Final Progress Report

Design, Modeling, and Computation of Active Thin Films
DA/DAAG55-98-1-0335

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1 Statement of Problem Studied

A new theory and numerical methods for the mechanical behavior of thin films were developed. The theory was applied to shape memory and ferromagnetic shape memory materials. This suggested several new designs for microactuators. One of these, a microvalve, was numerically simulated. It showed a reversible motion induced by temperature change and a nearly square hysteresis loop (valve opening vs. temperature). In addition, the deformation and transformation of a thin film by indentation and the disappearance of the indentation by heating and reverse phase transformation were numerically simulated.

A new scheme was developed for the passage from atomic to continuum level, applicable to nanoscale films, rods and tubes. This is being implemented in the context of carbon sheets, in joint work with Peter Chung of ARL. This implementation will continue at ARL jointly with Dr. Raju Namburu and Chung.

2 Summary of Most Important Results

Active martensitic thin films are increasingly being utilized in new and proposed technologies. The recent development by Palmstrom and James of techniques for the growth of single crystal martensitic thin films offers the promise of even larger work output per cycle. Bhattacharya and James have derived a thin film model for martensitic thin films from the geometrically nonlinear bulk theory of martensite. Luskin and his graduate student Pavel

Belik have utilized the Bhattacharya-James model to develop several finite element models for the deformation of active martensitic thin films.

Bělík and Luskin developed numerical methods and did simulations of an experiment performed by Cui and James. The goal of the experiment was to confirm the prediction of the thin film theory that certain martensitic alloys of specific composition and orientation support the tent deformation. In this experiment, a thin film of CuAlNi with a specific orientation was obtained, and an indenter in the shape of the predicted tent was used to deform the film appropriately. Upon removal of the indenter, the film remained in the tent-like shape in the upright position. A water bath was used to transform the film back to austenite, and the experiment was repeated several times.

Bělík and Luskin have developed a mathematical and computational model for the nucleation of the austenitie-martensite phase transformation and the propagation of the phase boundary as a single crystal thin film was heated and cooled from the boundary of the film. Our model has enabled us to begin to simulate the results of the experiment done by J. Cui and R. James on a thin slice of an alloy of CuAlNi.

A model for nucleation is necessary since the film would otherwise remain in a metastable local minima of the energy and would never transform at any temperature. We feel that the development of physical and efficient nucleation algorithms are necessary for the simulation and design of active materials based on phase transformation.

We have developed a Monte Carlo method that is implemented on each triangle of our finite element mesh that is based on a Maxwell-Bolzmann distribution of the states of the austenitic and martensitic phases. Another important aspect of our method was the development of an algorithm for the change of the phase of the crystal independently within each finite element triangle. For the phase change algorithm, it was crucial that we utilized the total variation surface energy developed earlier for this project.

We have developed a method for the direct passage from atomic to continuum scale for films. It relies on weak convergence methods to select in a natural way the continuum variables. The result of this work is a membrane theory for carbon sheets. For a film of n atomic layers the energy density is found to depend on $(\nabla u, b_1, \ldots, b_{n-1})$, where u describes the deformation of the "middle surface", and $(b_1, \ldots, b_{n-1})$ describe the relative displacements of the atomic layers that make up the film. An explicit formula for the energy is given that can be evaluated by atomic calculations. The approach is expected to give reliable results, as the entire procedure is justified by

asymptotic arguments resting on the atomic theory and mild assumptions about the deformations: the form of the continuum theory is not assumed. This will allow accurate calculations of the mechanical behavior of atomic scale films in a regime that are inaccessible to direct atomic simulation.

We are evaluating this energy for a carbon sheet with Peter Chung. We plan to do calculations on large arbitrarily deformed sheets, and treat defects with a quasi-continuum approach, and build up to the evaluation of the strength of materials. Chung is at the Army Research Laboratory doing an NRC postdoctoral fellowship under the direction of Dr. Raju Namburu (raju@arl.mil, (410) 278-0274). This work is of interest to the Army because of the potential use of nanoscale carbon nanotubes and sheets as a component in high strength composites or in monolithic material made from linked carbon nanotubes.

For the carbon sheets we first tried classical potentials of Stillinger-Weber and Tersoff type for carbon, but these were found to be innaccurate, by comparison to DFT calculations, for distorted states. We have now developed a suitable DFT method.

We are also currently doing theoretical work to understand the higher order asymptotics for atomic films; these are expected to deliver the bending energy at order $(1/k)^3$, where the film is a $k \times k$ sheet in its reference configuration.

James continued work on the behavior of thin films of active materials. It occurred in previous work that a small scale actuator could be driven by a certain time–dependent magnetic field. This led to the need for an expression for the driving force on a magnetoelastic interface. This has been treated in the literature, but the published expressions are incorrect. James derived the correct formula, which entailed a rather complete reworking of magnetism with careful attention to the presence of Dirac masses that arise in formulas for the force and energy. Using this formula for the driving force, a new theory was formulated for the behavior of hard magnetic materials with mobile interfaces (the interesting example: ferromagnetic shape memory materials in the martensitic phase) called Piecewise Rigid Magneto-Mechanics (PRMM). This theory is expected to allow us to simulate the dynamic behavior of small scale actuators. Of particular interest is the scale dependence of various quantities like natural frequency, gripping force. We have developed a fast numerical approach to PRMM.

3 Peer-reviewed Publications

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