SYMPOSIUM W
Mechanically Active Materials

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* Invited paper
9:30 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 electromechanically polarized and mechanically distorted states in a ferroelectric perovskite. These states coexist in characteristic domain patterns that 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 micro actuators. We will describe the theoretical background and the experimental validation in bulk materials. We will then describe how this approach can be adapted to thin films in geometries that can be obtained by standard micromachining tools, issues related to materials integration and the experimental validation.

9:45 AM W1.5 Superelastic Thin Film TiNi-Polymer-Composites. Eckhard Quandt1, Holger Rumpf2, Christiane Zamponi3, Christoph Bourouci2 and Dieter Drescher2, 1Smart Materials, caesar, Bonn, Germany; 2Poliklinik fuer Kieferorthopaedie, Universitaet Bonn, Bonn, Germany; 3Poliklinik fuer Kieferorthopaedie, Universitaet Dusseldorf, Dusseldorf, 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 treatment 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 [2] to be published [1] E. Quandt, H. Rumpf, B. Wehner, J. Frenzel, E. Quandt, Mat. Sci. and Eng. Tech., 2004, 35 No.5, 355-364

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/poivelectric devices for MEMS integration. To date, most ferroelectric 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, real and 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 BaTiO3 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 are obtained by low dispersion in fiber texture (≤ 4%) and also a narrow dispersion of in-plane orientations (≤ 5°). The MgO films form a template for heteroprestixs of perovskites. To date we have demonstrated epitaxial growth of PbSiAs1-xTe03/MgO/Si/Si by a sol-gel synthesis and BaTiO3/MgO/Si/Si by metalorganic chemical vapor deposition (MOCVD). An integration approach that yields truly single-crystal films is via wafer bonding and ion implantation-induced layer transfer. This technical 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 thermal chemical annealing 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 Thermomechanical 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 technology. 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 NiTi shape memory alloy (SMA). Previous work has shown that nanometer-scale indentations made in martensitic phase Ni-Ti SMA thin films recover spontaneously, thus showing 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 random microstructure 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 NiTi 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 Tyber², Ken Gall³ and Hans J. Maser³; 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 strength of the cast material was examined at various scales and is discussed in the context of resulting thermomechanical properties. The cast NiTi showed a spatial variance in grain size due to the solidification process ranging from approximately micro to millimeters. The 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 in grain size, minimal spatial variances in the thermomechanical properties 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% austenite and compressed to 5% martensite. 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 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 martensitic phase Ni-Ti SMA thin films recover spontaneously, thus showing 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 random microstructure 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 NiTi thin films are an appropriate medium for thermomechanical data storage.

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 Ni₅₀M₉₀₂₃G₆₇5₄ at room temperature were studied in the range of 300 to 350 K by room temperature x-ray diffraction (XRD). The temperature dependences of the elastic constants were determined by using a Varian FTIR spectrometer from 15 K to 300 K. The elastic constants of Ni₅₀M₉₀₂₃G₆₇5₄ exhibit a strong temperature dependence with a minimum at around 150 K. The temperature dependence of the elastic constants was analyzed using a modified version of the Landau-Devonshire theory which takes into account the effect of temperature on the shear modulus, and the results were compared to experimental data. The agreement between theory and experiment is good, indicating that the modified version of the Landau-Devonshire theory is appropriate for describing the temperature dependence of the elastic constants of Ni₅₀M₉₀₂₃G₆₇5₄.
The magnetostrictive stress induced Fe7P3 martensite has been investigated. The strain reaches a value 1980 ppm if this martensite is induced by a compressive stress of -12 MPa in the small temperature interval Ms<CT<Ms 10°C. It is proposed that the effect is associated with the tetragonal phase and that the interplay of stress and magnetic fields results in non-monotonic magnetostrictive behavior in the temperature range where it and the tetragonal phases can be stabilized.


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 or tetragonal lattice. Unlike the martensite shape memory effect in which the reversible strain is related to the diffusional 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 magneto-crystalline anisotropy of the low-symmetry martensitic phase. High twin boundary mobility, low twin boundary energy and high magneto-crystalline 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.


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 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 260K to above room temperature. Frontside and backside photolithography and selective etching procedures have been used to produce freestanding single crystal Ni2MnGa film structures. This 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 annealing from the substrate will be emphasized. Supported by NSF-NIRT DMS-0304326 and AFOSR-MURI AF/F49620-98-1-0433.

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 thin films of Tb0.4Fe0.6, Tb0.4Co0.6 and Tb0.4Fe0.6Co0.4 single layers 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 uniform magnetostrictive behavior of these films is due to random orientation of anisotropy axes produced by disorienting the substrate before deposition and then allowing it to assume its own flat shape after depositing the film. Different levels of tensile and compressive stresses induced by this method were considered. The heat treatment (combination of thermal and magnetostrictive (TM) treatments) was performed in situ 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 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 with thicknesses ranging from 0.1 to 1 m and a reference of 5 m. The deposition was performed at 200 W on alumina ceramic substrates using targets of Ni40.5Mn28.6Ga22.5 for thin films A and Ni52Mn24Ga24 for thin films B. All films were vacuum annealed at 1073 K for 24 hours. The temperature dependence 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 1 Tesla using a SQUID magnetometer. In the films A, the ferromagnetic transition at the Curie temperature, TC, occurs in the austenite state while in thin films B, TC 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 m. For thin films of type A, TC increases as a function of thickness by about 18K, while it decreases non-monotonically 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, with the highest ferromagnetic component is stronger in a perpendicular magnetic field. The magnetic susceptibility at high fields shows a sharp nonlinear decrease with increasing thickness, similar to the saturation magnetization. The opposite dependence is observed for the critical magnetic fields, which indicates 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 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 W2.8 Tunable multiferroic properties and the magnetoelectric effect in CoFe2O4-PbTiO3 nanocomposite thin film composition of Ni-Mn-Ga Martensitic Thin Films. Manfred Kohl1, Volodymyr A. Chenreno2,3, Makoto Ohtsuka3, Heike Reuter4 and Toshiyuki Takagi2, 1IMT, Forschungszentrum Karlsruhe, Karlsruhe, Germany; 2Institute of Magnetism, University of Kiev, Kiev, Ukraine; 3IMRAM, Tohoku University, Sendai, Japan; 4IFM, Forschungszentrum Karlsruhe, Karlsruhe, Germany. 

The tunable multiferroic properties of the nanocomposite thin films were created by means of a dual-layer structure with alternating layers of magnetic and ferroelectric properties. The deposition process without crystallizing the film. The thickness of the single layer thin films studied was between 400 and 1000 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 with thicknesses ranging from 0.1 to 1 m and a reference of 5 m. The deposition was performed at 200 W on alumina ceramic substrates using targets of Ni40.5Mn28.6Ga22.5 for thin films A and Ni52Mn24Ga24 for thin films B. All films were vacuum annealed at 1073 K for 24 hours. The temperature dependence 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 1 Tesla using a SQUID magnetometer. In the films A, the ferromagnetic transition at the Curie temperature, TC, occurs in the austenite state while in thin films B, TC 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 m. For thin films of type A, TC increases as a function of thickness by about 18K, while it decreases non-monotonically 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, with the highest ferromagnetic component is stronger in a perpendicular magnetic field. The magnetic susceptibility at high fields shows a sharp nonlinear decrease with increasing thickness, similar to the saturation magnetization. The opposite dependence is observed for the critical magnetic fields, which indicates 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 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.

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be a mechanical displacement that can be used to accomplish mechanical work. Despite several benefits (low operating voltages, conductive heating, and high power density), these materials also have unique properties such as superelasticity, shape memory effect (SME), 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-B bond (i.e., thermal displacement mode) - if bonding states are depleted or if anti-bonding states are populated. This study addresses these issues and aims to comprehensively investigate the contributions by studying the charge transfer dynamics on the surface of interacting nanotubes using in situ techniques. Laser resonance Raman spectroscopy (RRS) and to determine the associated parameters 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 Transitions in Amorphous NiTi Thin Films on Micromachined Membranes, Hai Ni, Hoo-Keong Lee and Aminas 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.


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 ago. The largest strain has been observed on polypyrrole film deposited electrochemically in methyl benzoate solution of tetra-n-butylammonium bis(trifluoromethanesulfonyl)imide. The strain is close to that of natural muscle. The force has been found to be 6.7 MPa, being smaller than that of natural muscle. The strain in polyaniline film has been found to exhibit more than 7% at pH 2.5 in concentrated NaCl solution.

W3.5 Advanced Experimental Approach for Probing Superelasticity in NiTi-Based Shape Memory Thin Films and Foils, P. Hasselbrink, J. Feydt, S. Thienhaus, L. Bufohn, N. Conte, O. Pykhov, K. Kruskik, N. Botkin and M. Moske; Research center caesar, Bonn, Germany; CSM Instruments SA, Peseux, Switzerland; Academy 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 advanced characterization techniques. One of them is nanoindentation with spherical tipped indenters 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 extension load. Therefore, for the above mentioned films, the width of the superelastic regime 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, microsensing 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 shape has completely been recovered. Notably, the structural 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 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_{2/3}Nb_{1/3})O_3-xPbTiO_3 single crystal and thin films, Youngho Park, J. L. Ruglovska, M. J. Dillon 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_{2/3}Nb_{1/3})O_3-PbTiO_3 (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. Polysilicon optical microscopy, X-ray diffraction, reflection 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 Gaitzsch, Stefan Roth, Norbert Mattern, Bernd F. Ringelmann and Ludwig Schultz; Institute for Metallic Materials, IW Dresden, Dresden, Germany; Institute of Solid State Analysis and Structural Research, IFW Dresden, Dresden, Germany.

Intermetallic compounds in a wide concentration range around the Ni-Mn-Ga composition are known to exhibit large magneto-induced strain (MFIS), the size of which is owed to a field driven movement of twin boundaries in the ferromagnetic tetragonal (martensite) low temperature phase of these Heusler alloys. Samples of Ni(100-x-y)Mn(x)Ga(y) with (x,y) = (26,20) and (x,y) = (20,20) were prepared by arc melting the pure elements in Argon. The martensitic start temperatures, Ms, and Curie temperatures, Tc, of the samples were measured by means of differential scanning calorimetry (DSC) and Parady magnetometry, respectively. Annealing at and below the B2-L21 ordering temperature (Tc ≈ 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) = (26,20) 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 (TM). 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, Ms, and below the thermodynamic L21 ordering temperature, Tc, 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. Thermal annealing at 6% in a magnetic anisotropy field by means of singular point detection (SPD) technique the magnetic anisotropy constant was determined to be roughly 1.5·10^6 J/m^3 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.


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. Compare to the silicon and piezoelectric-based microcantilevers, the MMC has following advantages: 1) remote/wireless driving and sensing; 2) easier 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. Vrachov Bouda, Lea Boudova and Denisa Haluzikova; 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 (adenosine triphosphate) to lower energy of ADP (adenosine 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 sarcosome 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 high 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 device. We show that a PEFS is capable of accurately measuring both the Youngs modulus and shear modulus of tissues in both regular and indentation experiments. Furthermore, we show that a PEFS can measure the Youngs 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 under both compression and under shear offer great potential to aid tumor malignancy test accuracy.


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 remote/wireless biosensors, 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)/Cu) microcantilevers were made from 20 micron thick freestanding PMN-PT films bonded by 600 micron thick Cu by electron beam deposition. 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/Cu microcantilever of different 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 nm thick, 600 nm thick bonded to a glass layer 150 μm 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, Huaidong 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 decreases 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 material, 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.

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 polished and deposed 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 energy release rates. 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
Pseudelastic Transformation at a Notch Tip in Polycrystalline CuAlNi. Adam Creuziger1, Thomas W. Shields1 and Wendy C. Cron2...

The copper-aluminum nickel (CuAlNi) system has held promise as an alternative 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 cylindrical samples under tension. 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

The giant magnetostrictive films exhibit promising applicability to devices for micro-machines, sensor systems due to high response of large magnetostrictive fields. The authors have shown that rapid-solidified melt spun Fe-29.6at%Pd and Fe-17at%Ga foils have large magnetostriction of 1000 and 270 ppm, respectively. For the application of non-magnetic materials for magnetic coating, we have developed thin films of Fe-Ga and Fe-Pd magnetic films. Monofunctional thiol-terminated poly(methacrylic acid-g-ethylene glycol) (SH-PMAA-g-PEG) with varying molecular weights (MW=7,000-17,000 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 at 1,100 g/mol, via thiol-ene click radical polymerization. Well-defined polymer brushes were then prepared on Au substrates via a "grafting to" chemosynthesis technique. Advancing contact angle (θa) measurements showed that the surface was hydrophilic with a θa of 19.3±3.8°. Chemically specific high resolution force spectroscopy (HRSF) with a combination of AFM and magnetic force microscopy, functionalized with 11-mercapto-1-undecanol, HS(CH\textsubscript{2})\textsubscript{11}OH, or 11-mercapto undecanoic acid, HS(CH\textsubscript{2})\textsubscript{11}COOH, were employed to measure the normal nanoscale interaction forces, F, 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 0.008 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 deprotonated in an acid medium. Thus, these stimuli-responsive polymer brushes may find applications as new tunable, pH-sensitive materials for biological or medical applications.
electrospinning technique from colloidally-stable suspensions of magnetite nanoparticles ($Fe_3O_4$) in polymer solutions. Magnetite nanoparticles are highly magnetic and can be used to produce nanofibers with specific properties. 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. The size of the magnetite increases from 200 nm to 600 nm, which increases the relaxation time from $10^{-1}$ to $1$, suggesting that it would be possible to modulate the fiber stiffness according to rate of deformation. The relative magnitude of such changes can be used to control the shape of the final product. The increased stiffness will also increase the sensitivity of the sensors or actuators made of electrosprayed magnetic fibers.

W3.23 On the Relationship between the Electric Double Layer and Actuation in Ionomeric Polymer Transducers.
Barbara Jawad Ateh and Donald J. Leo; Mechanical Engineering (CMSS), 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 by the application of an electric field. Ionomeric transducers are made of an ionomer such as Nafton, sandwiched between two high surface area electrodes. An electric double layer is formed on the interface between the cathode and the adsorbed Nafton polymer. 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 ionomer-electrode layers, which allows 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 transducers.

W3.24 Electromechanical Properties of Biaxially-Oriented Cellular Films.
Nathalie Chapleau, Emilie Lebon and Michel F. Champagne; Industrial Materials Institute, Boucherville, Quebec, Canada.

Cellular polyolefin films have been used for decades for products that need structural applications, enhanced barrier and optical properties, as well as superior thermal and electrical properties. The final performance can be improved by controlling the process parameters. It is therefore critical to understand how 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 control the orientation and the influence of processing conditions on the final properties of the films.

W3.25 The Use of Micro-Cantilevers for Actuation and Sensing Applications in Aqueous Environments.
Nabil Ibrahim AlOthman1,2,3, Marian Kabolek2,3, Yee Lam1, Bruce LawMatsumoto1, Robert Clark1,2 and Stefan Zaucha1,2; Mechanical Engineering and Materials Science, Duke University, Durham, North Carolina; Center for Biologically Inspired Materials and Material Systems, Duke University, Durham, North Carolina; Army 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) (pNIPAM) brushes responded to changes in temperature and solvent type, whereas cantilevers decorated with a copolymer composed of 70% pNIPAM and 30% vinylimidazole (VI) responded sensitively to changes in solution pH. The use of SRPs for cantilever actuation is exciting because common available micro-fabricated cantilever springs offer a simple and non-invasive way to sense changes in solution 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 deflect upon specific binding of mAb A32 to human immunodeficiency virus-1 (HIV-1) envelope glycoprotein 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.
Zhiyue 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, easy fabrication, and compact size. Sensor platforms based on MEMS, such as micro-cantilevers (including piezoelectric and silicon-based cantilevers), have been studied. Using of micro-electromechanical dimptherm (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 found to be much lower 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. Yang, Ken Gail1, Alicin Ortega1, Alan Greenberg1, Robin Shandas1,2, Kristi Anseth1,2,4 and Nick James Willett1; Mechanical Engineering, University of Colorado, Boulder, Colorado; Chemical and Biological Engineering, University of Colorado, Boulder, Colorado; Division of Cardiology, The Children’s Hospital, Denver, Colorado; Howard 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 dihydroxyethyl-dimethacrylate crosslinker. We first examined the...
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 MEMS-based designs. 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 magneto-mechanical coupling was found to be poor, resulting in insufficient signal amplitude. To obtain better performance, we are studying the use of alternative materials including an amorphous CoFeSiB alloy, CoNiZr, 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.

W3.28


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 temperature at a constant heating rate. Free strain recovery was determined to depend on the temperature during predeformation; lower predeformation temperatures (T < Tg) decreased the temperature required for free strain recovery. Constrained stress recovery shows a complicated response function of temperature, and also depends on the temperature during predeformation. Stress recovery after low temperature predeformation (T < Tg) shows a peak in the generated recovery stress, while stress recovery after high temperature predeformation (T > Tg) shows a 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.

W3.29

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 have 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-organic composites exhibit high electromechanical response under low applied field. For example, in a fully functionalized dielectric-percolative polymer in which the high dielectric filled 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 100 kg/m³ which is induced to a field of 25MV/m. Composites with conductive polymer nano-spheres as filler are also investigated and results will be presented.

W3.30


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 MEMS-based designs. 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 magneto-mechanical coupling was found to be poor, resulting in insufficient signal amplitude. To obtain better performance, we are studying the use of alternative materials including an amorphous CoFeSiB alloy, CoNiZr, 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.
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 & Hatzopoulos 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 shape reconfigurable systems. 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 technology. New magneto-rheological fluids employing carbonyl iron particles from 200nm - 10μm 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 potentially 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 50nm - 1μm in diameter enables the magnitude and onset point of 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 composite 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 these composites is further increased (by up to 10 times) due to viscous dissipation in the pores and rearrangement of the collapsible foam edges. As a result 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 loading of fluid. These new responsive composite materials thus have tremendous potential as adaptive energy absorbers.

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, there are only a 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 deforming. 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.

Shape memory polymers 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 jellyfish. We discuss how 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 Rigidly Constructed Flushing and Consequent Self-Assembly or Block Copolymer Peptide Folding and Self-Assembly. Darrin Pochan*1, Joel Schneider*1 and Tim Deming2; 1Materials Science and Engineering, University of Delaware, Newark, Delaware; 2Department of Materials, UCSD, Santa Barbara, California.

By using peptide molecules in the materials self-assembly design process, one can take advantage of inherent biomolecular attributes, intra- and inter-molecular folding cooperativity, and entropic and enthalpic contributions to more traditional self-assembling molecular attributes such as amphiphility, to define hierarchical material structure and consequent properties. Intramolecular folding events impart a molecular-level mechanism for environmental responsiveness at the material level, and viscoplastic carrier fluids, these materials do not require imposition of an external field systematically varied. For each type of fluid, a controllable shear-thickening colloidal fluids is also of particular interest for stress magnitude shows a dramatic increase (by up to 30 times the 'dry' foam) due to viscous dissipation in the pores and rearrangement of the collapsible foam edges. As a result 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 loading of fluid. These new responsive composite materials thus have tremendous potential as adaptive energy absorbers.

11:30 AM #W4.8

Mechanical Coupling in Endothelial Cell Development. M. Todd Thompson, Michael E. Berg, Michael F. Rubner and Krystyn J. Van Vliet; 1Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; 2Health Sciences and Technology, Massachusetts Institute of Technology, Cambridge, Massachusetts.

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 Ts or Tm. 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/m·K. In this work, we incorporated an inorganic filler featuring high thermal conductivity into a shape memory polymer, crosslinked polyacrylate, to increase its thermal conductivity and therefore shorten the heat transfer time. A simple mathematical model was developed that quantitatively correlated the material thermal conductivity and heat transfer time, r, that translates in shape recovery 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 performance was observed with the addition of this rigid thermal conducting filler.
Living biological cells are complex, mechanically active material systems that demonstrate coupling between chemical and mechanical fields. An example of such a material is the mechanical stimulus 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 through multilayer formation. We then correlate the effects of this mechanical compliance with the capacity for vascular endothelial cells to attach, spread, and express functions.

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 expression. Overlap 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 Crane
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 changes in tension/compression asymmetry. The simultaneous reverse transformation of self-accommodated and stressinduced martensite into austenite is also addressed. Different hardening functions are used to better capture the material response, as well as the role of detwinning and detwinned bilayers. 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 obtain 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, Coli Jannetti1, John L. Bassani1, and Sergio Turri1, 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 variety of applications including sensors and actuators. These materials, as well as pseudoelastic, 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, the continuum description is the ideal choice to model SMAs for use in applications on the 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 constitutive model for the thermomechanical behavior of martensitic phase transformations in single crystals is developed in the framework of irreversible thermodynamics with internal variables. The finite-strain kinematic 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 martensite 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 pseudelastic stress-strain branch and its dependence on the orientation of the loading axis relative to various crystallographic axes.

2:15 PM *W5.3
Kneumatic and Thermodynamic Models of Martensitic Interfaces, R. M. Reddi1, X. Ma2, 1Department of Materials Engineering, The University of Liverpool, Liverpool, United Kingdom; 2Department of Engineering, The University of Liverpool, Liverpool, United Kingdom; 713 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 property does not hold 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 diffuseness. The habit planes predicted by this model deviate in a systematic manner from the classical ones. The object of the present work 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. Serebrenskiy, 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 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 the mechanisms causing ferroelecteric 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 Ni 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, Habib S.2 and William A. Goddard III1, 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 (bulky) 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 transition between 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 huge changes in the material properties result at extremely high frequencies (over 10^9 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 and from this 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

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 solution 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. Byron D. Schmid, Peter Madden, John Madden, and Ian Hunter; 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 mecananoactive polypyrrole electrodes sandwiching an ion-permeable layer impregnated with a BF₄ Naf 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 25μm thick PPy films embedded in the trimorph and produced forces up to 0.2N and curvatures of 133m⁻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 thermomechanics 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

This paper addresses the development of a unified framework for quantifying hysteresis and constitutive nonlinearities inherent to ferroelectric, ferromagnetic and ferroelastic materials. 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 lower-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.