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This project developed mathematical models and computational methods for the design of new active thin films having applications as actuators. The focus was on magnetostrictive and shape memory materials, and a recently discovered class of active materials that combine shape-memory and ferromagnetism. A major part of the research was concerned with the behavior of these materials at small scales: the development of new models and computational methods that predict small scale behavior. Computational models were developed for simple micromachines that have applications as valves and pumps.

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FINAL TECHNICAL REPORT

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Active Thin Films
April 1, 1997 – December 31, 1997

Mitchell Luskin and Richard James
University of Minnesota
March 13, 1998

1 Research Accomplished

James and Luskin developed new models and computational methods for the behavior of thin films of active materials. This program of research concerns the problem of deriving the asymptotically limiting theory for a film of thickness h in the limit as $h \to 0$, and using these models for numerical simulations of active thin films and prototype micromachines.

Calculations were carried out for general micromagnetics by James and Gioia [7] and for the Ball-James theory of martensite by Bhattacharya and James [2]. During the past year substantial improvements have been obtained on the derivation of bending energies from this precedure. These represent the first calculations in which a thin film or plate theory has been derived from three dimensional nonlinear elasticity, including bending energy, but with no underlying ansatz or choice of asymptotic expansion. The resuling theory is expected to be a widely useful, accurate, theory of the mechanical behavior of thin films.

One of the unexpected results from [2] is that there exist energy minimizing deformations in properly oriented thin films with exact austenite/martensite interfaces, unlike in bulk where austenite/martesite interfaces are always finely twinned (This result also follows from bulk Ball-James theory). These interfaces can be used as a basis of various designs of "tents" and "tunnels" on a thin film which look promising as a basis of large work-output microactuator designs. During the past year, in joint work with Raefaella Rizzoni, James has extended the derivation to the case in which the film is loaded by an hydrostatic pressure, as would occur in applications to MEMS based miniature pumps and valves [8]. To put these ideas into practice, it will be necessary to make epitaxial thin films of, say, shape-memory or magnetostrictive materials. The authors have persuaded several experimental groups to begin this research (Palmstrøm at Minnesota, Schryvers at RUCA in Belgium), and the work of Palmstrøm along these lines looks promising: the first single crystal thin films of shape memory materials are emerging from this work. The patterning strategy of Palmstrøm follows precisely from the predicted designs for tents and tunnels.

Luskin and his graduate student, Tim Brule, utilized this theory to develop a collection of models of simple microvalves and micropumps which are suitable for numerical simulation. They have developed three-dimensional computational models and a code for the tents and domes described above, and they have begun to explore the behavior of various thin film designs during a temperature-driven phase change. The active thin films utilized in the proposed microvalves and micropumps will undergo large deformations, so they utilized frame-indifferent models which are accurate for large deformations and rotations.

James continued work on magneto-memory materials. These materials, which combine ferromagnetism and shape memory, have been predicted by theory and the search for these materials has been guided at every stage by modern mathematical theory of transforming materials. During the past year, James and Wuttig have demonstrated spectacular field induced strains of 4.5% in certain NiMnGa alloys; these strains are 40–50 times larger than the best giant magnetostrictive materials, so the current materials exhibit by far the largest known magnetostrictive effect [10]; this paper also gives a general theory of ferromagnetic shape memory. The design of magneto-mechanical experiments that achieves these strains was based on a new constrained theory of magnetoelasticity [6]. However there remain some discrepancies between the predictions and measurements, which has led to an intense period of recent activity on this area. A understanding of this discrepancy is expected to lead to further advances in active materials.

Luskin developed a theory of stability for microstructure which he utilized to give the first analysis of the numerical approximation of martensitic microstructure for a physically realistic, multi-dimensional crystalline energy in [18]. Using this theory, Luskin gave an analysis of the stability and numerical approximation of the orthorhombic to monoclinic (double well) transformation in [18], and he then (in joint work with his former graduate student and post-doc, Bo Li) used this this theory to give an analysis of the stability and numerical approximation of the cubic to tetragonal (triple well) transformation [13]. In [15], Luskin (in joint work with Li) has extended the class of laminates for which the stability analysis can be applied to those whose volume fractions vary in space.

Luskin has recently further extended this stability analysis (in joint work with K. Bhattacharya and B. Li) to the cubic to orthorhombic transformation. The fact that the energy density for the cubic to orthorhombic transformation has six wells makes this problem significantly more difficult than the cubic to tetragonal transformation which has three wells since additional wells give the crystal more freedom to deform without the cost of additional energy. The uniqueness of the microstructure for the cubic to orthorhombic transformation, which had been a long-standing open problem, is a consequence of this stability analysis. This analysis also gives some rigorous justification for the assumption made by all of the analytical and computational research on the Chu-James experiment that the deformation gradient takes values in only two of the wells. The techniques developed in this work should also allow the systematic study of a large class of martensitic phase transformations with applications to active thin films.

Luskin's stability analysis for microstructure has been used in the above works to obtain error estimates for the numerical approximation of microstructure by the finite element method. This analysis has given a theoretical basis for the computational program and has made possible the development of more effective and reliable algorithms for the simulation and design of active thin films.

Luskin (in joint work with Martin Kružík) developed algorithms and did computations to study the feasibility of using the rank-one convexification and the polyconvexification of the energy to compute three-dimensional martensitic microstructure. [12].

2 Personnel Supported

This grant funded the post-doctoral research of G. Gioia who did research on thin films of magnetostrictive materials and derived the limiting theory for a thin micromagnetic films [7]. It also partly supported Abdelhakim Bensaoula for predictions of material systems and substrate materials for the growth of single crystal films by molecular beam epitaxy.

This grant partially supported the post-doctoral research of Martin Kružík described above [12]. The research of Tim Brule on the computation of active thin films (described above) was also supported by this grant. More junior graduate students supported by this grant to work on computational methods for active thin films were Pavel Belik and Julia Liakhova.

This grant also supported the Ph.D. research of James Riordan on the development and analysis of nonconforming methods for martensitic microstructure [20]. Nonconforming finite elements are attractive for the computation of microstructure since they relax the constraint of continuity and sometimes allow a finer scale approximation than conforming methods when the microstructure is not aligned with the grid. Riordan collaborated with Bo Li and Luskin on a analysis of the piecewise linear, nonconforming finite element approximation [17, 20].

This grant supported the graduate student research of Q. Guo on a new family of composites of shape-memory material.

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