

SYMPOSIUM W
Mechanically Active Materials

November 30 - December 1, 2004

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* Invited paper

8:30 AM *W1.1

Domain Switching and Large Electrostriction in Ferroelectric Perovskites. Kaushik Bhattacharya, Mechanical Engineering and Materials Science, California Institute of Technology, Pasadena, California.

Symmetry breaking at the Curie temperature results in multiple spontaneously electrically polarized and mechanically distorted states in a ferroelectric perovskite. These states coexist in characteristic domain patterns, and can switch from one state to another depending on the applied electrical and mechanical boundary conditions. Interestingly, domain switching can form the basis of interesting nonlinear properties. This talk will describe an effort that explicitly exploits domain switching in ferroelectric perovskites to create materials capable of large electrostriction against significant forces. This work is motivated by the technological need to develop high energy density microactuators. We will describe the theoretical background and the experimental validation in bulk materials. We will then describe how this approach can be adopted to thin films in geometries that can be obtained by standard micromachining tools, issues related to materials integration and the experimental validation.

9:00 AM W1.2

Oxygen Vacancies, Domain Switching and Their Implication for Fatigue in Ferroelectric Perovskites. Yu Xiao and Kaushik Bhattacharya; California Institute of Technology, Pasadena, California.

The role of oxygen vacancy in dielectric breakdown and fatigue has been a topic of intense research in ferroelectric perovskites like BaTiO₃. This paper presents a comprehensive model that treats the ferroelectrics as polarizable wide gap semiconductors where the oxygen vacancies act as dopants. First, a fully coupled and nonlinear model is developed with space charges, polarization, electric potential and elastic displacements as variables without making any priori assumptions on the space charge distribution and the polarization profile. Both analytical and numerical results show that polarization profiles and space charge distributions change dramatically when the film thickness and doping level are varied. Particularly, a donor-doped Pt/BaTiO₃/Pt structure is considered in this paper in view of the fact oxygen vacancies are acting as donors in ferroelectric perovskite. Second, a 2-D FEM simulation show the interactions of oxygen vacancies with 180 and 90 degree domain walls. Numerical results show that 90 degree domain wall may play a significant role in the fatigue process. Finally the forced diffusion of oxygen vacancies under local electric fields due to nonuniform polarization and space charge generation is considered. The switching process and fatigue are then studied by examining the stability of the system. The probability of fatigue as intrinsic property of the system under different circumstances (film thickness, doping level, defects level etc.) are investigated. Comparison with experimental results and implications for device design are discussed.

9:15 AM W1.3

Electro-Mechanical Characterization of Free-Standing Thin Films of Ferroelectrics and Other Active Materials.

Rongjing Zhang, Doron Shilo, Jean-Thibault de Besombes, Guruswami Ravichandran and Kaushik Bhattacharya; California Institute of Technology, Pasadena, California.

This report describes a test-bed for the electro-mechanical characterization of free-standing thin films of ferroelectrics and other active materials. In this test bed, the mechanical loading is applied either through an indenter (for strips and membranes) or through the application of pressure (for membranes). The electrical excitation is applied by a Sawyer-Tower circuit. A micro-interferometer is used to observe the real-time displacement field. Finally polarized light microscopy and X-ray diffraction method are used to observe the stress-induced domain switching. Thus, this test bed not only provides the macroscopic electro-mechanical properties but also provides a means to cross-link it with microscopic mechanisms like domain switching. This report will describe results from single crystal BaTiO₃ thin film with thickness ranging from 1 to 100 microns, biaxially textured polycrystalline thin films of (BaxPb1-x)TiO₃ with thickness of 1 micron and amorphous silicon nitrate.

9:30 AM W1.4

Search For Low-hysteresis Thermoelastic Shape Memory Alloys Using Combinatorial Synthesis and Synchrotron X-ray Microdiffraction. Jun Cui¹, Yong S. Chu³, Jae Hatrick-Simpers¹, Olugbenga O. Famodu¹, Richard D. James², Ichiro Takeuchi¹ and

Manfred Wuttig¹; ¹Materials Science & Engineering, University of Maryland, College Park, Maryland; ²Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, Minnesota; ³APS, Argonne National Lab, Argonne, Illinois.

Recent advances in the geometric nonlinear theory of martensites have explained the cause of large thermal/stress hystereses commonly exhibited by known shape memory alloys (SMAs) and prescribed a set of conditions that an ideal SMA must satisfy. An ideal SMA is defined as having a hysteresis width approaching zero. These conditions are a set of constraints on the lattice parameters that might be satisfied by fine-tuning the compositions of the materials. The combinatorial thin film synthesis technique can be used to prepare hundreds of samples with different compositions within a short period of time, and thus, it is the ideal method to search for the composition of the ideal SMA. Here, we report on preliminary results of our search using the combinatorial technique. The work involves synchrotron x-ray analysis on hundreds of free-standing thin film specimens prepared by combinatorial thin film synthesis on a single wafer. We have demonstrated that x-ray analysis can be used to precisely determine the lattice constants of predominantly textured SMA thin films. Systematic change in the lattice parameters are traced on ternary composition spread samples fabricated in a combinatorial co-sputtering system.

9:45 AM W1.5

Superelastic Thin Film TiNi-Polymer-Composites.

Eckhard Quandt¹, Holger Rumpf¹, Christiane Zamponi¹, Christoph Bouraue² and Dieter Drescher³; ¹Smart Materials, caesar, Bonn, Germany; ²Poliklinik fuer Kieferorthopaedie, Universitaet Bonn, Bonn, Germany; ³Poliklinik fuer Kieferorthopaedie, Universitaet Duesseldorf, Duesseldorf, Germany.

Superelastic shape memory materials are of special interest in medical applications due to the large obtainable strains, the constant stress level and their biocompatibility. Superelastic TiNi-polymer-composites have the potential to be used for novel applications in orthodontics and medical instrumentation as well as in certain areas of mechanical engineering. Especially, using TiNi thin films these composites have the potential to substantially reduce those forces compared to conventional TiNi wires and tubes. In orthodontic applications lowering the forces during arch wire treatment is of special importance due to tooth root resorption, which can be caused by the application of oversized forces during arch wire treatment [1]. Furthermore, the use of superelastic materials or composites enables the application of constant forces independent of diminutive tooth movements during the therapy due to the superelastic plateau. Superelastic TiNi thin films have been fabricated by magnetron sputtering using extremely pure cast melted targets [2]. Special heat treatment were performed for the adjustment of the superelastic properties and the transformation temperatures. A superelastic strain of up to 4.5% at 37 C was obtained. In this paper the fabrication of superelastic thin film TiNi-polymer-composites is presented and their characteristics are compared to wires and tubes in view of orthodontic applications. [1] D. Drescher et al., to be published [2] C. Zamponi, H. Rumpf, B. Wehner, J. Frenzel, E.Quandt, Mat. Sci. and Eng. Techn. 2004, 35 No5, 359-364

10:30 AM *W1.6

Integration of Textured Polycrystalline and Single Crystalline Ferroelectric Thin Films on Si. Harry Atwater, Applied Physics, California Institute of Technology, Pasadena, California.

Ferroelectric thin film integration with Si and other integrated device substrates has the potential to enable new modes of photonics integration as well as a new class of high work/volume piezoelectric devices for MEMS integration. To date, most ferroelectrics integration efforts have focused either on growth of polycrystalline films with poor control of microstructure or on perovskite epitaxial growth using the Si substrate or a bulk oxide substrate as a template. However, realistic integration schemes with electronic and photonic devices probably will not allow growth on a single crystal silicon substrate, but rather will require perovskite oxide integration on top of amorphous dielectrics separated from CMOS electronic devices. Thus we have focused on two approaches for integration of PbxBa1-xTiO₃ and LiNbO₃ on Si using biaxially-textured MgO templates and direct wafer bonding and layer transfer of single crystal films. Biaxially textured MgO is formed by ion-beam assisted deposition on amorphous silicon nitride, and films are obtained with a narrow dispersion in fiber texture (< 4°) and also a narrow dispersion of in-plane orientations (< 7°). The MgO films form a template for heteroepitaxy of perovskites. To date we have demonstrated epitaxial growth of PbxBa1-xTiO₃/MgO/SiN/Si by a sol-gel synthesis and BaTiO₃/MgO/SiN/Si by metallorganic chemical vapor deposition (MOCVD). An integration approach that yields truly single-crystal films is via wafer bonding and ion implantation-induced layer transfer. This technique enables fabrication of BaTiO₃ and LiNbO₃ single

crystal thin films with excellent control of crystallographic and domain microstructure relative to other thin film fabrication methods. Details of the microstructural characterization of BaTiO₃ and LiNbO₃ single crystal thin films will be discussed with an eye toward new integrated photonic and MEMS device applications.

11:00 AM W1.7

Applying NiTi Shape-Memory Thin Films to Thermo-mechanical Data Storage Technology. Wendy C. Crone¹ and

Gordon A. Shaw²; ¹Engineering Physics, Univ. of Wisconsin - Madison, Madison, Wisconsin; ²Manufacturing Metrology, National Institute of Standards and Technology, Gaithersburg, Maryland.

As the data storage density in cutting edge microelectronic devices continues to increase, the superparamagnetic effect poses a problem for magnetic data storage media. One strategy for overcoming this obstacle is the use of thermomechanical data storage technology. In this approach, data is written by a nanoscale mechanical probe as an indentation on a surface, read by a transducer built into the probe, and then erased by the application of heat. An example of such a device is the IBM millipede which uses a polymer thin film as the data storage medium. It is also possible, however, to use other kinds of media for thermomechanical data storage, and in the following work, we examine the possibility of using thin film Ni-Ti shape memory alloy (SMA). Previous work has shown that nanometer-scale indentations made in martensite phase Ni-Ti SMA thin films recover substantially upon heating. This study examines the effect of repeated thermomechanical cycling of indentations as well as the effect of indent proximity, both of which are critical for a device to carry out write, read, and erase operations repeatedly. The data are compared to Johnson's expanding spherical cavity model and a new Hertzian model for indentation, showing good agreement for the parameters tested. A preliminary data array with a storage density of 10 Gbit/in² is also demonstrated. While there are still problems to be solved, the experimental evidence and theoretical predictions show SMA thin films are an appropriate medium for thermomechanical data storage.

11:15 AM W1.8

Cast NiTi Shape Memory Alloys. Alicia M. Ortega¹, Carl P.

Frick¹, Jeffrey Tyber¹, Ken Gall¹ and Hans J. Maier²; ¹Mechanical Engineering, University of Colorado, Boulder, Colorado; ²Institute für Werkstoffkunde, University of Paderborn, Paderborn, Germany.

The purpose of this study is to investigate the structure and properties of polycrystalline NiTi in its cast form. Although it is commonly stated in the literature that cast NiTi has poor shape memory properties, we demonstrate that with appropriate nano/micro structural design, cast NiTi possesses excellent shape memory properties. Cast NiTi shape memory alloys may give rise to a new palette of low-cost, complex-geometry components. Three different compositions of cast NiTi were examined: 50.1 at.%Ni, 50.5 at.%Ni, and 50.9 at.%Ni. The structure of the cast material was examined at various scales and is discussed in the context of resulting thermo-mechanical properties. The cast NiTi showed a spatial variance in grain size due to the solidification process ranging from approximately a hundred microns to several millimeters. This spatial variance was also seen in the grain orientation, which showed a random distribution throughout the cast material, except for a <100> texture along the direction of primary solidification. Despite the spatial variance of grain size, minimal spatial variances in the thermo-mechanical response of the cast material resulted. The transformation temperatures were minimally affected by the radial location from which the material was extracted from the casting, showing slightly more diffuse transformation peaks from the material near the center of the ingot, possibly due to micro-compositional segregation. Mildly aged 50.5 at.%Ni and 50.9 at.%Ni materials were capable of full shape memory strain recovery after being strained to 5% under both tension and compression, while the 50.1 at.%Ni demonstrated residual plastic strains near 1%. The superior recovery in the more Ni rich materials was linked by TEM to a larger density of nanometer scale precipitates after aging. The symmetric response under tensile and compressive loading is a result of the measured random grain orientation distribution, which also resulted in an isotropic behavior of the cast material, showing minimal differences in the stress-strain response as a function of loading-axis orientation. Typically, wrought NiTi materials are highly textured in the <111> direction and show a considerably asymmetric stress-strain response in tension and compression, with recoverable strains of only 3% in compression. Preliminary tensile pseudoelastic low cyclic fatigue tests, conducted on the cast material with a 50.9 at.%Ni composition, demonstrated cyclic stability on par with wrought materials. The favorable recovery properties in the cast material are primarily attributed to the presence of the nanometer scale precipitates, which inhibit dislocation motion and favor the martensitic transformation.

11:30 AM W1.9

Thermal Processing of Polycrystalline NiTi Shape Memory

Alloys. Carl Pieter Frick¹, Ken Gall¹, Alicia Ortega¹, Jeffrey Tyber¹, Hans Maier² and Yinong Liu³; ¹Mechanical Engineering, University of Colorado, Boulder, Colorado; ²Materials Science, University of Paderborn, Paderborn, Germany; ³Mechanical Engineering, University of Western Australia, Crawley, Western Australia, Australia.

The objective of this study is to examine the effect of heat treatment on polycrystalline Ti-50.9 at.%Ni in hot-rolled and cold-drawn states. In particular we examine microstructure, transformation temperatures, as well as, mechanical behavior in terms of both uniaxial monotonic testing and instrumented Vickers micro-indentation. The results constitute a comprehensive understanding of the effect of heat treatment on thermal/stress induced martensite and resistance to plastic flow in NiTi, all of which are critical for optimizing the mechanical properties. The high temperature of the hot-rolling process caused recrystallization, recovery and hindered precipitate formation, essentially solutionizing the NiTi. The subsequent cold-drawing induced a high density of dislocations and martensite. Heat treatments were carried out on hot-rolled, as well as, hot-rolled then cold-drawn materials at various temperatures for a duration of 1.5 hours, inducing Ti₃Ni₄ precipitates. Based on transmission electron microscopy (TEM) observations, these precipitates progressively increased in size from coherent to incoherent, as a function of increased heat treatment temperature. Precipitate size and coherency were observed to systematically shift the transformation temperatures, bringing out the R-phase and multiple-stage transformations. Room temperature stress-strain tests illustrated a variety of mechanical responses for the various heat treatments from pseudoelastic to shape memory, which were related to the shift in the primary martensite transformation temperatures, rather than changes in the nature of the R-phase transformation. The results confirm that Ti₃Ni₄ precipitates can be used to elicit a desired isothermal stress-strain behavior in polycrystalline NiTi. In addition, instrumented micro-indentation tests were performed in an attempt to correlate Vickers force-displacement behavior during indentation with traditional stress-strain properties, although, such a link was difficult to establish. However, using Atomic Force Microscopy (AFM) to measure indentation depth before and after heating more distinctly confirmed shape memory or pseudoelastic behavior. The Martens (Universal) Hardness revealed that small coherent precipitates were more effective at blocking plastic flow than incoherent or even larger coherent precipitates. Although, preexisting dislocation density is shown to be more influential than precipitates at inhibiting plasticity and hence increasing hardness. Based on comparison of hardness and the stress required to induce martensite, it is shown that the resistance to dislocation motion and the ease of the martensite transformation cannot be simultaneously maximized, although an optimal combination should exist.

SESSION W2: Magnetomechanical Coupling

Chair: Krystyn Van Vleet

Tuesday Afternoon, November 30, 2004

Room 209 (Hynes)

1:30 PM *W2.1

Elasticity of Ferromagnetic Shape Memory Alloys. Liyang Dai, James Cullen and Manfred Wuttig; Materials Science and Engineering, University of Maryland, College Park, College Park, Maryland.

The dependence of a solid's elastic properties on temperature in the vicinity of a structural transformation provides insight into the nature of the transition. Therefore, the temperature dependences of the elastic constants of both martensitic and austenitic Ni_{0.50}Mn_{0.284}Ga_{0.216}, MS_≈318K, and Ni_{0.49}Mn_{0.2345}Ga_{0.2755}, MS_≈273K were studied in the temperature ranges 428K > T > 200K and 413K > T > room temperature, respectively. An ultrasonic continuous wave method was used and a suitably oriented 0.8 T magnetic field was applied to the sample to select the desired single domain state. Anomalous behaviors of the elastic constants were observed. All elastic constants of Ni_{0.50}Mn_{0.284}Ga_{0.216} at 218K indicate an intermartensitic transition from a tetragonal (c/a < 1) to a possibly another tetragonal (c/a > 1) phase as the temperature is lowered. The temperature dependence of the elastic constants in the austenitic Ni_{0.49}Mn_{0.2345}Ga_{0.2755} apparently show a pre-martensitic transformation around 333K, i.e. in between the Curie (380K) and martensite start (273K) temperatures. We also studied both the temperature and magnetic field dependences of elastic constants in Fe₃Pd. A possible magnetic field induced transition was observed. In this paper we will discuss the details of these measurements. In addition to the experimental study, we developed a Landau-type model to interpret the variation of the shear elastic constants C* and C' of Ni_{0.50}Mn_{0.284}Ga_{0.216}. This model reproduces said temperature dependences reasonable well.

2:00 PM W2.2

Magnetostriction of Stress-Induced Martensite. Jun Cui¹, Tom Shield² and Manfred Wuttig¹; ¹Materials Science & Engineering, University of Maryland, College Park, Maryland; ²Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, Minnesota.

The magnetostriction of stress induced Fe7Pd3 martensite has been investigated. The striction reaches a value 1980 ppm if this martensite is induced by a compressive stress of -12 MPa in the small temperature interval $M_s \leq T < M_s + 10^\circ\text{C}$. It is proposed that the effect is associated with the adaptive phase and that the interplay of stress and magnetic fields results in non-monotonous magnetostrictive behavior in the temperature range where it and the tetragonal phases can be stabilized.

2:15 PM W2.3

Temperature Dependence of Magneto-Mechanical Response in Ni-Mn-Ga Magnetic Shape Memory Alloys. Leon Cheng,

Garrett Landry, Shannon Farrell and Calvin Hyatt; Emerging Materials Section, Defence R&D Canada - Atlantic, Dartmouth, Nova Scotia, Canada.

Ferromagnetic shape memory alloys have received much attention since a large reversible, magnetic-field-induced strain was observed in Ni-Mn-Ga alloys in 1996. So far, up to 10% reversible magnetic field induced strains have been observed in Ni-Mn-Ga alloys with an orthorhombic seven-layered (7M) martensite. Unlike the conventional shape memory effect in which the reversible strain is related to the diffusionless structural phase transformation from a high-temperature high-symmetry phase to a low-temperature low-symmetry martensitic phase; it is generally accepted that the magnetic shape memory (MSM) effect is due to the rearrangement of twin variants in the martensite by an applied magnetic field leading to an overall change of shape. The main thermodynamic driving force for twin boundary motion in the presence of a magnetic field is the high magnetocrystalline anisotropy of the low-symmetry martensitic phase. High twin boundary mobility, low twin boundary energy and high magnetocrystalline anisotropy energy are the key factors for large magnetic field induced strain. In this work, a systematic investigation is being carried out on single crystals of varying composition near the stoichiometric Ni₂MnGa Heusler alloy to determine the effect of temperature on the magneto-mechanical behaviour of the Ni-Mn-Ga alloys. Repeated mechanical and magnetic forces have been applied to Ni-Mn-Ga samples at various temperatures below the martensite finish temperature. Twin boundary motions and evolution of martensite variant structure during mechanical and magnetic loading were observed by means of an optical microscope stage capable of applying longitudinal stress and transverse magnetic field simultaneously. In addition, influence of additional alloying elements (such as Fe) on the magneto-mechanical response of Ni-Mn-Ga alloys are also being investigated.

2:30 PM W2.4

Ferromagnetic Resonance Enhancement of Magnetomechanical Coupling in Magnetostrictive Materials. J. R. Petrie¹, N. C. Woo^{2,1}, J. A. Lieberman¹ and R. B. van Dover¹; ¹Materials Science and Engineering, Cornell University, Ithaca, New York; ²Chemistry and Chemical Biology, Cornell University, Ithaca, New York.

Magnetostriction is an induced strain in ferromagnetic materials caused by the reorientation of their spins due to an applied field. An AC magnetic field results in an oscillating magnetostrictive strain. We have studied the feasibility of enhancing the magnetoelastic coupling by applying an AC field at the ferromagnetic resonance (FMR) frequency. The magnons produced at this frequency should transfer their energy to phonons at the same frequency, thus increasing the amplitude of the strain oscillations. To explore this effect, we examined a YIG platelet with low magnetic anisotropy using a custom-built single-turn permeameter. The dissipative component of the UHF permeability (μ'') was found to exhibit distinct peaks when the FMR frequency corresponds to an integral number of acoustic wavelengths in the sample, consistent with acoustic resonance (AR). We are currently studying the coincident AR/FMR effect in a variety of metallic and rare-earth materials, such as Ni and (Tb,Dy)Fe thin films. This effect could be particularly useful for improving insertion loss in magnetically-transduced SAW (MTSAW) devices, which employ magnetostrictive transducers to generate surface acoustic waves on arbitrary substrate surfaces. These devices have been proposed for a number of applications, notably including 'electronic nose' sensor technology on silicon integrated circuits.

2:45 PM *W2.5

Ferromagnetic Shape Memory Alloys and Other Active Materials. R. C. O'Handley, S. M. Allen, D. I. Paul, S. R. Hall, M.

Marioni, M. Richard, J. Feuchtwanger, B. W. Peterson, J. Chambers, R. Techapiesancharoenkij and D. Bono; MIT, Cambridge, Massachusetts.

Ni-Mn-Ga magnetic shape memory alloys appeared on the scene of active materials in 1996 with a 0.2% field-induced strain and 6% field-induced strain at room temperature in 2000. Since then, the advantages and challenges of this material have been discovered. It remains a promising candidate for many high-strain, moderate stiffness applications, an area not well served by piezoelectric and magnetostrictive materials. Cyclic and pulse-field actuation show 6% field induced strain with bandwidths up to 2 kHz. More recently, promising results have been realized with Ni-Mn-Ga used in combination with either piezoelectric stack actuators or as fillers in polymer composites. The 4 kOe to 5 kOe field strength needed to fully actuate Ni-Mn-Ga crystals can be significantly reduced by application of a modest acoustic signal (50 V, 1 kHz). Ni-Mn-Ga particles aligned into chains in a polymer matrix show superior vibration energy absorption compared to visco-elastic materials or Terfenol-filled polymers. The data will be interpreted in terms of phenomenological and microscopic models of field-induced and stress induced twin-boundary motion.

3:30 PM *W2.6

Growth, Processing and Characterization of Free-Standing Single Crystal Ferromagnetic Shape Memory Alloy Thin Film Structures. C. J. Palmstrom¹, T. C. Shih¹, S. K. Srivastava¹, J. W. Dong^{1,2}, C. Adelman¹, S. McKernan¹, M. Luskin³ and R. D. James⁴; ¹Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota; ²SVT Associates, Inc., Eden Prairie, Minnesota; ³School of Mathematics, University of Minnesota, Minnesota; ⁴Department of Aerospace Engineering and Mechanics, University of Minnesota, Minnesota.

The development of microelectromechanical systems (MEMS) requires materials that undergo mechanical motion with the application of an external stimulus. In order for a material to demonstrate the shape memory effect it must undergo martensitic phase transformation with temperature. Furthermore, in the martensite during plastic deformation, twin boundary motion must be energetically favored over dislocation motion. In bulk, most full Heusler alloys in the L21 crystal structure are ferromagnetic and some show the shape memory effect. This combination of ferromagnetism and shape memory effect suggests that some Heusler alloys may display the ferromagnetic shape memory effect, which can result in very large magnetostriction. Ni₂MnGa is one such material, which in bulk single crystals can display 9.5% magnetostriction (1). Epitaxial Ni₂MnGa films have been grown on GaAs (001) by molecular beam epitaxy. By adjusting the composition of Ni₂MnGa, the martensitic phase transformation temperature has been varied from 200K to above room temperature. Frontside and backside photolithography and selective etching procedures have been used to produce freestanding single crystal Ni₂MnGa film structures. The shape memory effect has been demonstrated in such freestanding films. In this presentation, molecular beam epitaxial growth and characterization of Ni₂MnGa films on GaAs (001) and their magnetic, shape memory and ferromagnetic shape memory properties before and after releasing from the substrate will be emphasized. Supported by: NSF-NIRT DMS-0304326 and AFOSR-MURI AF/F49620-98-1-0433 I.A. Sozinov, et al., Appl. Phys. Lett., 80, 1746 (2002)

4:00 PM W2.7

Effect of Stress-Induced Magnetic Anisotropy on the Properties of Giant Magnetostrictive Single Layer and Multilayer Thin Films. Jin-Hui Tan¹, Wayne A. Anderson¹, Victor H. Guerrero² and Robert C. Wetherhold²; ¹Electrical Engineering, State University of New York at Buffalo, Amherst, New York; ²Mechanical Engineering, State University of New York at Buffalo, Amherst, New York.

Giant magnetostrictive thin films deposited on nonmagnetic substrates can constitute effective sensors and actuators for microdevices. In this work, we investigated the effects of a stress-induced anisotropy on the magnetic and magnetostrictive properties of Tb_{0.4}Fe_{0.6}, Fe_{0.5}Co_{0.5} single layer films and [Tb_{0.4}Fe_{0.6}/Fe_{0.5}Co_{0.5}]_n multilayers deposited on Si substrates. The magnetostrictive thin films were fabricated by means of RF sputtering and were subjected to a post-deposition annealing treatment. The uniaxial magnetic anisotropy was induced by bending the substrate before deposition and then allowing it to resume its original flat shape after depositing the film. Different levels of tensile and compressive stresses induced by this method were considered. The heat treatment was performed either in a furnace in which there was forming gas flowing through at a rate of 1 ml/min or in a vacuum system whose pressure is maintained at 10⁻⁶ Torr. The magnetic properties of the specimens fabricated were measured using a SQUID. SEM and XRD analyses were performed to ensure that the thermal treatment would relax the internal stresses induced during

the deposition process without crystallizing the film. The thickness of the single layer thin films studied was between 400 and 1000 nm. Typical multilayer samples consisted of 4-20 layers, whose thickness ranged from about 10 to 50 nm. Typical multilayer sample results exhibited saturation magnetization of about 0.24T with coercive field of 100 Gauss. Three main factors which influence the properties of the deposited films were identified: sputtering process parameters, amount of external stresses applied and post-deposition annealing. The sputtering and heat treatment parameters were optimized aiming at improving the low field magnetostriction and the magnetostrictive susceptibility of the films.

4:15 PM W2.8

Magnetic Properties of Submicron Ni-Mn-Ga Martensitic Thin Films. Manfred Kohl¹, Volodymyr A. Chernenko^{2,1}, Makoto Ohtsuka³, Heike Reuter⁴ and Toshiyuki Takagi⁵; ¹IMT, Forschungszentrum Karlsruhe, Karlsruhe, Germany; ²Institute of Magnetism, University of Kiev, Kiev, Ukraine; ³IMRAM, Tohoku University, Sendai, Japan; ⁴IMF III, Forschungszentrum Karlsruhe, Karlsruhe, Germany; ⁵IFS, Tohoku University, Sendai, Japan.

Ferromagnetic thermoelastic martensites formed as a result of a martensitic transformation in a ferromagnetic matrix represent a new type of materials. Due to the coupling of the structural and magnetic degrees of freedom they exhibit extreme magneto-mechanical properties which open up new technical applications as sensors and actuators. Concerning the development of novel sensors, the development of thin film technology of such materials is of paramount importance. In this work, r.f.-magnetron sputtering technique was used to deposit two series of thin films (A and B). Each series consists of five films with thicknesses ranging from 0.1 to 1 μ m and a reference of 5 μ m. The deposition was performed at 200 W on alumina ceramic substrates using targets of Ni_{49.5}Mn_{28.0}Ga_{22.5} for thin films A and Ni₅₂Mn₂₄Ga₂₄ for thin films B. All films were vacuum annealed at 1073 K for 36 ks. The temperature dependences of the electrical resistivity in all films are typical for the ferromagnetic Heusler alloys transforming martensitically. X-ray diffraction patterns reveal a 10M and 14M crystal structure for films A and B, respectively. The magnetic properties of the thin films have been characterized by the in-plane and out-of-plane field dependences of magnetization, M(H), at 300 K and the temperature dependences of saturation magnetization, M_s(T), upon heating in the temperature range 250-400 K at the field of 2 Tesla using a SQUID magnetometer. In thin films A, the ferromagnetic transition at the Curie temperature, T_C, occurs in the austenite state while in thin films B, T_C occurs in the martensitic state. We find that the magnetic properties of the thin films exhibit a considerable thickness variation in the submicron range, which is not present in the range of 1-5 μ m. For thin films of type A, T_C increases as a function of thickness by about 18 K, while it decreases non-monotonously by about 20K for thin films of type B. Up to the maximum field of 5 Tesla, no saturation is observed. Therefore, it can be assumed that the magnetic moments are inclined to the film plane at certain angles. This conclusion is supported by magnetic force microscopy measurements showing a pronounced magnetic contrast, which is stronger in the presence of a perpendicular magnetic field. The magnetic susceptibility at high fields shows a sharp nonlinear decrease with increasing thickness, similar to the susceptibility at low fields. The opposite dependence is observed for the critical magnetic fields, which indicate the starting points of perfect linear behavior of the M(H) curves at high fields, reflecting the change of magnetic anisotropy of the thin films. These magnetic results can be interpreted by assuming a more uniform distribution of the in-plane components of the magnetic moments and a less uniform distribution of their out-of-plane components showing larger inclination angles in the thinner films.

4:30 PM *W2.9

Tunable multiferroic properties and the magnetoelectric effect in CoFe₂O₄-PbTiO₃ nanocomposite thin film composition spreads. Chiro Takeuchi, ¹Materials Science and Engineering, University of Maryland, College Park, Maryland; ²Center for Superconductivity Research, University of Maryland, College Park, Maryland.

The magnetoelectric effect can be achieved in composite systems as a product property arising from the elastic coupling of piezomagnetic and piezoelectric components. In order to systematically explore the multiferroic properties and the magnetoelectric effect in thin film structures, we have fabricated nanocomposite structures using a composition spread technique. We have used the layout of the spread where two end compositions are pure PbTiO₃ (PTO) and CoFe₂O₄ (CFO) and there is gradual mixing of the two materials and the two ferroic properties in the middle of the spread. In order to create nanocomposite structures, we originally put down CFO and PTO at 600 °C in the "superlattice spread" geometry where the wedge thickness is multiples of the lattice constants of CFO and PTO. Microwave microscopy and room temperature scanning SQUID

microscopy are used to map the ferroelectric and ferromagnetic properties of the spreads, respectively. There is a region in the middle of the spread where the material is clearly multiferroic. From high resolution transmission electron microscopy, we have found that depending on the wedge thickness and the average composition, the deposited heterostructure results in a rich variety of nanocomposite configurations. They include the intended superlattice like layered-structure and structures where one of the components is formed as nanopancakes or nanopillars. X-ray microdiffraction is used to map the structural change of the components. We have found that the ferroelectric transition temperature of the PTO component can be continuously tuned all the way from 500 °C down to below the room temperature. We have observed the magnetoelectric effect using the microwave microscope at 1 GHz in a range of composition on the spread. 10 Oe ac magnetic field is used, and the change in the dielectric properties of the nanocomposite is detected. This work was performed in collaboration with M. Murakami, K.-S. Chang, C. Gao, C.-L. Lin, L. A. Bendersky, M. A. Aronova, S. E. Lofland, and M. Wuttig.

SESSION W3: Poster Session
Tuesday Evening, November 30, 2004
8:00 PM
Exhibition Hall D (Hynes)

W3.1

Raman Imaging of Grain Growth Mechanisms in Highly Textured Pb(Mg_{1/3}Nb_{2/3})O₃-PbTiO₃ Piezoelectric Ceramics. Philippe L. Colombari¹ and Mai Pham Thi²; ¹LADIR UMR7075 UPMC, CNRS, Thiais, France; ²Ceramics and Packaging Dept, Thales R and T France, Orsay, France.

The piezoelectric performance of relaxor single crystals provides excellent opportunities for improvements in medical ultrasonic imaging, sonar applications, active damping, and high strain actuation, if the costs can be reduced. PMN(PZN)-PT single crystals exhibit unique electromechanical properties when poled along the non-polar <100> direction. This is related to the fact that single crystal domains easily orient during poling so that the maximum response is obtained. A longitudinal coupling coefficient k₃₃ of 90% and an exceptional piezoelectric coefficient d₃₃ > 2000 pC/N can be obtained (1-2). The key to the improved properties observed in single crystals is the ease with which the crystal and poling directions can be aligned. While expensive crystal growth techniques are advancing, it is of great practical importance to develop an alternative low-cost production method based on strongly oriented or textured ceramics. We present the thermal expansion and Raman spectroscopy study of Pb(Mg_{1/3}Nb_{2/3})O₃-PbTiO₃ solid solution (PMN(1-x)-PTx) ceramics prepared by homo-epitaxial templated grain growth (HTGG) using cubic PMN-PT single crystal seeds as templates and nanoparticles as ceramic matrix. Relationships between Raman parameters such as band component or area versus x-composition are proposed. Wavenumber and peak area shifts from single crystal seeds centre to growth periphery are assigned to composition change. Representative medium to highly textured ceramics with Lotgering factors of 0.7 and 0.9 were sintered at 1150C and 1200C, respectively, and studied by direct and smart Raman imaging. Raman peak centre of gravity depends on solid solution x composition whereas peak intensity is correlated to the unit-cell distortion and related short-range structure. Two different growing mechanisms are evidenced: below 1200C sharp corner and straight edged single crystal seeds develop through liquid I phase at the crystal/matrix interface; at higher temperature, the matrix is consumed and crystal growth develops in contact with liquid II phase, through the help of the high PbO partial pressure. Smart Raman imaging shows that the final composition is very close to that of the matrix. Formation of short-range ordered B/b domains is expected. A phase diagram is proposed.

W3.2

Investigations on Single-Wall Carbon Nanotube Actuator Mechanism. Sanju Gupta, Mark Hughes and John Robertson; Physics, NCSU, Raleigh, North Carolina.

The isothermal conversion of chemical energy into mechanical work underlies the motility of all living systems - natural muscles. In this presentation, actuators built from a macro scale sheets of single-wall carbon nanotubes (bucky paper), which is among the growing list of several actuator materials since its pioneer demonstration, will be presented. They are therefore dubbed as artificial muscles lying under the category of electro-chemo-mechanical devices, whereby the transformation of chemical energy into mechanical energy is triggered by electrical signal or dc bias. They operate as a result of double-layer (i.e. electrochemical double layer; ECDL) charge injection in electrodes having very high gravimetric surface areas and gravimetric/specific capacitances and the output of the actuators may

be a mechanical displacement that can be used to accomplish mechanical work. Despite several benefits (low operating voltages, conducting nature, high temperature performance, and unusual electro-mechanical coupling), some open questions concerning the actuation principle/mechanism remain. They stretch if they are electrically charged and stretching is due to the elongation of C-C bond (i.e. tangential displacement mode) - if bonding states are depopulated or if anti-bonding states are populated. This study addresses these issues and aim to comprehend the various contributions by investigating the charge transfer dynamics on the surface of single-wall carbon nanotubes using in situ resonance Raman spectroscopy (RRS) and to determine the associated parameters include microscopic strain, fractional charge transfer and the corresponding shift in Fermi level through modeling [1]. The cyclic voltammetry and ac electrochemical impedance spectroscopy results will be discussed briefly which help to demonstrate well-developed capacitive behavior of single-wall carbon nanotubes sheet and to estimate the gravimetric/specific capacitances as well. [1] S. Gupta, M. Hughes, A. H. Windle, and J. Robertson, *J. Appl. Phys.* 95, 2038 (2004) and references therein.

W3.3

Crystallization and Phase Transformations in Amorphous NiTi Thin Films on Micromachined Membranes. Hai Ni, Hoo-Jeong Lee and Ainissa G. Ramirez; Mechanical Engineering, Yale University, New Haven, Connecticut.

Amorphous sputtered nickel-titanium thin films were deposited onto micromachined silicon-nitride membranes and subjected to heating and cooling conditions. Their associated microstructure was monitored directly and simultaneously with in situ transmission electron microscopy. These electron-transparent micromachined membranes constrained the NiTi films and rendered it possible for observation of the complete transformation cycle, which includes: the crystallization of the amorphous phase to austenite phase (cubic B2 structure) with heating; and the conversion of austenite (B2) to martensite (monoclinic B19' structure) with cooling. Electron micrographs show the nucleation and growth of grains occurs at temperature of 470°C and at a rate that indicates a polymorphic transformation. The onset of martensitic transformation occurs between 25 and 35°C. Calorimetric measurements are consistent with the observed crystallization. Actuation properties were also measured by wafer curvature methods.

W3.4

Enhanced Strain and Force in Electrochemical Deformation of Conducting Polymers, Polyaniline and Polypyrrole.

Keiichi Kaneto, Life Science and Systems Engineering, Kyusshu Institute of Technology, Kitakyushu, Japan.

Strain and force of conducting polymers generated by electrochemical oxidation and reduction have been improved greatly, since the beginning of the research started approximately 15 years. The largest strain has been obtained to be 26.5% in Polypyrrole film deposited electrochemically in methyl benzoate solution of tetra-n-butylammonium bis(trifluoromethanesulfonyl)imide. The strain is closing to that of natural muscles. The force has been found to be 6.7 MPa, being ten times larger than the typical natural muscle. The strain in polyaniline film has been found to exhibit more than 7% at pH > 2 in concentrated NaCl solution.

W3.5

Advanced Experimental Approach for Probing Superelasticity in NiTi-Based Shape Memory Thin Films and Foils.

R. Hassdorf¹, J. Feydt¹, S. Thienhaus¹, L. Buforn², N. Conte², O. Pykhteev¹, M. Kruzik^{1,3}, N. Botkin¹ and M. Moske¹; ¹Research center caesar, Bonn, Germany; ²CSM Instruments SA, Peseux, Switzerland; ³Academy of Sciences, Prague, Czech Republic.

With the advent of functional vapor-deposited thin films, the incorporation of shape memory and superelastic materials into coatings and lithographically processed microstructures has gained high prospects and technological importance. This holds specifically for their use in medical devices and thermal actuators. However, with shrinking size scale, characterization of the nonlinear superelastic behavior has become more and more demanding. In this respect, we present a study demonstrating the use of different advanced characterization techniques. One of them is nanoindentation with spherical tipped indenter tested on MBE-grown submicron NiTiCu alloy thin films. By applying Hertzian contact mechanics, the full range of mechanical response can be obtained from elastic, through the yield point, to permanent deformation. Moreover, using an analytical approach the indentation data can be converted into a stress-strain scenario aimed at simulating uniaxial tension load. Therefrom, for the above mentioned films, the width of the superelastic region is determined to be around 1-1.5% strain which complies with finite-element simulations used to fit the indentation

curves. In extension to nanoindentation experiments, microtensile tests and knife edge imprints combined with simultaneous X-ray diffraction analysis enable instant correlation of load deformation and microstructural changes. In favor of this advantage, commercially available NiTi foils have been probed. They reveal a superelastic plateau, here, in the order of 6.5%, at the end of which the parent austenite has completely disappeared. Notably, the microstructural change is fully reversible upon lowering the deformation as referred to X-ray reflex positions and intensity values. Further characterizations of free-standing MBE-grown NiTi films are in progress. The implementation of the characterization techniques discussed above enables a more systematic approach to superelasticity in thin films and foils. In this respect, our results provide a basis for comparing different microstructures in terms of functionality. Supported by BMBF under contract no. 03N4031A.

W3.6

Abstract Withdrawn

W3.7

Study of ferroelectric domain structure of (1-x)Pb(Mg_xNb_y)Ti_{3-xPb}TiO₃ single crystal and thin films. Youngbae Park, J. L.

Ruglovsky, M. J. Dicken and Harry A. Atwater; Thomas J. Watson Lab. of Applied Physics, California Institute of Technology, Pasadena, California.

Ferroelectric and piezoelectric properties of the relaxor ferroelectric single crystal Pb(Mg_xNb_y)TiO₃-PbTiO₃ (PMNT-PT) single crystals grown by Bridgman method have been characterized. The local ferroelectric domain properties of the relaxor PMNT-PT single crystals and thin film with different compositions are investigated using voltage modulated scanning force microscopy (SFM) which enables the out-of-plane (OPP) and in-plane (IPP) polarizations to be measured. Polarized optical microscopy, x-ray diffraction, Reflected high energy electron diffraction (RHEED), electron backscattering selected diffraction and Raman spectroscopy have been used to characterize the crystallographic structure, the microstructure and texture. Polarization-field measurements and laser interferometry were used to measure the macroscopic polarization hysteresis and d₃₃ value after poling. We have investigated the composition dependent ferroelectric and piezoelectric properties. Different compositions near the morphotropic phase boundary show rhombohedral and tetragonal structures with different Curie temperatures confirmed by in situ Raman spectroscopy and RHEED. Domain orientation at the surface of each ferroelectric domain is determined via a combination of the out-of-plane and in-plane polarizations and allows one to reconstruct the three dimensional domain orientation.

W3.8

Influence of Thermal Treatment and Composition on Structure and Magnetic Properties in Ni-Mn-Ga Shape Memory Ferromagnets. Uwe Gaitzsch¹, Stefan Roth¹, Norbert Mattern², Bernd F. Rellinghaus¹ and Ludwig Schultz¹;

¹Institute for Metallic Materials, IFW Dresden, Dresden, Germany; ²Institute of Solid State Analysis and Structural Research, IFW Dresden, Dresden, Germany.

Intermetallic compounds in a wide concentration range around the Ni₂MnGa composition are known to exhibit a large magnetic field induced strain (MFIS), the size of which is owed to a field driven movement of twin boundaries in the ferromagnetic tetragonal (martensitic) low temperature phase of these Heusler alloys. Samples of Ni(100-x-y)Mn(x)Ga(y) with (x,y) = (26,22) and (x,y) = (30,20) were prepared by arc melting the pure elements in Argon. The martensitic start temperatures, M_S, and Curie temperatures, T_C, of the samples were measured by means of differential scanning calorimetry (DSC) and Faraday magnetometry, respectively. Annealing at and below the B2 - L2₁ ordering temperature (T_O ≈ 750°C) followed by water quenching was found to affect the structure of the low temperature martensitic phase. XRD investigations revealed that the structure was tetragonal for the sample with (x,y) = (26,22) and orthorhombic with some monoclinic distortion of the unit cell for the sample with (x,y) = (30,20), thereby indicating the seven-layered type of martensite (7M). Compression tests at pressures of up to 50 MPa resulted in permanent deformations of the samples. Thermal annealing at temperatures of about 20 K above the martensitic transformation temperature, M_S, and below the thermodynamic L2₁ ordering temperature, T_O, allowed to fully recover the original shape of the sample, thereby providing evidence for the occurrence of the shape memory effect (SME) in these alloys. However, the application of external magnetic fields of up to 2 T did not result in any permanent shape change of the deformed sample. From measurements of the magnetic anisotropy field by means of singular point detection (SPD) technique the magnetic anisotropy constant was determined to be roughly 1.5·10⁵ J/m³ for samples which were annealed at 800°C for 6 hours and subsequently cooled to room temperature at a rate of 2 K/min. Magneto-mechanical tests with and without a magnetic field

applied perpendicular to the force direction revealed a significant influence of the field on the stress-strain-curves.

W3.9

Magnetostrictive Microcantilever - A Novel Platform for High Performance Biosensors. Suiqiong Li, Zhimin Li and Z.-Y. Cheng; Materials Engineering, Auburn University, Auburn, Alabama.

Biosensors for detecting and quantifying the presence of a small amount of biological threat agents in a real-time manner are urgently needed for a wide range of applications. In this paper, a novel type of micro-biosensor platform - magnetostrictive microcantilever (MMC) - is reported. Compared to the silicon and piezoelectric-based microcantilevers, the MMC has following advantages: 1) remote/wireless driving and sensing; 2) easy to fabricate. The resonance behavior and the sensitivity of MMC as sensor platform are characterized and compared to the theoretical calculation. It is found that the sensitivity of MMC is about 50% higher than that of piezoelectric-based microcantilevers. More importantly, it is found experimentally that the quality merit factor (Q value) of MMC can reach more 250, which is much higher than other cantilevers. Therefore, the development of MMC-based biosensors will significantly advance the capability to identify the biological threatening agents. The detection of yeast cells and Salmonella typhimurium cells using the biosensor made of MMC was carried out. The specifications of the biosensor is reported and compared to other biosensors.

W3.10

Abstract Withdrawn

W3.11

Classical Contractile Mechanism of Muscle Cell versus Contraction as a Phase Transition. Vaclav Bouda¹, Lea Boudova² and Denisa Haluzikova²; ¹Mechanics and Material Science, Czech Technical University, Prague, Czech Republic; ²Institute of Sports Medicine, Charles University, Prague, Czech Republic.

Despite numerous modification, biological skeletal muscle has maintained a uniform construction. Skeletal muscle are built of micron-sized contractile units called sarcomere, which contain two main filaments: thin, and thick. Swinging of the myosine heads drives the thin filaments toward the centre of the sarcomere in this classical mechanism, thereby shortening the sarcomere and the muscle. Myosin heads convert the higher energy of ATP (adenosin triphosphate) to lower energy of ADP (adenosin diphosphate) and Pi during their swinging. There are many reasons for considering this classical mechanism inadequate. We believe in the paradigm of the significant role of the phase transition of the system of the myosin heads. The sarcomere contraction is interpreted as a calcium induced mechanical rearrangement and swing of myosin heads, which result in a relative actin-myosin sliding. The proposed mechanism can be applied both for the actuators in mechanical systems and for the biomechanical implants.

W3.12

Measurement of Tumor Stiffness and Mobility Using Piezoelectric Fingers. Hakki Orhan Yegingil, Wan Young Shih and Wei-Heng Shih; Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennsylvania.

It is known that tumors or cancerous cells have higher stiffness than their surroundings. Measurement of tissue stiffness could aid early detection of tumor/cancer location. The goal of this study is to use piezoelectric fingers (PEFS) of various designs to measure tumor stiffness both under compression and under shear for potential early cancer detection. A PEFS is a piezoelectric cantilever consisting of a highly piezoelectric layer, e.g., lead zirconate titanate (PZT) bonded to nonpiezoelectric layer, e.g., stainless steel. Using a unique dual-electrode design, a PEFS can both apply a force and detect the resultant displacement with one single device. We show that a PEFS is capable of accurately measuring both the Young's modulus and shear modulus of tissues in both regular and indentation experiments. Furthermore, we show that a PEFS can measure the Young's modulus and shear modulus variations in model tumor tissues with less than one-millimeter spatial resolution to a depth of up to several centimeters. Results on experiments with PEFS on real breast tissues and prostates that have tumors inside will also be carried out. The ability of a PEFS to measure the stiffness of tumors both under compression and under shear offers great potential to aid tumor malignancy test accuracy.

W3.13

Detection Sensitivities of Piezoelectric PMN-PT/Cu Microcantilever Biosensors. Qing Zhu, Hongyu Luo, Wan Y. Shih and Wei-Heng Shih; Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennsylvania.

A piezoelectric microcantilever biosensor is consisted of a piezoelectric layer bonded to a nonpiezoelectric layer. Receptors of a target species, e.g., molecules, or cells, are immobilized at the cantilever tip. Detection of the target species is achieved by monitoring the cantilever resonance frequency shift due to the binding of the target species to the immobilized receptors at the cantilever tip. Compared to other sensors, a piezoelectric microcantilever has the advantages of real-time, in-situ detection using simple electrical means. Piezoelectric lead magnesium niobate-lead titanate solisolution (PMN-PT)/copper (Cu) microcantilevers were made from 20 micron thick freestanding PMN-PT films bonded to 5 micron thick Cu by electroplating. Previous humidity monitoring studies using a 500 micron long, 500 micron wide PMN-PT/Cu microcantilever suggested that the cantilever exhibited a better than picogram per Hz detection sensitivity. In this study, PMN-PT microcantilever of various sizes will be used to detect yeast and salmonella T and their mass detection sensitivities will be determined. Piezoelectric cantilevers consisted of a lead zirconate titanate (PZT) layer 125 μ m thick, 600 μ m long bonded to a glass layer 150 μ m thick with a 2 mm long glass tip of a know mass detection sensitivity, 10-10g/Hz will be used for comparison and calibration.

W3.14

Microfabrication of miniaturized highly piezoelectric microcantilevers for rapid, direct, and multiple biosensing. Zuyan Shen, Huidong Li, Wan Y. Shih and Wei-Heng Shih; Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennsylvania.

Miniaturized highly piezoelectric cantilevers offer the advantages of simple electrical detection and better capabilities to withstand damping in water. It is especially suitable for in-situ aqueous detection of bioagents or microbes. Binding of antigens to the antibody immobilized on the cantilever surface increases the cantilever mass and reduces its resonance frequency, which is detected by monitoring the resonance frequency shift. Our earlier work, both theoretical and experimental, indicated that piezoelectric microcantilevers less than 100 microns in length will provide femtogram/Hz mass detection sensitivity (the mass of a single virus). In this work, we focused on the development and incorporation of micron-thick highly piezoelectric lead zirconate titanate (PZT) thin films by a Sol-gel method and their subsequent patterning using SF6-based Reactive Ion Etching (RIE) or Cl-based Inductively Coupled Plasma (ICP) etching. Integrated with the microelectronic fabrication technology, freestanding PZT piezoelectric microcantilevers less than 100 microns long were made to realize such sensitivities. A nonpiezoelectric tip of an optimal length included at the free end of cantilever will further enhance the mass detection sensitivity. Results of the PZT microcantilever development and the theoretical calculations that helped optimize the sensing sensitivity will be presented.

W3.15

The Effects of Materials used during Synthesis on the Material and Actuation Properties on Polypyrrole. S. Naomi Davidson, Patrick A. Anquetil and Ian W. Hunter; Mechanical Engineering, MIT, Cambridge, Massachusetts.

Use of Polypyrrole based conducting polymer actuators is commonly limited by low strain rates during actuation (1%/s for strain amplitudes of 2% at 0.25 Hz was a typical average value for actuators tested). In this paper we show how synthesis conditions, namely the choice of the deposition electrode, affects this property. Polypyrrole films were synthesized on a range of electrode materials such as stainless steel, gold, nickel, and glassy carbon. The resulting actuators were then characterized for mechanical and electrical properties. We show that variation of the deposition electrode material can increase the strain rate performance by as much as 93%. Possible sources for these effects were investigated by measuring differences in surface roughness, porosity, conductivity. A comparison of the actuators is presented and design choices based on the selection of deposition materials are discussed.

W3.16

Micro-fluidics applications of telephone cord delamination blisters. Alex A. Volinsky and Patrick Waters; Mechanical Engineering, University of South Florida, Tampa, Florida.

Telephone cord buckling delamination blisters are commonly observed in compressed thin films. These mechanically active features form by a loss of adhesion between the film and the substrate due to residual stress relief, and exhibit directional growth under certain conditions. This paper considers telephone cord delamination channels for micro-fluidics applications.

W3.17

Fracture Behavior of the Dielectric Ceramics Containing a Conductive Crack. Xiaosheng Gao and Tianhong Wang; Mechanical

Internal electrodes are widely adopted in electronic and electromechanical devices made from dielectric ceramics. These internal electrodes may be regarded as pre-conductive cracks or notches. Our previous fracture tests on poled and depoled lead zirconate titanate (PZT) ceramics indicate that purely electric fields are able to propagate conductive cracks (notches) and fracture the samples. To understand the fracture behavior of conducting cracks in dielectric ceramics, a polarization saturation-free zone (SFZ) model was proposed to establish a failure criterion for the conductive cracks under electric and/or mechanical loads. The SFZ model treats the dielectric ceramics as mechanically brittle and electrically ductile materials and allows the local intensity factors of the electric field strength and electric displacement as well as the local stress and strain intensity factors to have finite nonzero values. Failure occurs when the local energy release rate exceeds the critical value. The predictions of the SFZ model are in good agreement with the experimental results. To further understand the fracture behavior of a conductive crack in the dielectric materials, microstructure simulations are also conducted in this study. The mechanism of the microstructural modeling is based on a domain-switching model, which is introduced to explain why the electric fracture toughness is higher than the mechanical fracture toughness. We use a discrete electric dipole to represent the local spontaneous polarization and the force couples to represent the local strains respectively, and consequently a domain structure is simulated with a grid of points where the polarization and strains vary with the applied loads. The entire material response is then captured by the behavior of the isotropic background medium and the superimposed point defects. In the two-dimensional computer simulation, the orientations of all the domains are within a plane. The crack tip singularity and the interactions between domains in the crack tip zone are also considered. The computer simulation reproduces the hysteresis curves and butterfly loops under uniform loading for a finite medium with a single edge conductive crack. With the critical local energy release rate adopted as the fracture criterion, the domain-switching simulation can explain the experimental results that the critical mechanical load for fracture decreases with the increase of the applied electric field and the critical electric field for fracture decreases with the increase of the applied mechanical load. The results of the domain-switching simulation also facilitate us to establish a failure criterion for conductive cracks in piezoelectric ceramics under combined mechanical and electrical loads.

W3.18

Pseudoelastic Transformation at a Notch Tip in Polycrystalline CuAlNi. Adam Creuziger², Thomas W. Shield³ and Wendy C. Crone¹; ¹Engineering Physics, Univ. of Wisconsin - Madison, Madison, Wisconsin; ²Engineering Mechanics Program, Univ. of Wisconsin - Madison, Madison, Wisconsin; ³Aerospace Engineering and Mechanics, Univ. of Minnesota, Minneapolis, Minnesota.

The copper aluminum nickel (CuAlNi) system has held promise as an alternate shape memory alloy (SMA) to nickel titanium (NiTi). Unfortunately this system is crippled by intergranular fracture at low cycles. Thus, after very few loading cycles, understanding the fracture processes in CuAlNi is of interest. We present data from experiments on notched polycrystalline samples loaded in bending. Electron backscatter diffraction was performed prior to testing to determine the orientation of the grains near the notch. During testing we observed the martensite formation using differential interference contrast microscopy. From the orientation data, stress field solutions were calculated for each sample. An available work criterion was used to analytically predict martensite microstructure formation, and this was correlated with experimental observations.

W3.19

Development of Magnetostrictive Fe-Ga and Fe-Pd Thin Films. Teiko Okazaki, Fac. Science and Technology, Hirosaki University, Hirosaki, Japan.

The giant magnetostrictive films exhibit promising applicability to devices for micro-machines, sensor systems due to high response velocity and huge stress created by the magnetostriction. The authors have showed that rapid-solidified melt-spun Fe-29.6at%Pd and Fe-17at%Ga foils have large magnetostriction of 1000 and 270 ppm, respectively. However, saturation magnetostriction is required applying of large magnetic field of 10 kOe. In this study, we developed the Fe-Ga/Al/Ni and Fe-Pd/Al/Ni thin films by magnetron sputtering system. Magnetostriction of these films measured by a bedding cantilever beam method reaches to 250-300 ppm at small magnetic field of 0.5 kOe and exhibits little hysteresis. Moreover, the magnetostrictive characteristics do not change under low alternating magnetic field. The magnetoelastic energy of these films is 25-30 Mpa, which compares with one of PZT. These metallic sensor/actuator materials are useful for application of magnetostrictive 2D-Scanner.

W3.20

Magnetic Field Control of a Ferrofluid Interface in Wetting Contact with a Vertical Wall. Shihab Elborai¹, S.-H. Lee¹, R. E. Rosensweig² and M. Zahn¹; ¹EECS, MIT, Cambridge, Massachusetts; ²Exxon Corporate Research (retired), Summit, New Jersey.

The height and shape of the meniscus formed by a non-magnetic fluid wetting a vertical wall is governed by fluid weight, interfacial surface tension and the contact angle for a particular fluid and wall material combination. The height and shape of a ferrofluid meniscus, however, can be changed by an applied magnetic field. The study of the effects of uniform and non-uniform magnetic fields on ferrofluid surface deformation is the first step in determining the contribution of magnetic surface forces to ferrofluid spin-up flows in rotating magnetic fields. Meniscus shape measurements were performed for different configurations of applied magnetic field. These measurements were compared to the predictions of a simple analytical model that extends Bernoulli's equation to account for magnetic effects. Preliminary results show that the effects of an applied uniform magnetic field are more complicated than the predictions of the simple analytical model because of the non-uniform demagnetizing fields at the interface of the ferrofluid. Measurements show that horizontal applied magnetic fields tend to lower the meniscus, whereas vertical fields tend to raise the meniscus, opposite to the predictions of the simple model. To account for non-uniform demagnetizing field effects, finite element analysis was used to iteratively solve for a self-consistent meniscus shape and magnetic field distribution. The numerical solution for a uniform horizontal applied magnetic field shows that the magnetic field on the fluid side of the top surface is weaker at the wall than in the bulk while in a uniform applied vertical magnetic field the reverse is true. Because ferrofluid is attracted to the stronger field regions, these numerical results indicate a tendency for the meniscus height to decrease in a horizontal applied field and increase in a vertical field, in directional agreement with the experiments.

W3.21

Stimulus-Responsive Polymer Brushes for the Control of the Interfacial and Nanomechanical Properties. Miao Ye, Dong Zhang and Christine Ortiz; Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Surfaces with chemically end-grafted stimulus-responsive polymers have great potential for a variety of applications, e.g. transport, separation, and detection of biomolecules, controlled adhesion, friction, and lubrication in microfluidic systems, and force or displacement generation in micro- and nanoscale devices. In this study, we have investigated one particular class of stimulus-responsive polymers; pH-sensitive comb-type graft copolymers with ionizable main chain segments. Mono-functional thiol-terminated poly(methacrylic acid-*g*-ethylene glycol) (SH-PMAA-*g*-EG) with varying molecular weights ($M_w=7,000\sim 17,000$ g/mol as measured by gel permeation chromatography), PEG graft densities (1.9~8.4% as measured by ¹H nuclear magnetic resonance), and a PEG molecular weight = 1,100 g/mol, have been synthesized via atomic transfer radical polymerization. Well-defined polymer brushes were then prepared on Au substrates via a "grafting to" chemisorption technique. Advancing contact angle (θ_a) measurements using deionized water as a function of chemisorption incubation time showed that an equilibrium density was achieved after 72 hours with a final $\theta_a=19.33\pm 3.77^\circ$. Chemically specific high resolution force spectroscopy (HRFS) with Au-coated probe tips that had been functionalized with 11-mercapto-1-undecanol, HS(CH₂)₁₁OH, or 11-mercapto undecanoic acid, HS(CH₂)₁₀COOH, were employed to measure the normal nanoscale interaction forces, F_z , as a function of probe-tip sample separation distance, D , in a series of aqueous buffer solutions of varied pH (pH=4-9) and a constant ionic strength of 0.005 M. As the pH was reduced, the polymer brushes were observed to undergo a dramatic conformational change from a negatively charged, hydrophilic, expanded state to neutral, hydrophobic, and collapsed state in the pH range of 5.0~6.0, due to the H-bonding and hydrophobic complexation interactions between MAA segments on the main chain and the PEG side chains as the MAA groups become protonated. Ongoing theoretical modeling using Poisson-Boltzmann based polyelectrolytic electrostatic double layer theory is yielding fundamental structure-nanomechanical property relationships of these stimulus-responsive polymer brushes, such as the conformation and surface charge density per unit area.

W3.22

Development of Field-responsive Polymeric Magnetic Composite Nanofibers via Electrospinning. Mao Wang, Harpreet Singh, T. Alan Hatton and Gregory C. Rutledge; Department of chemical engineering, Massachusetts institute of technology, Cambridge, Massachusetts.

Polymeric magnetic composite nanofibers were produced via an

electrospinning technique from colloidal-stable suspensions of magnetite nanoparticles (Fe_3O_4) in polymer solutions. Magnetite nanoparticles with an average diameter of 7.5 nm were synthesized by an aqueous co-precipitation technique in the presence of a polymer that attaches to the particle surfaces and confers steric stabilization to the nanoparticle dispersion in the polymer solutions. Uniform fibers of poly(ethylene oxide) with an average diameter of 400 nm, and of poly(vinyl alcohol) with an average diameter of 140 nm, each containing magnetite nanoparticles, were electrospun from the aqueous polymer/magnetite suspensions. The magnetite nanoparticles were found to align in columns parallel to the fiber axis direction within the fiber by the electrospinning process. Magnetite nanoparticles within the fibers were easily magnetized by an external magnetic field and the magnetic composite fibers exhibit superparamagnetic behavior at room temperature. A mathematical model was developed to predict changes in shape or stiffness of the composite nanofibers in an external magnetic field. In a nonuniform field, the nanofiber is predicted to deflect in the direction of magnetic gradient, with the magnitude of deflection proportional to the magnitude of the external magnetic field gradient. This prediction compares favorably with experimental results for the magnetic poly(vinyl alcohol) nanofibers deflected in a nonuniform magnetic field. In a uniform magnetic field, the bending stiffness of the fiber is predicted to increase due to the coupling between the magnetic nanoparticles and the external field. In addition to depending on the magnitude of the external magnetic field, the increased stiffness is predicted to depend strongly on the size of the magnetic particles, which determines the relaxation time of the particles, and thus the time scale of the application. As the size of the magnetite increases from 7.5 nm to 16 nm, the Neel relaxation time increases from 10^{-8} s to 1 s, suggesting that it would be possible to modulate the fiber stiffness according to rate of deformation. The relative magnitude of such changes in shape or stiffness within an external field is increased significantly as the diameter of the embedding polymer fiber is reduced, which would increase the sensitivity and reduce the response time of sensors or actuators made of electrospun magnetic fibers.

W3.23

On the Relationship between the Electric Double Layer and Actuation in Ionomeric Polymer Transducers.

Barbar Jawad Akle and Donald J. Leo; Mechanical Engineering (CIMSS), Virginia Tech, Blacksburg, Virginia.

Ionic polymer transducers are soft actuators that perform large bending deflections when voltages on the order of 1-5 V are applied across their thickness. Previous work showed that actuation performance of ionic polymer transducers is strongly correlated with the capacitance due to surface charge accumulation. Increasing the capacitance of the actuator increases the motion of the charges and increases the strain produced under the application of an electric field. Ionomeric transducers are made of an ionomer such as Nafion, sandwiched between two high surface area electrodes. An electric double layer is formed on the interface between the cathode and the adsorbed positive ions. Traditional models of the electric double layer such as Gouy-Chapman are used to compute the electric field and predict the charge motion across the transducer membrane. A novel plating technique which was previously developed is used to vary the morphology of the polymer-electrode interface to investigate the parameters of importance to the formation of the electric double layer. Electromechanical transducer tests are performed as a function of electrode morphology to correlate surface charge accumulation with force and deflection generated by the transducer.

W3.24

Electromechanical Properties of Biaxially-Oriented Cellular Films. Nathalie Chappleau, Emilie Lebon and Michel F. Champagne; Industrial Materials Institute, Boucherville, Quebec, Canada.

Cellular polyolefin films have been used for decades for products that are now in flat markets, such as ribbons and labels. In recent years, the interest for foamed films with high added-value properties has grown, especially in the fields of communications and electronics. This is particularly true for biaxially-oriented foamed films, which exhibit superior electromechanical thickness response and can be used as actuators or sensors. The electromechanical effect is enhanced by the presence of the voids, which make the film soft and elastic in the thickness direction. Also, the biaxial orientation processes allows to obtain very thin, flexible films. Biaxial orientation processes are commonly used to enhance the performance of polymeric materials. The development of molecular orientation during biaxial forming processes enables to produce materials that can be utilized in a wide variety of uses that need structural applications, enhanced barrier and optical properties, as well as superior thermal and electrical properties. The final performance can be remarkably improved by controlling the process parameters. It is therefore critical to understand how the processing variables affect the film crystallinity, orientation and morphology, and how this microstructure correlates

with the final film properties. In this work, a chemical blowing agent was used to produce foamed polyolefin sheets. A laboratory biaxial stretcher was used to perform biaxial orientation and study the influence of processing conditions on the final properties of the films. The structure development during stretching was investigated. The biaxially-oriented foamed films were characterized in terms of morphology (microstructure, orientation), mechanical performance (tensile, impact), thermal, dielectric and electromechanical properties, which were correlated to biaxial processing conditions.

W3.25

The Use of Micro-Cantilevers for Actuation and Sensing Applications in Aqueous Environments.

Nehal Ibrahim Abulail^{1,2}, Marian Kaholek^{1,2}, Yee Lam¹, Bruce LaMattina³, Robert Clark^{1,2} and Stefan Zauscher^{1,2}; ¹Mechanical Engineering and Materials Science, Duke University, Durham, North Carolina; ²Center for Biologically Inspired Materials and Material Systems, Duke University, Durham, North Carolina; ³Army Research Office, Research Triangle Park, Durham, North Carolina.

We show that mechanically active micro-cantilevers can be used in aqueous environments to detect conformational changes of polymer brushes or specific molecular recognition events between proteins. In the first respect, micro-cantilevers decorated with stimulus-responsive polymer (SRP) brushes can be reversibly deflected by induced conformational changes in the polymer brush. This conformational change induces a change in the surface stress on the cantilever, and ultimately causes cantilever bending. SRP brushes were synthesized on one side of the cantilever using surface-initiated atom transfer radical polymerization (ATRP). Cantilevers decorated with poly(N-isopropylacrylamide) (pNIPAAm) brushes responded to changes in temperature and solvent type, whereas cantilevers decorated with a copolymer composed of 70% pNIPAAm and 30% vinylimidazole (VI) responded sensitively to changes in solution pH. The use of SRPs for cantilever actuation is exciting because commonly available micro-fabricated cantilever springs offer a simple and non-intrusive way to sense changes in solvent type, temperature, and pH, promising great potential for sensing applications in micro-fluidic devices. Similarly, micro-cantilevers can be used to detect specific molecular recognition events between proteins efficiently. We show that micro-cantilevers decorated with monoclonal antibodies (mAb) A32 defect upon specific binding of mAb A32 to human immunodeficiency virus-1 (HIV-1) envelope glycoprotein gp120 (HIV-1 Env gp120). In this case, cantilever deflection results from the surface stress induced by molecular recognition mediated protein binding. The specific binding between the two proteins was confirmed through force spectroscopy measurements. Our results encourage the use of micro-cantilever deflection as a sensitive detection tool of molecular recognition events. Due to its rapid response, this biosensor can offer a simple, efficient, and sensitive technique for the diagnosis of HIV-1.

W3.26

Electroactive Polymer Based MEMS as Biosensor Platform. Zhimin Li, Suiqiong Li and Z.-Y. Cheng; Materials Engineering, Auburn University, Auburn, Alabama.

There is an urgent need for real-time biodetectors with high performance, such as high sensitivity, small size, easy deployment. Sensor platforms based on MEMS, such as microcantilevers (including piezoelectric and silicon-based cantilevers), have been studied. Using of micro-electromechanical diaphragm (MEMD) as micro-sensor platform is induced in this article. The principle and the simulation results are presented. It is found that the sensitivity of MEMD is about 100 times higher than that of microcantilever. The method used to characterize the device is discussed. The high sensitivity of MEMD is demonstrated by MEMD made of electroactive polymer - P(VDF-TrFE). Additionally, it is found experimentally that the quality merit factor (Q value) of MEMD is higher than that of microcantilever. More importantly, the damping effect of liquid media on MEMD is much smaller than that on cantilever, which makes MEMD a strong candidate for developing high performance biosensor used in liquid media.

W3.27

Shape Memory Polymers for Biomedical Applications.

Christopher M. Yakacki¹, Ken Gall¹, Alicia Ortega¹, Alan Greenberg¹, Robin Shandas^{1,3}, Kristi Anseth^{2,4} and Nick James Willett¹; ¹Mechanical Engineering, University of Colorado, Boulder, Colorado; ²Chemical and Biological Engineering, University of Colorado, Boulder, Colorado; ³Division of Cardiology, The Children's Hospital, Denver, Colorado; ⁴Howard Hughes Medical Institute, Boulder, Colorado.

We examine the shape memory effect in polymer networks intended for biomedical applications. The polymers were synthesized by photo-polymerization from a tert-butyl acrylate monomer with a diethyleneglycol-dimethacrylate crosslinker. We first examine the

fundamental link between the polymer structure (fraction and type of crosslinker) and the resulting shape memory recovery properties. Ideal shape recovery performance was obtained for a moderate crosslinking density and the optimized material was used for subsequent testing. The glass transition temperature, T_g , of the optimized polymer system was tailored to the necessary levels by changing the length of the crosslinking agent. We systematically investigated the thermomechanics of shape storage (predeformation) and shape recovery in the polymer using three-point bending. The polymers show a sigmoidal free strain recovery response as a function of increasing temperature at a constant heating rate. Free strain recovery was determined to depend on the temperature during predeformation; lower predeformation temperatures ($T < T_g$) decreased the temperature required for free strain recovery. Constrained stress recovery shows a complex evolution as a function of temperature, and also depends on the temperature during predeformation. Stress recovery after low temperature predeformation ($T < T_g$) shows a peak in the generated recovery stress, while stress recovery after high temperature predeformation ($T > T_g$) is sigmoidal. The isothermal free strain recovery rate was found to increase with increasing temperature or decreasing predeformation temperature. We also examine basic photo-polymerization issues in the polymer for the patterning of complex biomedical devices. Finally, the thermomechanical results are discussed in light of potential biomedical applications, and several prototype devices are presented.

W3.28

Force Generation and Electrical Voltage Induction in Miniaturized Piezoelectric Fingers for Cellular Elasticity Measurements.

Wei-Heng Shih, Hui Li and Wan Y. Shih; Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennsylvania.

Piezoelectric fingers (PEF) are piezoelectric cantilevers consisting of a highly piezoelectric layer, e.g., lead magnesium niobate lead titanate solid solutions (PMN-PT) bonded to nonpiezoelectric layer, e.g., copper with various tip designs. With a dual electrode design, a PEF can simultaneously generate force (from the driving electrode) and measure the corresponding displacement (from the sensing electrode), making it ideal for in-vivo palpation for early disease detection. PEFs have been shown to accurately measure both tissue stiffness under compression and tumor mobility under shear and stand to greatly improve tumor malignancy test accuracy. The goal of this study is to construct miniaturized PEFs made of 20 microns thick PMN-PT films developed in our lab for cellular elasticity measurements and examine the piezoelectric response of the PEFs both theoretically and experimentally for optimal performance. We include PEFs a bottom sensing PMN-PT layer. The effective spring constant, the axial displacement generated by the applied voltage, and the induced voltage in the sensing PMN-PT layer were examined in terms of the ratio of the length of the sensing PMN-PT layer to the length of the driving PMN-PT layer and the thickness of the non-piezoelectric layer. We showed that the spring constant to decrease with an increasing cantilever length and the induced voltage to increase with a decreasing thickness of the nonpiezoelectric layer, which was quantitatively confirmed with the experiments. Results of cellular elasticity measurements using miniaturized PEFs will be discussed.

W3.29

High Dielectric Constant Nano-Polymer Composites as Actuator Materials.

Cheng Huang¹, Qing Wang² and Q.M. Zhang¹; ¹Materials Research Institute and Electrical Engineering Department, The Pennsylvania State University, University Park, Pennsylvania; ²Materials Science and Engineering Department, The Pennsylvania State University, University Park, Pennsylvania.

For many electronic and electromechanical applications, flexible polymeric material with high dielectric constant is highly desirable. Although the dielectric constant of intrinsic dipolar response polymers is far below that of inorganic materials (< 100), recently, we demonstrated that by making use of nano-composite approach in which organic fillers with high dielectric response are incorporated into insulating polymer matrix, high dielectric nano-composites with their mechanical properties very similar to the polymer matrix can be developed. Furthermore, these high dielectric nano-all-organic composites exhibit high electromechanical response under low applied field. For example, in a fully functionalized dielectric-percolative polymer in which the high dielectric constant copper phthalocyanine and conductive polyaniline are grafted to a polyurethane backbone, a dielectric constant of 1,000 can be achieved. The fully functionalized polymer exhibits an electromechanical strain of 13% with an elastic density near $1\text{J}/\text{cm}^3$, which is induced under a field of $25\text{MV}/\text{m}$. Composites with conductive polymer nano-spheres as filler are also investigated and results will be presented.

W3.30

Improved Magnetostrictively Transduced SAW Devices.

N. C. Woo^{1,2}, J. R. Petrie², X. Ho² and R. B. van Dover²;

¹Chemistry and Chemical Biology, Cornell University, Ithaca, New York; ²Materials Science & Engineering, Cornell University, Ithaca, New York.

Surface acoustic wave (SAW) transducers can be made with magnetic materials using magnetostriction as a means of electromechanical coupling. Unlike conventional piezoelectrically transduced SAW devices, the magnetically transduced SAWs do not require an exotic single-crystal substrate or high temperature processing, and therefore may be easily integrated into Si-based integrated circuits. These devices have many potential applications, biosensors being one of the most promising. When the substrate between a transmitter and a detector transducer is functionalized with specific bio-receptors, a binding event will affect propagation of the SAW wave that can be detected with simple electronics. In previous MTSAW devices, the magnetomechanical coupling was found to be poor, resulting in insufficient signal amplitude. To obtain better performance, we are studying the use of alternative magnetostrictive materials including an amorphous CoFeTaZr alloy, CoNbZr, and compositions in the Terfenol family (TbFe₂, etc.). We are using combinatorial materials science (continuous composition spread approach) to identify optimum alloy compositions. The devices are also being redesigned to yield better performance.

W3.31

Abstract Withdrawn

W3.32

Abstract Withdrawn

SESSION W4: Mechanically Active Liquids and (Macro)Molecules

Chair: Patrick Mather

Wednesday Morning, December 1, 2004

Room 209 (Hynes)

8:30 AM *W4.1

Dynamic Tuning of Microfluidics by Electrowetting. Shu Yang, Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania.

The ability to dynamically tune surface properties would provide attractive opportunities in many applications, ranging from photonics to biotechnology. On the tens to hundreds of micrometer length scale, the behavior of liquids is strongly influenced by the surface tension. Recently we have demonstrated to dynamically tune the microfluid using electrowetting, which has the advantage of low power consumption and fast response. For example, a liquid micro lens has been studied to reversibly position itself in three dimensions by applying a small biased voltage. An electrowetting pump has been fabricated to move liquid in microchannels and guide the light propagation and transmission. We then apply the electrowetting on a nanostructured surface, which dramatically reduces the contact area of a liquid droplet, and thereby allow interactions between the liquid and the substrate to be varied by a factor of hundred to a thousand. Combined with MEMS, the ability to dynamic switch wetting behavior by electrowetting will find potential applications as high through-put, high sensitivity actuators and sensors.

9:00 AM W4.2

Magnetoviscosity and Torque Measurements on Ferrofluid Cylinders in Rotating Magnetic Fields.

Carlos Rinaldi¹, Arlex Chaves¹, Fernando Gutman¹, Xiaowei He² and Markus Zahn²; ¹Chemical Engineering, University of Puerto Rico, Mayaguez, Mayaguez, Puerto Rico; ²Department of Electrical Engineering and Computer Science and Laboratory for Electromagnetic and Electronic Systems, Massachusetts Institute of Technology, Cambridge, Massachusetts.

The effective viscosity of magnetic nanoparticle suspensions (ferrofluids) is studied using the rotating magnetic field generated by a two-pole three phase magnetic induction motor stator winding. Measurements of the torque required to rotate a spindle submerged in ferrofluid subjected to co-rotating and counter-rotating fields yields the first experimental observation of a "negative magnetoviscosity." Further measurements are presented for the torque required to restrain a spindle when it is (i) entirely filled with ferrofluid, (ii) entirely surrounded with ferrofluid, and (iii) both entirely filled and surrounded with ferrofluid. The results for the spindle either entirely filled or entirely surrounded with ferrofluid are compared to theoretical expressions obtained from the ferrohydrodynamic equations using a regular perturbation expansion in the small parameter $\Omega\tau$, where Ω is the applied field frequency and τ is the effective magnetic relaxation time of the suspension.

9:15 AM *W4.3

Field-Responsive Fluids: Rheology and Applications in Adaptive Energy Dissipation. Gareth H. McKinley, Suraj Deshmukh and Giorgia Bettin; Department of Mechanical Engineering, Institute for Soldier Nanotechnology & Hatsopoulos Microfluids Laboratory, MIT, Cambridge, Massachusetts.

Field-Responsive fluids such as magneto-rheological (MR), electrorheological (ER) and shear-thickening (ST) fluids offer numerous applications in controllable and adaptive energy dissipation. However there are also numerous difficulties associated with controlling the magnitude of the response, and in fluid deployment and longevity. Many of these issues can be overcome by the use of new nanoparticle syntheses, microfluidic assembly and novel macroscale deployment mechanisms. New magnetorheological fluids employing carbonyl iron particles from 200nm - 10 μ m and viscoplastic carrier fluids have been prepared and the dependence of the yield-stress on the magnetic field strength has been compared to commercially available MR fluids. The use of core-shell nanoparticles and chained-particles assembled in microchannels can further enhance the magnitude of the resulting MR response. Analysis of creep and large amplitude oscillatory shear flow behavior below and beyond the yield stress is particularly useful in providing information on the macroscopic rheological properties of such field-responsive fluids and can be correlated with structural information obtained using high speed digital videomicroscopy in microchannels. The behavior of shear-thickening colloidal fluids is also of particular interest for possible applications in ballistic impact, energy shunting and load dissipation, as well as in biomedical applications. In contrast to MR fluids, these materials do not require imposition of an external field but are activated beyond a critical deformation rate by formation of shear-induced structures. The availability of monodisperse silica particles from 50 nm - 1 μ m in diameter enables the magnitude and onset point of the shear thickening response to be customized and systematically varied. For each type of fluid, a controllable energy-absorbing material can be constructed consisting of an open-cell elastomeric foam impregnated with the field-responsive fluid. The mechanical properties of the resulting fluid-solid composites are investigated under various loading conditions. The viscoplastic flow of the particles inside the pores of the reticulated foam alters the mechanical properties of the composite. The energy absorbing capacity of the materials shows a dramatic increase (by up to 30 times that of the 'dry' foam) due to viscous dissipation in the pores and stiffening of the cellular foam edges. In the case of MR fluids this can be user-controlled by changing the magnetic field to vary the yield-stress of the MR fluid; for ST fluids, the material exhibits a strongly nonlinear response to the rate of loading. These new responsive composite materials thus have tremendous potential as adaptive energy absorbers.

9:45 AM *W4.4

Photoactuation in Liquid Crystal Elastomers. Miguel Camacho-Lopez¹, Heino Finkelmann², Jeremy Neal³, Peter Palfy-Muhoray³, Tibor Toth-Katona³ and Michael Shelley⁴; ¹School of Physics and Astronomy, University of St. Andrews, St. Andrews; ²Institute für Macromolekulare Chemie, Albert-Ludwigs Universität, Freiburg, Germany; ³Liquid Crystal Institute, Kent State University, Kent, Ohio; ⁴Courant Institute of Mathematical Sciences, New York University, New York, New York.

Liquid crystal elastomers are rubbers whose constituents are orientationally ordered. Due to the coupling between orientational order and strain, external stimuli which change the orientational order give rise to mechanical deformations. We present the results of experiments probing light induced stresses and shape changes in liquid crystal elastomers. In dye doped samples, the deformations can be very fast (70 ms) and very large (70° bend). We describe unusual optomechanical phenomena, such as swimming away from light by samples floating on water, and the behavior of light-driven artificial goldfish. We discuss the physics underlying light induced shape changes in nematic elastomers and momentum exchange between samples of these materials and their surroundings. We consider the issues of efficiency, impedance matching and the possible utilization of 'soft elasticity' for device applications.

10:30 AM *W4.5

Shear Responsive Hydrogels with Tunable Rigidity Constructed Via Peptide Folding and Consequent Self-Assembly or Block Copolyptide Folding and Self-Assembly. Darrin Pochan^{1,4}, Joel Schneider³ and Tim Deming²; ¹Materials Science and Engineering, University of Delaware, Newark, Delaware; ²Department of Materials, UCSB, Santa Barbara, California; ³Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware; ⁴Delaware Biotechnology Institute, University of Delaware, Newark, Delaware.

By using peptidic molecules in the materials self-assembly design process, one can take advantage of inherent biomolecular attributes, intramolecular folding events and secondary structure, in addition to more traditional self-assembling molecular attributes such as amphiphilicity, to define hierarchical material structure and consequent properties. Intramolecular folding events impart a molecular-level mechanism for environmental responsiveness at the material level (e.g. infinite change in viscosity of a solution to a gel with changes in pH, ionic strength, temperature). Importantly, since the networks are physically associated, they readily shear thin for ease of processing but immediately reassemble into rigid networks after the cessation of shear. The utility in responsive material design with two classes of peptidic molecules will be discussed. First, small, 20 amino acid beta-hairpin peptides will be discussed. The self-assembly construction process is predicated on the peptides first intramolecularly folding into the beta-hairpin conformation from a random coil conformation. Importantly, the scaffold assembly is completely reversible with pH or temperature by reversibly folding and unfolding the constituent peptides that, in turn, assembles or disassembles the scaffold, respectively. In addition, the rigidity of the gel scaffold can be tuned via the magnitude of the environmental stimuli, e.g. gels triggered with temperature form a more rigid network when assembled at higher temperatures due to faster folding and self-assembly kinetics. The molecular design and self-assembly principles, including a model to explain the inherent tunability of the final gel networks that underlie the observed morphological and rheological material, will be presented. Secondly, the self-assembly of block copolyptides with desired secondary structure will be presented. The ultimate rigidity of the resultant hydrogel networks is directly related to the secondary structure of the anchoring hydrophobic blocks. In addition, the connectivity of the network is directly dependent on the molecular weight of the block copolyptides.

11:00 AM W4.6

Prospects for ER Gels as Mechanically Active and Reactive Materials. Montgomery T. Shaw, Polymer Program and Dept. of Chemical Engineering, University of Connecticut, Storrs, Connecticut.

Electrorheological materials have been known for some time as substances that undergo large changes in stiffness on application of an electric field. In spite of their relatively high actuation speed and simplicity, they are used commercially in very few applications. Best known as fluids that turn into solids, they also can be formulated as soft solids that stiffen considerably, e.g., by a factor of 3 or more. Less known are ER materials that are configured to change shape, leading to bending, shrinking or shearing deformations. Not surprisingly, they can also act in reverse as transducers. This talk will describe how such materials can be made, their achieved performance, and the physical limitations on ultimate performance. Comparisons will be drawn with the analogous magnetorheological materials that are activated with a magnetic field.

11:15 AM W4.7

A Shape Memory Polymer with Improved Shape Recovery. Changdeng Liu and Patrick T. Mather; Polymer Graduate Program and Chemical Engineering Department, University of Connecticut, Storrs, Connecticut.

Thermally actuated shape memory polymers have aroused great interest, both academically and industrially, due to their ability to memorize a permanent shape that is set during processing and a temporary shape that is later programmed by manipulation above a critical temperature, usually T_g or T_m . However, the thermal triggering process is usually retarded compared to cousin materials, shape memory alloys, due to the comparatively low thermal conductivity for polymers that is usually less than 0.30 W/m²K. In this work, we incorporated an inorganic filler featuring high thermal conductivity into a shape memory polymer, crosslinked polycyclooctene, to increase its thermal conductivity and therefore shorten the heat transfer time. A simple mathematic model was developed that quantitatively correlated the material thermal conductivity and heat transfer time, τ , that translates in shape recover to an induction time. The model fit nicely with our experimental data that showed near doubling of thermal conductivity and an associated reduction in induction time. As an additional benefit, mechanical reinforcement was observed with the addition of this rigid thermal conducting filler.

11:30 AM W4.8

Mechanical Coupling in Endothelial Cell Development. M. Todd Thompson^{1,2}, Michael C. Berg¹, Michael F. Rubner¹ and Krystyn J. Van Vliet¹; ¹Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; ²Health Sciences and Technology, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Living biological cells are complex, mechanically active material systems that demonstrate coupling between chemical and mechanical fields. The extent to which chemical signals and mechanical stimuli independently direct cell behavior is not well understood, nor is the degree to which both operate in concert to induce cellular processes. Here, we present the mechanical characterization of polymeric electrolyte multilayers for which chemical composition is maintained constant and mechanical compliance is varied as a function of pH during multilayer formation. We then correlate the effects of this mechanical compliance with the capacity for vascular endothelial cells to attach, proliferate and express functional phenotypic molecules. Under controlled chemical environment, we find that there exist critical levels of substrate compliance and surface roughness beyond which vascular endothelial cells do not maintain typical phenotypic presentation. Quantification of mechanical determinants of cellular behavior in a chemically decoupled environment has direct applications for tissue engineering, as well as research on inflammation and wound healing.

SESSION W5: Modeling of Mechanically Active Materials

Chair: Wendy Crone

Wednesday Afternoon, December 1, 2004

Room 209 (Hynes)

1:30 PM *W5.1

Thermomechanical Constitutive Modeling of Shape Memory Alloys. Dimitris C. Lagoudas and Peter Popov; Aerospace Engineering, Texas A&M University, College Station, Texas.

A comprehensive thermomechanical constitutive model for Shape Memory Alloys (SMAs) is presented. The model is a result of a systematic effort to develop a three-dimensional constitutive model for SMAs with special features, dictated by new experimental observations. The model accounts in a unified manner for the different effects of the martensitic transformation observed during non-proportional loading, such as detwinning and reorientation of the martensitic variants, as well as tension/compression asymmetry. The simultaneous reverse transformation of self-accommodated and stress induced martensite into austenite is also addressed. Different hardening functions are used to better capture the material response in pseudoelastic and detwinning regimes. A numerical implementation of the model, using return-mapping algorithms, is also discussed. The model is tested on a wide range of thermomechanical paths in order to attain robust numerical implementation. Numerical simulations of different SMA actuated devices are finally presented.

2:00 PM W5.2

A Thermodynamically-Based Model for Martensitic Phase Transformations with an Application to Shape-Memory Alloys. Carl Jannetti¹, John L. Bassani¹ and Sergio Turteltaub²; ¹Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, Pennsylvania; ²Aerospace Engineering, Delft University of Technology, Delft, Netherlands.

As an important class of active materials, shape-memory alloys (SMAs) derive unique properties from martensitic phase transformations and are used in a wide variety of applications including sensors and actuators. These unique properties, such as pseudoelasticity, are a result of a solid-to-solid phase transformation, which occurs on the level of the crystal lattice. Although the underlying mechanism for the phase transformation is microscopic, a continuum-level description is the ideal choice to model SMAs for use in applications on the size scale of devices such as stents, sensors and actuators. Therefore a link between the microscopic phenomena and its influence on the macroscopic response is required. A continuum-level constitutive model for martensitic phase transformations in single crystals is developed in the framework of irreversible thermodynamics with internal variables. The finite-strain kinematical representation adopted is appropriate for a multi-phase composite microstructure comprising several phases of martensite as well as austenite. Central to the model is the notion that the rate of progression of microscale structural rearrangements depends on the stress state through the thermodynamic forces conjugate to the rearrangements. These thermodynamic forces, which are taken to be the driving forces for the phase transitions, are shown to have a significant contribution from changes in the effective elastic properties that occur during transformations. Finite-element simulations for single crystal NiTi capture the macroscopic effects of phase transformations and demonstrate important implications of the thermodynamic theory. In particular, we consider the tension-compression asymmetry associated with the pseudoelastic stress-strain response, and its dependence on the orientation of the loading axis relative to various crystallographic axes.

2:15 PM *W5.3

Kinematic and Topological Models of Martensitic Interfaces. R. C. Pond¹, X. Ma¹ and J. P. Hirth²; ¹Department of Engineering, The University of Liverpool, Liverpool, United Kingdom; ²113 E Ramsey Canyon Rd, Hereford, Arizona.

According to the classical theory of martensitic crystallography, the interface between parent and daughter is a geometrically invariant plane of the shape transformation. Moreover, the displacements occurring as a result of transformation are homogeneous, increasing linearly with distance from the interface. This proposition is at variance with experimental observations using transmission electron microscopy which show such interfaces to be terraced at the atomic level with short-range inhomogeneous displacement fields. A model of martensitic interfaces has been developed recently which is consistent with experimental observations, and also demonstrates explicitly that the mechanism of interface motion proposed in diffusionless. The habit planes predicted by this model deviate in a systematic manner from the classical ones. The object of the presentation is to explain the physical origin of the discrepancies between the two approaches, and consider the implications in martensitic transformations.

2:45 PM W5.4

Modelling of Fatigue in Ferroelectrics. Santiago A. Serebrinsky, Irene Arias and Michael Ortiz; Graduate Aeronautical Laboratories, California Institute of Technology, Pasadena, California.

Ferroelectrics are attractive electro-mechanically active materials due to their large strain actuation and applications in non-volatile memories. Nevertheless, the fatigue of their material properties at relatively low number of cycles N hinders a more widespread use of ferroelectrics. Two forms of fatigue, which may be related, are typically encountered: (i) polarization fatigue, whereby the remanent polarization decreases with N ; (ii) mechanical fatigue, i.e., the nucleation and propagation of cracks. Understanding and predicting ferroelectric fatigue becomes thus highly desirable. We present here a phenomenological model for ferroelectric fatigue crack nucleation and growth, based on cohesive theories of fracture. The central feature of the model is a hysteretic cohesive law which couples the mechanical and electrical fields. The model is also suitable for polarization damage due to the electromechanical coupling at the cohesive level. The cohesive law is used in conjunction with general constitutive relations of bulk behavior, including domain switching, in order to predict fatigue cracking and damage under arbitrary electro-mechanical loading conditions. A particularly appealing feature of the model is its ability to deal with both crack nucleation and propagation. We apply the model to both types of fatigue, irrespective of their possible relation. Under the assumption that for smooth samples the number of cycles N_i required to nucleate a fatigue crack is a sizable part of the total fatigue life, we compare our calculations with experimental results. Despite the scarcity and uncertainty of the experimental data, comparisons with PZT fatigue-life data are encouraging. In particular, the model is able to predict the loss of remanent polarization under repeated electro-mechanical cycles observed in experiment.

3:30 PM W5.5

First Principles-Based Modeling of Ferroelectric Polymers: Computational Design of a PvdF-Based Nano-Actuator. Alejandro Strachan¹, Haibin Su² and William A. Goddard, III²; ¹Los Alamos National Laboratory, Los Alamos, New Mexico; ²Materials and Process Simulation Center, Caltech, Pasadena, California.

We use first principles methods to study the static and dynamical mechanical properties of the ferroelectric polymer Poly(vinylidene fluoride) (PVDF) and its copolymer with trifluoro ethylene (TrFE). We use density functional theory [within the generalized gradient approximation (DFT-GGA)] to calculate structures and energetics for various crystalline phases for PVDF and P(VDF-TrFE). We find that the lowest energy phase for PVDF is a non-polar crystal with a combination of trans (T) and gauche (G) bonds; in the case of the copolymer the role of the extra (bulkier) F atoms is to stabilize T bonds. Using the MSXX first principles-based force field (FF) with molecular dynamics (MD) we calculate that the energy necessary to nucleate a G bond in an all-T crystal is much lower (14.9 kcal/mol) in P(VDF-TrFE) copolymer than in PVDF (24.8 kcal/mol). This correlates with the observation that the polar phase of the copolymer exhibits a solid-solid transition to a non-polar phase under heating while PVDF directly melts. We also find that the interface between a polar and non-polar phases has a smaller threshold stress and a higher mobility in the copolymer as compared with PVDF. We then use molecular modeling to design and test a PVDF nanoactuator. Our simulations predict that large electrostrictive strains (5%) at extremely high frequencies (over 109 Hz) can be obtained in a PVDF nano-actuator if the inter-chain packing density is appropriately chosen. We control the packing density by assembling the polymer chains on a Si <111> surface with 1/2 coverage. Under these

conditions the equilibrium conformation of the polymer contains a combination of Gauche and Trans bonds which can be easily transformed to an all-Trans conformation by applying an electric field. Such molecular transformation is accompanied by a large deformation along the polymer chain direction. We find that the strain-polarization curves show a typical electrostrictive behavior with strain proportional to polarization squared. This work exemplifies the increasingly important role that modeling will play in the design of new materials with improved properties.

3:45 PM W5.6

Quantum-mechanical design of molecular actuators based on π -stacking. Damian Scherlis^{1,4}, Timothy Swager^{2,4}, Ian Hunter^{3,4} and Nicola Marzari^{1,4}; ¹Materials Science and Engineering, MIT, Cambridge, Massachusetts; ²Chemistry, MIT, Cambridge, Massachusetts; ³Mechanical Engineering, MIT, Cambridge, Massachusetts; ⁴Institute for Soldier Nanotechnologies, Cambridge, Massachusetts.

The π -stacking between aromatic compounds has been intensely studied by experimental and theoretical groups for over three decades. Nevertheless, exploiting this phenomenon as the driving force in molecular actuators is a novel concept. In the present work we explore how thiophene oligomers can be linked to calixarene crowns to design molecular actuators with the ability for expansion and contraction as a function of the electrochemical potential. In such systems, oligothiophenes constitute the electroactive component, while calixarenes perform the role of hinges between oligomer segments. We use first-principles quantum mechanics at the density-functional theory level to screen a variety of calixarene molecules in different conformations and to optimize the overall design. Moreover, correlated quantum-chemistry approaches are applied to describe the stacking interactions between the thiophene oligomers and to show how these can be switched on and off by the electrochemical potential to achieve molecular actuation. The effects of solvation and of oligomer length are explored, and the proposed architectures tested with first-principles molecular dynamics simulations.

4:00 PM W5.7

Modeling and Analysis of Conducting Polymer-Based, Trimorph Bending Actuators in Air. Bryan D. Schmid¹, Peter Madden¹, John Madden² and Ian Hunter¹; ¹Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; ²Electrical and Computer Engineering, University of British Columbia, Vancouver, British Columbia, Canada.

Ionic electroactive polymers, particularly polypyrrole (PPy), were analytically modeled and experimentally characterized in a non-aqueous, bending actuation configuration. The PPy trimorph design is composed of two mechanoactive polypyrrole electrodes sandwiching an ion-permeable layer impregnated with a BF_4 gel electrolyte. The developed analytical models introduce a moment equilibrium analysis of the PPy trimorph and its geometrical constraints as the PPy films undergo a linear strain previously described by J. Madden. The analytical models predict both the trimorph's force and curvature as a function of the applied charge density. Non-aqueous experimental characterization of fabricated trimorph films using a dynamic mechanical analyzer verifies the analytical model within the error bounds of the trimorph's physical properties. Such PPy trimorphs were typically composed 25 μm thick PPy films embedded in the trimorph and produced forces up to 0.2N and curvatures of 133 m^{-1} .

4:15 PM W5.8

Thermomechanics of the Shape Memory Effect in Polymers. Yiping Liu, Ken Gall, Martin L. Dunn and Alan R. Greenberg; Department of Mechanical Engineering, University of Colorado, Boulder, Colorado.

Shape memory polymers (SMPs) have the capacity to store and recover relatively large strains when subjected to a unique thermomechanical cycle. Owing to their ability to provide reliable low-cost actuation, shape memory polymers have potential biomedical, aerospace, and microsystem applications. Although shape memory properties exist in various polymer systems, and novel applications are emerging, little work has been done to understand or predict thermomechanical couplings in SMPs. In this study, the thermomechanics of shape storage and recovery are systematically investigated in a SMP deformed under tension and compression. During heated recovery, three cases of constraint are examined: unconstrained strain recovery, stress recovery at full strain constraint, and stress recovery at reduced strain constraint. The unconstrained strain recovery implies the absence of the external stress and the free recovery of the induced strain. The stress recovery at full strain constraint implies the fixing of the pre-deformation strain and the gradual recovery of the pre-deformation stress. The reduced strain constraint level equals the pre-deformation strain minus the strain

caused by glassy state unloading. Based on the experimental results, a one-dimensional constitutive model is developed using a micromechanics approach. The model is motivated by the shape memory mechanism of the polymer network and thermodynamics (changes in entropy and internal energy). The foundation of the model is that the entropy change is gradually stored during cooling and released during reheating as free recovery strain or constrained recovery stress. When fit to free strain recovery data, the model can predict the trends of the stress evolution during shape fixation and constrained stress recovery with/without low temperature unloading.

4:30 PM *W5.9

A Unified Framework for Modeling Hysteresis in Ferroic Materials. Stefan Seelecke¹ and Ralph C. Smith²; ¹Dept of Mechanical & Aerospace Engineering, North Carolina State University, Raleigh, North Carolina; ²Dept of Mathematics, Ctr for Research in Scientific Computation, North Carolina State University, Raleigh, North Carolina.

This paper addresses the development of a unified framework for quantifying hysteresis and constitutive nonlinearities inherent to ferroelectric, ferromagnetic and ferroelastic compounds. Because the mechanisms which produce hysteresis vary substantially at the microscopic level, it is more natural to initiate model development at the mesoscopic, or lattice, level where the materials share common energy properties along with analogous domain structures. In the first step of the model development, Helmholtz and Gibbs energy relations are combined with Boltzmann theory to construct mesoscopic models which quantify the local average polarization, magnetization and strains in ferroelectric, ferromagnetic and ferroelastic materials. In the second step of the development, stochastic homogenization techniques are invoked to construct unified macroscopic models for non-homogeneous, polycrystalline compounds exhibiting nonuniform effective fields. The combination of energy analysis and homogenization techniques produces low-order models in which a number of parameters can be correlated with physical attributes of measured data. Furthermore, the development of a unified modeling framework applicable to a broad range of ferroic compounds facilitates material characterization, transducer development, and model-based control design. Attributes of the models are illustrated through comparison with piezoceramic, magnetostrictive and shape memory alloy data and prediction of material behavior.