between distinct configurations, which may have long waiting times. Recently Voter introduced a method called "hyperdynamics," which changes the underlying potential to make transitions more frequent, then corrects for errors associated with modification of the potential [30]. This method is generating great excitement in the materials science community. It seems a natural object for mathematical analysis, to reveal its power and limitations, and perhaps to make improvements.

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