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13. ABSTRACT (Maximum 200 Words) THE RESEARCHERS DEVELOPED NEW COMPUTATIONAL METHODS AND THEORETICAL MODELS APPROPRIATE TO THE PASSAGE FROM ATOMIC TO CONTINUUM SCALES. THE METHODS WERE DEVELOPED IN THE CONTEXT OF SMALL SCALE FLIGHT. MAJOR ADVANCES WERE MADE ON DISCRETE SIMULATION MONTE CARLO METHODS, COMPUTATIONAL FLUID MECHANICS, COMPUTATIONAL MATERIALS SCIENCE AND DENSITY FUNCTIONAL THEORY. METHODS FOR THE GROWTH OF FERROMAGNETIC SHAPE MEMORY MATERIALS BY MOLECULAR BEAM EPITAXY WERE DEVELOPED, AND SEVERAL NEW CONCEPTS FOR ACTUATORS WERE DISCOVERED.				
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I. Introduction

Several main computational methodologies were developed under this program. The Effective Hamiltonian method produced continuum scale energy from DFT calculations; it produces accurate values of energy at scales that are many orders of magnitude larger than accessible by DFT alone. The second is a methodology for combining computational fluid mechanics with atomic methods based on the Boltzmann equation; it is successful for aerodynamics at scales where the Navier-Stokes equations of traditional fluid mechanics fail. A new concept for microactuation has been developed based on the use of released films of active material energized by a remotely applied field. Guided by theory, the first single crystal films of an active material (the ferromagnetic shape memory material Ni₂MnGa) were grown.

These methods will enable scientists and engineers to explore quickly new concepts for sensors and actuators and new designs of micro-aircraft that will be the basis of new military systems with a high degree of awareness.

A detailed report of activities can be found at the web site of this project, <http://www.multiscale.umn.edu/program.html>, including the presentations of the participants at all of the reviews. Below is a summary of those activities.

II. Summary of Activities

a) Particle methods for flows at very small scale

Boyd introduced the Information Preservation (IP) method in the early phase of this MURI project, as a way of overcoming major limitations of DSMC arising from statistical scatter at Reynold's numbers typical of microscale flows. In the IP method, macroscale information is carried along with the statistical information of particle interactions, and macroscopic conservation laws are used to update macroscopic quantities.

In the first DSMC-type simulations of a MEMS experiment he simulated flow in a micro channel using ordinary DSMC and DSMC/IP and compared with experiment. This is a challenging problem for particle based methods, because of the 1.2 x 1.2 x 3000 micron dimensions and low speed. Both DSMC and DSMC/IP gave good agreement with the experimental data for the (nonlinear) pressure drop vs. position along the channel, but DSMC had significantly more statistical scatter and similar accuracy of the two methods was only obtained with a factor 5 greater computational time of the older DSMC method. In flow over a flat plate at Reynold's numbers of 0.1 to 100, DSMC methods with 760,000 particles/cell gave entirely unacceptable statistical scatter in density and pressure fields, but the DSMC/IP method gave smooth fields and good agreement with experiment. In fact, the DSMC results also gave reasonable results of the drag coefficient vs. Re. Thus despite the statistical scatter that makes DSMC completely useless

for the prediction of local fields, some overall (averaged) quantities seem to be predicted well. But in any case DSMC/IP is much faster.

A hybrid DSMC/IP-NS code was developed. This comprises the seamless integration of Navier-Stokes computations with DSMC/IP calculations. Excellent matching of velocity profiles was achieved in a Couette flow with a DSMC/IP layer near the wall and Navier-Stokes in the central part. External flows are relevant to microscale aircraft, and good comparisons between full DSMC/IP and the hybrid code were also achieved in flow over a flat plate.

Some comparisons on more complex flows were made.

There is almost no experimental data for external, microscale gas flows. This data will be needed for future tests of codes like the hybrid code. A microscale wind tunnel facility was designed at the University of Michigan. Its design was based on the DSMC/IP and hybrid code predictions of Boyd.

b) Complex microscale aerodynamics

Candler developed new computational fluid dynamics approaches for the simulation of insect-like aircraft. This work involves the solution of the Navier-Stokes equations on three-dimensional Cartesian meshes, with the moving geometry described by a time-dependent masked region of the grid. A sub-cell masking approach is used where the grid mask crosses grid cells to produce accurate simulations for arbitrary masks. This allows the simple and efficient analysis of complex geometry flapping insect-like micro-air vehicles at low Reynolds numbers. This work builds on the previous approach of using Bezier hyperpatches to describe the moving geometry. This method is also promising, but is less efficient than the current masking approach.

Progress was made on the algorithm for the Navier-Stokes solver. A key bottleneck is the Poisson solver used to determine the pressure. A new parallelized conjugate gradient solver was developed that involves low memory and scales perfectly with number of processors. In addition, new multigrid-based solvers and improved preconditioning techniques are being investigated that should reduce the number of iterations required to obtain pressure solves.

A revealing study of microscale to milliscale flapping objects was done for the first time. Abrupt "wake transitions" were found at certain frequency and Re leading to a high degree of wake asymmetry. This in turn led to large increases in lift and thrust. A critical relation between Re and frequency was found where the transition takes place. Any design of microscale aircraft will need to be aware of such transitions and perhaps to take advantage of them. Intriguing extrapolations to higher frequencies were presented.

Three-dimensional simulations of flapping geometries show that the wing tip vortices intertwine to form a highly complex wake structure. For the low aspect ratio simulations,

the three-dimensional wake does not transition to the asymmetric mode seen in the two-dimensional simulations. These wake transitions were found to lead to greatly enhanced lift and thrust.

c) First principles calculations and atomic to continuum for transforming materials

Work at Rutgers by Rabe focused on first-principles investigation of the structural energetics of NiTi and the related compounds PdTi and PtTi. Taken together with the earlier studies of NiAl, and the ferromagnetic Heusler alloy Ni₂MnGa (which played a prominent role in the experimental part of this project; see below), these studies gave a complete picture of the diverse structural energetics and the mechanisms of transformation of these alloys. In addition, they laid the groundwork for the development of Effective Hamiltonians for these alloys, which in turn are able to deliver subtle predictions like transformation temperatures and latent heats of transformation.

A striking prediction was made. Through painstaking investigations, reproduced repeatedly with several different implementations of Density Functional Theory (DFT), Rabe and her students found that the accepted crystal structure of the low temperature martensitic phase in the important alloy NiTi is not the accepted B19' structure, but a rather different B19' structure with orthorhombic symmetry. Rabe and co-workers believed that these results are indeed reliable, and acceptance of this fact certainly would lead to a complete revision of the thinking about this alloy. They suggest a mechanism based on stress that has apparently stabilized the accepted structure.

Tijssens and James developed Karin Rabe's method of Effective Hamiltonians (EH). Their goals were to: 1) present the theory in a "geometrically exact" large strain format, 2) pass all the way to continuum level (As presently formulated, EH is designed to make finite temperature predictions, but not to do general inhomogeneous deformations), 3) automated implementation, and 4) to link EH with the kind of continuum theory used by Bhattacharya, James and Luskin. Progress was made on all fronts. In particular, some of the concepts were developed in a more precise way and led to explicit formulas for quantities used in the construction of the basis; this is expected to speed implementation.

d) Efficient simulation of "tents" and progress on the nucleation problem for microactuators

Luskin completed work in two areas related to the efficient simulation of microactuators: 1) the development and implementation of a new physically accurate and computationally efficient model of interfacial energy for martensitic materials, and 2) the implementation of a Monte Carlo method for dealing with nucleation.

A key problem was the accurate simulation of the effects of hysteresis in the microactuators. These effects have origins in the spatial fluctuations due to the presence of defects and the temporal fluctuations due to the vibrations of atoms that occur at finite temperature. Luskin developed a Monte Carlo method based on a distribution of the states of the austenitic and martensitic phases. Since the distribution of the states

used in the algorithm is general and can come from theoretical and/or experimental information, the method can be used to model nucleation due to either defects and/or thermal fluctuations. Another important aspect of this method was the formulation of an algorithm for the change of the phase of the crystal independently within each finite element triangle. A thin film version of the algorithm was developed and utilized to numerically simulate the phase transformation of an active thin film.

For predictions of nucleation in martensitic materials, it is crucial to have an accurate model of interfacial energy. Interfaces in these materials tend to be localized at atomic scale. Gradient models (having an additive contribution of the energy of the form $\text{const.}|\text{grad } F|^2$, where F is the deformation gradient) have difficulty reconciling the measured value of the interfacial energy with the very sharp measured profile of the interface in these materials. Briefly, if the interfacial energy is modeled correctly then the profile of the interface is often way too broad, especially in the "hard" but highly reversible materials with big transformation strains that dominate this project. As an alternative, Luskin developed a total variation surface energy as part of this project. The total variation is a natural mathematical object for measuring jumps of quantities across interfaces, and there is a natural "calculus" that goes with it. Luskin discovered that the total variation could be adapted to the modeling of interfacial energy and that numerical algorithms could be built around the natural calculus. He used the total variation surface energy with the nucleation method described above to simulate the indentation and collapse of the "tent" that was studied experimentally in the project. The simulation matched nicely the observed shape of the tent during collapse.

e) Atomic/continuum studies of crystalline solids undergoing phase transformation

A key obstacle for the description of motion in small scale actuators is the derivation of the laws that govern the propagation of phase boundaries. These laws are not in general given by the overall balance laws (or constitutive equations) of continuum mechanics and require new multiscale methods. The effort in Caltech led by Bhattacharya focused on understanding the kinetics of phase boundaries. One part of the effort concentrated on the motion of phase boundaries in slender objects like strings and rods made of phase transforming materials, and the use of such objects in generating propulsion at extremely small scales. The main effort concentrated on the direct derivation of kinetic relations from atomic simulation.

Simulations on atomic strings having pairwise interactions that lead to a phase transformation were conducted by Bhattacharya and his students. The free energies of such strings exhibit, after suitable application of statistical mechanics to account for small atomic vibrations, a double well character. Bhattacharya chose a pair potential to deliver this free energy in a realistic way and did direct MD simulations at atomic level. These simulations revealed a structure after averaging in time that has a lot in common with the predictions of continuum theory, that is, nonlinear elastic bar theory with the same free energy. These solutions were of Riemann-type: isolated propagating phase boundaries, preceded by acoustic waves, with a small amount of superimposed noise. Some of this noise appeared more organized than expected based on continuum theory, and this

deserves further study. From the simulations Bhattacharya calculated a driving force and plotted the speed of the boundary vs. the driving force for all simulations. All data collapsed to a single curve. This is a comforting confirmation of what is often done in continuum theory. More will be needed for a first principles' prediction of the kinetic relation in a real alloy, but these simpler simulations give confidence that these might be feasible.

As an alternative intermediate step, Bhattacharya proposed that these could be done in structures with reduced geometry like strings and beams. During the project he developed a framework for these kinds of kinetic laws, and discovered that kinetics influences only certain kinds of interfaces in these. For example, in a string with a kink – a sharp discontinuity of slope that coincides with a phase boundary– the speed of the kink is completely determined by the conventional balance laws. He designed experiments to test these predictions.

Bhattacharya also investigated the interaction of a moving phase boundary with a defect, with particular focus on the effect of the presence of the defect on the macroscopic kinetic relation. He also improved the methods used to model the free energies of transforming materials, making use of ideas from algebraic geometry.

At small scales, due to the competition between bulk energy and interfacial energy on phase and twin boundaries, James found that typical equilibrium configurations have only a few interfaces. Most of the designs for microactuators that we have found are of this type: a few interfaces that move around, subject to magneto-mechanical driving forces, giving rise to a large shape change. Magnetically and elastically hard materials like Ni_2MnGa are nearly rigid in regions between the interfaces. In addition, as a consequence of their magnetic hardness, the magnetization stays closely attached to the easy axes. According to his analysis, which was later confirmed by MFM studies, even the strong demagnetization effects which tend to make the magnetization lie in the plane of thin film only rotate the magnetization slightly, less than 1 degree in Ni_2MnGa films with out-of-plane easy axes. Based on these observations, James and R. Rizzoni gave a new dynamic model for the motion of microactuators, called Piecewise Rigid Body Mechanics (PRBM, and its generalizations Piecewise Rigid Thermodynamics, PRT, and Piecewise Rigid Magneto-Mechanics, PRMM). This gives a tractable approach to the fully 3-D motion of microactuators and was coupled to fluid flow simulations. The basic input for PRMM is only fundamental material constants – lattice parameters any symmetries of the phases, easy axes, saturation magnetization, mass density – together with the kinetic laws for the interfaces.

Simulations were done on the purely mechanical version of this theory, with kinetic relation of the type found by Bhattacharya. They revealed an important effect of frequency. Amplitudes of twin boundaries were sensitive to frequency, and, with apparently reasonable choice of material constants and kinetic relation, the amplitude was significantly degraded at frequencies of 1-2KHz. In short, with what appeared to be realistic kinetics, the twin boundaries could not “keep up” with the oscillating applied load at these frequencies. The effect of this freezing of interfaces was that the overall

amplitudes of vibration of the cantilever were greatly reduced. This important effect vehemently deserves further study, especially at small scales and with various geometries, to see if there is any way large amplitudes are attainable at very high frequency.

f) Growth of Ni₂MnGa and related films

Palmstrøm, together with his student J. Dong, made major improvements to the growth of Ni₂MnGa films on GaAs and excellent films can now be grown routinely. Free standing bridges and cantilevers were made using front and back side photolithography and preferential substrate removal, and these processing techniques were also refined. This gave sharper features than presented previously on the cantilevers and bridges. On released films of Ni₂MnGa the reversible martensitic transformation was observed many times in an optical microscope using polarized light induced by heating and cooling: the martensitic phase was found to be much stiffer than the austenitic phase. In addition, for the first time magnetic field induced motion of a cantilever was observed.

Palmstrøm and his students also grew a potential new ferromagnetic shape memory alloy Co₂NiGa, discovered by Wuttig and co-workers. This alloy is a Heusler alloy like Ni₂MnGa, and has some attractive features like low symmetry of the martensite. However, no ferromagnetic shape memory effect has been observed, and maybe this is due to its polycrystallinity. It is an interesting candidate to look at experimentally, with the full flexibility that MBE growth offers, and Palmstrøm began growth of films of Co₂NiGa. It was found that, depending on the growth temperature, either the austenite or the martensite phase could be stabilized. This had a dramatic effect on the magnetic anisotropy.

A great many devices were made on Ni₂MnGa films. Many shapes like "tents" and "hip roofs" were seen and these suddenly collapsed to the flat shape on cooling the film. However, they were not the structures expected based on the original predictions. This in hindsight is expected as Palmstrøm had actually and somewhat unexpectedly grew a new phase of Ni₂MnGa, not previously reported, not the expected austenite (We called this new phase appropriately P-phase). Palmstrøm and James rationalized the observed structures: they found that these structures are the low energy structures defined by special compatible interfaces between P-phase and a martensite, but this martensite is also not the usual thermal martensite in this alloy.

g) Two clusters MSCALE and NSCALE were built using matching funds for the project. The positive and negative aspects of building and using these for high performance computations were transmitted to DoD personnel.