Nanoscale Shape Memory Actuators and Swimming Bugs - Theory, Computing, and MBE Synthesis

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This interdisciplinary collaboration brings to bear multiscale methods to predict the behavior and guide the development of nanoscale shape memory devices. In particular, methods of Γ -convergence and newly developed schemes for passing from atomic to continuum scale are being used for this purpose. The proposed program of research fully integrates theoretical, computational, and experimental work.

The shape memory effect at macroscale is the following. A large, apparently permanent plastic deformation is imposed on a specimen at its transformation temperature. After heating to a moderate temperature the specimen returns to its original shape. In the alloys of interest here, the phenomenon is due to a diffusionless martensitic phase transformation, Figure 1.

We are designing and growing martensitic shape memory alloys since they exhibit the largest work output per unit volume of any actuator system (Krulevitch et al. 1996), and therefore are interesting candidates for small scale applications. At small scales, the slow process of heat transfer that hampers applications at macroscale is vastly improved. Shape memory actuators can be produced as free standing films, cantilevers, tents, tunnels, and other configurations, and therefore provide a wide array of methods to produce motion, unhampered by the friction that restrains many electrostatic actuators.

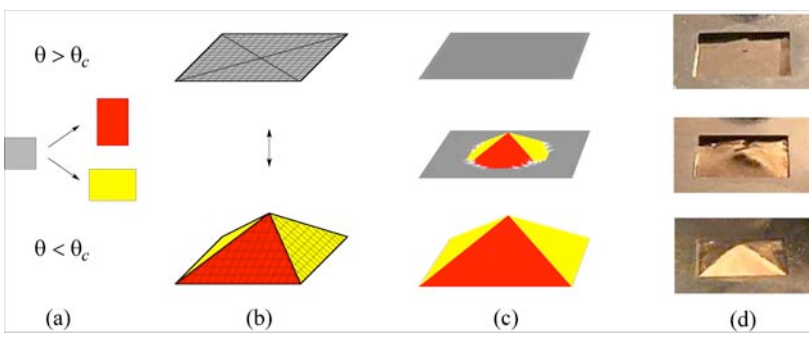

Figure 1. Nanoscale partially released thin film actuator design using a first-order structural phase transformation. (a) The gray phase is stable at high temperature and the symmetry-related yellow and red rectangular phases are stable at low temperature. (b) In the theoretical design of Bhattacharya and James, the film is flat and in the gray phase at high temperature. At low temperature, the upper and lower triangular regions of the film transform to the red rectangular phase, and the left and right triangular regions transform to the yellow rectangular phase. By satisfying precise conditions for a three-dimensional shape transformation and crystal orientation, the released film remains attached to the substrate as it transforms reversibly from flat to tent, and the tent structure will grow and shrink with temperature as the transformation proceeds in either direction. (c) Numerical simulation using the computation model of Belik and Luskin (d) Experiment at microscale of what we plan to do at nanoscale.

A new family of *ferromagnetic* shape memory (FSM) alloys such as Ni_2MnGa undergoes a martensitic transformation, exhibits the shape memory effect, but also is ferromagnetic. Because the different variants of martensite have approximately orthogonal easy axes, a shape change can be produced by applying appropriate magnetic fields to rearrange the variants. Studies that are emerging on FSM indicate that under magnetic actuation, these not only have the very high work output of shape memory materials, but they are also amenable to remote actuation. This has great potential for applications; for example, in biomedical applications of very small scale ferromagnetic shape memory actuators, the applied field could be produced by magnets external to the body.

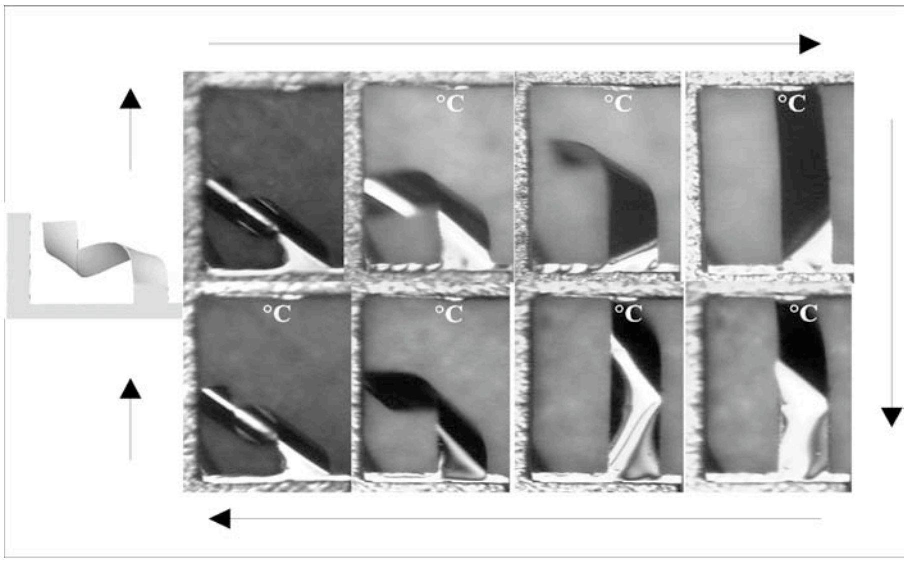

Figure 2. Optical micrograph of a free-standing epitaxially grown single crystal 90 nm thick, 400 μm long, and 100 μm wide Ni_2MnGa cantilever produced by front and backside photolithography and selective etching. The micrograph at the upper left shows the released film at room temperature in the martensitic phase, and it is coiled into a spiral shape. Upon heating above the martensite-austenite transformation temperature, the spiral unwinds and the optical micrograph on the upper right shows that the cantilever is almost straight. Upon cooling, the cantilever transforms back to the shape in the upper left micrograph. These shape changes are reversible with temperature.

Project Objectives:

- Develop multiscale analytic and computational methods for small scale motion utilizing single crystal films of shape memory alloys. Develop patterning strategies appropriate for these designs using e-beam lithography
- Build a flexible MBE growth system with flux controls, particularly designed for precise composition control. Grow single crystal films of NiTi and Ni_2MnGa. Investigate the shape memory effect and pseudoelasticity systematically at nanoscale. Formulate e-beam lithography techniques for patterning films and pattern according to predictions. Extend investigations to other SMA and FSM systems such as Fe_3Pd and Fe_3Pt.

Project Results:

Molecular beam epitaxy has been used by Palmstrøm's group to grow single crystal Ni_2MnGa ferromagnetic shape memory thin films on GaAs. The structural and magnetic properties of each sample have been characterized by reflection high energy electron diffraction, x-ray diffraction (for lattice parameter), Rutherford backscattering spectrometry (for compound determination), RBS channeling (to examine the quality of crystallization), transmission electron microscopy (for microstructure analysis), and vibrating scanning magnetometry (magnetic properties). In order to observe the shape memory effect and the austenite to martensite phase transition, free standing films have been prepared. A number of procedures for simplifying the processing to form free standing films have been investigated. One procedure involves lithographic patterning of the Ni_2MnGa film and selective bonding of the Ni_2MnGa film to another substrate, such as a glass slide, using a spin on glass, followed by complete removal of the GaAs substrate. One aim of the new processing procedures has been to investigate the detection of the phase transformation by measuring changes in the electrical resistivity of the films. This is hoped to result in a simpler determination of the phase transformation than optical detection when measurements are being performed in a cryostat where optical access is difficult.

Luskin and Belik have developed a computational model and code for the martensitic first-order structural phase transformation in a single crystal thin film. They have developed a free energy density to model a structural first-order phase transformations from a high-temperature cubic phase to a low-temperature tetragonal phase. The free energy density models the softening of the elastic modulus controlling the low-energy path from the cubic to the tetragonal lattice, the loss of stability of the tetragonal phase at high temperatures and the loss of stability of the cubic phase at low temperatures, the effect of compositional fluctuation on the transformation temperature, and the effect of spatial temporal noise.

James developed, within a mathematical context, the method of effective Hamiltonians. This is a multi-scale method that uses softness to derive a basis for atomic displacements that then can be used in statistical mechanics formulations to predict temperature dependent properties. James has also discovered some mathematical relations (originating from the analysis of microstructure) that correlate extremely well with low hysteresis; a patent based on these relations was applied for by the U of Minnesota. These can therefore be used as a basis for the search for new shape memory materials. He is trying to better understand the theoretical basis of these relations; there is a heueristic but the rigorous basis is unclear. It appears that a search for new materials based on these relations is feasible and this possibility is being explored.

Project Outreach:

A presentation was given in Spring, 2004 entitled “Mathematical Models for Crystal Microstructure” to high school students in the University of Minnesota Talented Youth Math Program provided an interdisciplinary experience in mathematics, science, and engineering. Talented high school students were also hosted at our lunch meetings to interact with undergraduate and graduate students working on this project. A “Perspectives” article was submitted to Science describing our objectives and recent work.

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