SYMPOSIUM CC

Coupled Nonlinear Phenomena–Modeling and Simulation for Smart, Ferroic, and Multiferroic Materials

March 29 - 31, 2005

Chairs

Robert M. McMeeking
Dept. of Mechanical & Environmental Engr
University of California-Santa Barbara
Santa Barbara, CA 93106
805-893-8434

Marc Kamlah
Institut für Materialforschung II
Forschungszentrum Karlsruhe GmbH
Postfach 3640
Karlsruhe, D-76021 Germany
49-7247-82-5860

Stefan Seelecke
Dept. of Mechanical & Aerospace Engineering
North Carolina State University
3211 Broughton Hall
Raleigh, NC 27695-7910
919-515-5282

Dwight Viehland
Dept. of Materials Science & Engineering
Virginia Tech
201 Holden Hall (0237)
Blacksburg, VA 24061
540-231-2276

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* Invited paper

SESSION CC1: Modeling of Constitutive Properties
Chair: John A. Shaw
Tuesday Morning, March 29, 2005
Room 2020 (Moscone West)

8:30 AM CC1.1
Material Characterisation of Piezoceramic Actuator Hystereses for Actuation Strain Prediction in Smart Structures. Ruediger Schmidt, Heiko Bossong and Sven Lentzen; General Mechanics, RWTH Aachen University, Aachen, Germany.

Piezoelectric ceramics are often used as actuators in smart structures technology. In the vast majority of papers dealing with modelling and simulation of shape and vibration control only linear constitutive relations are used. However, the electric field-strain relations of such actuators show hysteretic behaviour, which means that the piezoelectric coupling coefficient is not constant. The induced strain of an embedded actuator is accurately predictable, when the coupling coefficient is considered as a function of the actual strain. In this study the hysteresis of a mechanically unconstrained actuator is determined using a direct measurement procedure, the Michelson Interferometry. The hysteretic behaviour, including the input history of the system, is modelled by a Preisach Model. Using these experimental data, for the modelling of an active structure with embedded piezoelectric actuators the actual coupling coefficient can then be determined with the help of the Preisach Model. Thus, with this procedure the actuation strain of an embedded actuator, including the physical nonlinearities, can be calculated using the material characteristics obtained for an unconstrained actuator. For an experimental validation of the method outlined above, a Lead Zirkonate Titanate (PZT) actuator is characterised experimentally and then glued to a cantilever beam. Then, the tip displacement of the actuated beam is determined experimentally and simulated numerically using the above method. The experimental and numerical results agree reasonably well if, in addition, the shear lag due to the bonding layer between the actuator and the structure is taken into consideration.

8:45 AM CC1.2
Self-Consistent Modeling of Ferroelectrics. Maziar Motahari[1,2], Ersan Ustundag[2], Robert Rogan[3] and Chad Landis[4]; [1]Applied Mechanics, California Institute of Technology, Pasadena, California; [2]Ames Laboratory and Department of Materials Science and Engineering, Iowa State University, Ames, Iowa; [3]Materials Science, California Institute of Technology, Pasadena, California; [4]Mechanical Engineering and Material Science, Rice University, Houston, Texas.

The remnant electrical polarization in ferroelectrics can be switched by the application of an electric field or mechanical stress. Several nonlinear constitutive models have been developed to describe the response of ferroelectric ceramics to electromechanical loading. One such model (Huber et al. J. Mech. Phys. Solids 47 (1999) 1663) used progressive domain wall motion as the basis of the microelectromechanical response of individual crystals. Intergranular interactions were then accounted for using a self-consistent approach to yield the macroscopic polycrystalline behavior. In this research, we adapt this model to evaluate lattice strains as a function of electromechanical loads. We also modify the model to allow direct comparison with diffraction data. The modeling predictions are then compared with data collected from several X-ray and neutron diffraction experiments on PZT and $BaTiO_3$ ceramics.

9:00 AM *CC1.3
Experimental Investigation and Constitutive Modeling of the Magnetic Shape Memory Effect Caused by Martensitic Variant Rearrangement. Dimitris C. Lagoudas[1], Ibrahim Karaman[2] and Bjoern Kiefer[1]; [1]Aerospace Engineering, Texas A&M University, College Station, Texas; [2]Mechanical Engineering, Texas A&M University, College Station, Texas.

Magnetic shape memory alloys (MSMAs) have recently emerged as a new class of active materials that can be used in the design of magnetomechanical actuators. For actuation, one takes advantage of their characteristic nonlinear, hysteretic strain response, which is caused by a martensitic phase transformation of the crystal structure or alternatively the rearrangement of variants in martensite. The focus of this presentation is placed on the rearrangement of martensitic variants, which is either magnetic field or stress-induced. The induction of large ($<10\%$) strains in MSMA single crystals, caused by the magnetic field-controlled reorientation of martensitic variants, is accompanied by the magnetization of the material. Several phenomena influence the evolution of the magnetization, namely the reorientation of magnetic easy axes in the rearrangement of variants, the local rotation of magnetic moments and magnetic domain wall motion. It is therefore evident that the nonlinear evolution of strains and magnetization are coupled. Any modeling approach that captures the constitutive response of MSMAs has to reflect this effect. From standard experiments, however, it is difficult to distinguish the individual contributions of each of these mechanisms to the macroscopic magnetization of the multivariant MSMA single crystal. The experimental work recently conducted on MSMA single crystals presented here is aimed at resolving this problem by correlating various data such as the strain-magnetic field response curves with the associated magnetization-magnetic field curves. In this manner mechanisms that for example contribute to the evolution the magnetization but not the development of macroscopic strain can be identified. The presentation of experimental observations includes the description of a thermo-magneto-mechanical test frame that has been designed and built for these experiments. The discussed experimental observations are used to improve the accuracy and applicability of a constitutive model previously introduced by the authors. The model is based on the postulation of a free energy functional in which the dissipative nature of the material behavior is captured by internal state variables such as the reorientation strain and the martensitic variant and magnetic domain volume fractions. A phase diagram based approach in stress-magnetic field space is used to define activation functions for the variant rearrangement process and to derive evolution equations for the internal state variables. The analysis of magnetization mechanisms is utilized in incorporating the local rotation of magnetic moments and the associated magnetic anisotropy, as well as in the description of the evolution of magnetic domains. For some specific cases model predictions are verified with the available experimental data. It is pointed out how the constitutive model can conversely be used to further improve the current experimental testing procedures.

9:30 AM CC1.4
Investigations on Multi-axial Domain Switching Criteria for Piezoceramics. Bernd Laskewitz, Dayu Zhou and Marc Kamlah; Institute for Materials Research II, Forschungszentrum Karlsruhe GmbH, Karlsruhe, Germany.

The spreading of applications of piezoceramics requires a mature level of understanding their multi-axial behavior and the distributions of the stress and the electric fields. One important issue is the determination of so-called switching criteria for the onset of electrically and mechanically induced domain switching processes in piezoceramics. Experimental and theoretical work on this topic is still rare. Initially unpoled soft PZT was subjected to a proportional, coaxial electromechanical loading. The ratio of compressive stress to electric field was changed between the experiments. From this a series of nonlinear polarization and strain responses were obtained. Based on an offset method, initial domain switching states in the two-dimensional stress-electric field space were determined. Furthermore, experiments with non-proportional, coaxial electromechanical loadings in the switching regime were carried out. The results are compared with two constitutive models developed earlier in order to verify the representation of the pronounced history dependency in the switching regime of piezoceramics. In continuum mechanics, thin walled tubes are used to investigate the multi-axial stress states. However, simple linear dielectric analysis indicates an inhomogeneous electric field distribution in such geometries. Therefore, the suitability of thin walled tubes for multi-axial electromechanical experiments has to be investigated. Simulations with a finite element tool based on a phenomenological constitutive model for ferroelectric and ferroelastic hysteresis behavior were performed. The results confirm inhomogeneous distributions of electric fields and stresses after poling. A geometry variation is discussed to minimize these effects.

9:45 AM CC1.5
Hysteresis Modeling in Ferroelectric Materials using Dry Friction Analogy. Daniel Guyomar[1], Kaori Yuse[2] and Gael Sebald[3]; [1]LGEF, INSA de Lyon, Villeurbanne, France; [2]GEMPPM, INSA de Lyon, Villeurbanne, France; [3]Institute of Fluid Science, Tohoku University, Sendai, Japan.

Ferroelectric ceramics are widely used as a piezoelectric material in many sensor and actuator applications due to their high electromechanical properties. Most ferroelectric materials behave as piezoelectric for low driving levels. However, for high driving levels a major limitation of the actuators is their lack of accuracy due to nonlinearities and hysteresis. Modeling hysteresis related behaviors could be achieved using a dry friction analogy, considering that the motion of domain walls can be compared to the motion of a mass on a plane and subjected to dry friction resistive force. Starting from that analogy, a model using a dry friction spectrum is developed to take into account hysteresis loops of the polarization (major and minor loops). This spectrum comes more specifically from experimental considerations that are detailed in the paper. Piezoelectric materials are a joint between two kinds of physical quantities (mechanical and electrical) and the electromechanical coupling links the respective behaviors. Heavy nonlinear behaviors follow the same coupling rules and it is a wrong way to model electrical and mechanical behaviors separately. In the approach presented here, a scaling effect is detailed

between electric field and the stress multiplied by the polarization. Experimental validation of this scaling is presented. Some experimental comparisons (conducted on soft PZT ceramic type Navy II) are finally shown on hysteresis loops of the polarization versus electric field and stress to show the global viability of the approach

10:30 AM CC1.6
A Free Energy Model for the Inner Loop Behavior of Pseudoelastic Shape Memory Alloys. Olaf Heintze and Stefan Seelecke; Dept. of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, North Carolina.

A free energy model for shape memory alloy behavior based on a statistical thermodynamics approach and the theory of thermally activated processes is presented. Through the inclusion of an energy balance, the model accounts for the fully coupled thermo-mechanical behavior caused by the rate-dependent release and absorption of latent heats. The original single crystal version is extended to include inhomogeneities and effective stress concepts by a stochastical homogenization procedure. The method is shown to reproduce the experimentally observed inner loop behavior of pseudoelastic SMAs over a large range of strain rates.

10:45 AM CC1.7
A Two-Dimensional Free Energy Model for Single Crystalline Ferroelectrics. Sang-Joo Kim[1], Stefan Seelecke[2] and Ralph C. Smith[3]; [1]Dept. of Mechanical and Information Engineering, University of Seoul, Korea, Seoul, South Korea; [2]Dept. of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, North Carolina; [3]Dept. of Mathematics, North Carolina State University, Raleigh, North Carolina.

In the present paper, the one-dimensional free energy model of Smith et al.(2004) is generalized to a two-dimensional model. The proposed two-dimensional energy potential has four energy wells that correspond to respective four in-plane variants of the material, four saddle points through which 90° domain switchings occur, and one local energy maximum through which 180° switchings occur. The free energy potential is combined with thermal activation-based evolution equations. A recently observed hysteresis curve for a BaTiO3 single crystalline material is predicted successfully with the present model. The responses of the model to an application of in-plane multi-axial electric field at various loading rates are calculated and the roles of 90° and 180° domain switchings are discussed.

11:00 AM *CC1.8
A Stress-Dependent Hysteresis Model for Ferroelectric and Ferromagnetic Compounds. Brian L. Ball and Ralph C. Smith; Mathematics, North Carolina State University, Raleigh, North Carolina.

This paper addresses the development and validation of a stress-dependent model for polycrystalline ferroelectric and ferromagnetic compounds. The theory is based on the homogenized energy framework of Smith et al. [2004] which characterizes hysteretic phenomena through a combination of energy principles at the lattice level and macroscopic stochastic homogenization techniques. The proposed model incorporates stress effects by extending the energy framework to include both 90 and 180 degree domain switching as a function of input fields and stresses. Properties of the model are illustrated through comparison and prediction of experimental PLZT data.

11:30 AM *CC1.9
Modeling the Behavior of Heterogeneous Materials with Non Linear Couplings using Translated Fields. Stephane Berbenni, Veronique Favier and Marcel Berveiller; LPMM- UMR CNRS 7554, ENSAM, Metz, France.

The determination of the behavior of heterogeneous materials with complex physical and mechanical couplings constitutes a challenge in the design of new materials and the modeling of their effective properties. In real heterogeneous materials, the simultaneous presence of elastic mechanisms and non linear inelastic ones (viscoplastic, magnetic, ferroelectric, shape memory effect etc.) leads to a complex non linear coupling between the mechanical fields which is tricky to represent in a simple and efficient way. Hence, for many situations the effective global behavior does not follow the same structure than the local constitutive one. Regarding space-time couplings for instance, a heterogeneous material composed of phases described by Maxwell elements can not be considered as a Maxwellian solid at the macro scale. This presentation introduces a new micro-macro approach based on translated fields in its generalized form to be applied to different coupled phenomena. The local total strain (rate) is composed additively of an elastic strain (rate) and an inelastic one which is no more limited to be stress free as considered originally by Kroener. An extended (non conventional) self-consistent model is then proposed starting from the integral equation for a translated strain (rate) field and the projection operators introduced by Kunin and Kroener. The chosen translated field is the compatible inelastic strain (rate) of the fictitious inelastic heterogeneous medium submitted to a uniform unknown boundary condition. The self-consistency condition amounts to define analytically these boundary conditions so that a relative simple and compact strain (rate) concentration equation is obtained. In order to illustrate the method, the case of a non linear elastic-viscoplastic coupling is developed and applied to different classes of composites and polycrystals.

SESSION CC2: Experimental Characterization
Chair: Stefan Seelecke
Tuesday Afternoon, March 29, 2005
Room 2020 (Moscone West)

1:30 PM *CC2.1
Estimation of Strain from Piezoelectric Effect and Domain Switching in Morphotropic PZT-Ceramics. Michael J. Hoffmann and Hans Kungl; IKM, University of Karlsruhe, Karlsruhe, Germany.

Morphotropic PZT compositions are the state of the art materials for ferroelectric actuators. Strain and hysteresis are essential performance parameters for these materials. On a microscopic scale the strain provided by an application of an electric field is due to two different mechanisms. The piezoelectric effect causes an elongation of the unit cells in the direction parallel to the electric field. Domain switching is changing the crystallographic orientation of the unit cells by aligning the polarization towards field direction. With the orientation of polarization changing from perpendicular to parallel to the field, this process also results in an expansion of the material parallel to the field direction. Hysteresis and fatigue are attributed in particular to the domain switching mechanism. The contribution of the two mechanisms to total strain can be estimated by combining macroscopic strain measurements and X-Ray diffraction data. Starting point of the procedure is an analysis of the remnant state after poling. The remnant strain is only due to effects from domain switching because no piezoelectric effect occurs at zero electric field. Evaluation of the changes in texture from unpoled to poled state provides information on the corresponding amount of domain switching. From these data the effects of the texture change on strain can be calculated, giving as a result a strain efficiency factor of domain switching. With an electric field applied to the poled material, texture changes caused by the electric field were measured by in-situ X-ray diffraction. Using the strain efficiency factor and the data on texture, the strain from domain switching along with the electric field can be calculated. Information on total strain is provided by macroscopic strain measurement. The strain from the piezoelectric effect can be calculated from the difference between total strain and strain from domain switching.

2:00 PM *CC2.2
Characterization of the Electro-Thermo-Mechanical Constitutive Behavior of Relaxor Ferroelectric Single Crystals. Chris S. Lynch[1], Tieqi Liu[1] and Elizabeth A. McLaughlin[2]; [1]Mechanical Engineering, Georgia Tech, Atlanta, Georgia; [2]Devices, Sensors, and Materials R&D Branch, NUWCDIVNPT, Newport, Rhode Island.

Recently techniques have been developed for growing large ferroelectric single crystals. Relaxor rhombohedral single crystals of PMN-32%PT display very large piezoelectric coefficients with low loss when cut and poled in the [001] and [011] orientations. Under uniaxial electric field these cuts are stable against domain wall motion. At field levels above the transformation field, combinations of stress and electric field drive phase transformations. Data will be presented that is indicative of a rhombohedral to orthorhombic transformation in the [011] poled crystal. Combinations of stress, electric field, and temperature that induce this transformation are experimentally mapped out. This has resulted in the identification of the transformation start and transformation finish functions. Internal energy and free energy are determined through numerical integration of the path integrals represented by the data. The result is a scalar criterion for the multivariable driven phase transformation.

2:30 PM CC2.3
Experimental Investigation of Rate-Dependent Inner Hysteresis Loops in PZT. Alexander York and Stefan Seelecke; Dept. of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, North Carolina.

The rate-dependence of piezoelectric material resulting from the kinetics of domain switching is an important factor that needs to be included in realistic modeling attempts. This paper provides a systematic study of the rate-dependent hysteresis behavior of a commercially available PZT stack actuator. Experiments covering full loop as well as first, second, third and forth order reversals are conducted at different loading rates with polarization and strain recorded. Creep behavior at different constant levels of the electric field is also observed. The kinetics are characterized by strongly varying relaxation times that can be associated with different switching mechanisms. Inner hysteresis loops in the (P, E) diagram are also shown to have different characteristics depending on the electric field level at the reversal points.

2:45 PM CC2.4
In-Situ Characterization of Ferroelectric Constitutive Behavior Using Diffraction. Robert Rogan[1,2], Ersan Ustundag[1], Maziar Motahari[1,2], Mark Daymond[3] and Ulrich Lienert[4]; [1]Ames Laboratory and Department of Materials Science and Engineering, Iowa State University, Ames, Iowa; [2]Materials Science, California Institute of Technology, Pasadena, California; [3]Mechanical and Materials Engineering, Queens University, Kingston, Ontario, Canada; [4]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois.

Electromechanical loading was applied to monitor strain and texture (domain switching) evolution in various Pb(Zr,Ti)O3 (PZT) and BaTiO3 ceramics using neutron and high energy X-ray diffraction. In-situ uniaxial compression experiments were performed on various PZTs using neutron diffraction to determine their ferroelastic behavior. PZTs near the edge of the morphotropic phase boundary as well as single phase (tetragonal and rhombohedral) specimens were investigated. Analysis of the diffraction patterns allowed for observation of the onset and culmination of domain switching through modeling of the sample texture using the March-Dollase approach. Diffraction data suggested a high degree of anisotropy and a complicated internal stress state in all specimens. In-situ uniaxial electrical cycling experiments on (Pb0.92La0.8)(Zr0.65Ti0.35)O3 or PLZT and BaTiO3 polycrystalline electroceramics were conducted using high energy synchrotron diffraction. Using a two-dimensional detector, complete biaxial elastic lattice strains were measured simultaneously. The results will be interpreted in comparison with a self-consistent model.

3:30 PM CC2.5
Deformation Instability and Pattern Formation in Superelastic Shape Memory Alloy Microtubes. Q. P. Sun, Department of Mechanical Engineering, Hong Kong University of Science and Technology, Kowloon, Hong Kong.

This talk reports the deformation instability and band morphology evolution during stress-induced phase transformation in a superelastic NiTi polycrystalline shape memory alloy microtube. High-speed data and image acquisition techniques were used to investigate the dynamic as well as quasistatic events which happened during displacement controlled quasi-static tensile loading/unloading process of the tube. These events include dynamic formation, self-merging and the front instability of a macroscopic deformation band. The reported phenomena are highly nonlinear in nature and have brought up several issues in the fundamental understanding of the instability and pattern evolution in polycrystal NiTi under mechanical force. These issues are believed to be essential in the theoretical modeling and worth further investigation in the future.

3:45 PM CC2.6
Quantitative Studies of Phase Fraction Evolution in Near-Equiatomic TiNi Films. Bo-Kuai Lai, [1]Physics, U of Arkansas, Fayetteville, Arkansas; [2]Materials Science and Engineering, Case Western Reserve University, Cleveland, Ohio.

The focus of previous TiNi thin film studies has generally been on macroscopic properties, such as stress and resistivity, and on microstructure. The thermomechanical properties and phase content of TiNi thin films depend on film composition, thermomechanical history, and sputtering conditions if the thin films are formed by sputter deposition. It is generally accepted that stress evolution is closely related to the phase fraction "evolution" of martensite or austenite in TiNi thin films, whereas resistivity is closely related to the presence of R-phase. However, quantitative understanding of phase fraction evolution and phase distribution in TiNi thin films and how these relate to macroscopic properties and microstructure is not available. In the absence of experimental results, several computational models, involving phenomenological constitutive models and micromechanical models have been proposed. However, conclusive insight on the exact behavior is still lacking. Furthermore, the phase distribution and the presence of R-phase are usually not considered in these models, due to the complexity of modeling and the lack of experimental results. A transmission electron microscopy (TEM) study of TiNi thin films has shown the importance of intermediate phases, such as Ti2Ni or Ti3Ni4, and the role of dislocations and grain boundaries on the transformations involving R-phase, austenite-R-phase (A-R) and R- phase-martensite (R-M). To date, however, the dynamic phase transformation behavior between austenite, martensite, and R-phase is poorly understood. TiNi thin films with near-equiatomic compositions exhibited transformation temperatures between 65 and 100C, low residual stresses at room temperature, and high recoverable stresses, thus making them suitable for microactuators in microelectromechanical systems. Phase transformations in near-equiatomic TiNi shape memory alloy thin films were studied, and their phase fraction evolutions were quantitatively correlated to the stress and resistivity of the films. To author's knowledge, such quantitative correlation has never been reported experimentally. Using elevated temperature x-ray diffraction, combined with quantitative Rietveld analysis, phase fraction evolutions during complete thermal cycles (heating and cooling) were obtained. Sheet resistance, thus resistivity, of TiNi films was measured using 4-point probe. By comparing stress-temperature and resistivity-temperature evolutions to the phase fraction evolution of austenite, martensite and R-phase, it is evident that the stress and resistivity behavior correspond to the phase evolution of martensite and R-phase, respectively. It was also found that the phase distribution through the film thickness, which occurs even film thickness is less than 1um, also affected the stress-temperature behaviors in TiNi films.

4:00 PM *CC2.7
Domain Switch Toughening in Polycrystalline and Single Crystal Ferroelectrics. Chad M. Landis, Mechanical Engineering, Rice University, Houston, Texas.

Mode I steady crack growth is analyzed to determine the toughening due to domain switching in ferroelectric ceramics. Multi-axial, electromechanically coupled, incremental constitutive theories for polycrystalline and single crystal ferroelectrics are applied to model the material behavior. The constitutive laws are then implemented within the finite element method to study steady crack growth. The effects of domain switching on the fracture toughening are investigated. Specific attention is paid to the anisotropy induced in the switch toughening by electrical and mechanical poling and crystal orientation. Results for the predicted fracture toughness, remanent strain and remanent polarization distributions, and domain switching zone shapes and sizes are presented.

4:30 PM CC2.8
The Electric Permittivity Interior to Cracks in PZT as a Function of Time and Applied Electric Field Measured by Scanning Probe Microscopy. Frank Martin Felten and Gerold A. Schneider; Advanced Ceramics Group, Technical University of Hamburg-Harburg, Hamburg, Germany.

An indentation crack in a poled PZT ceramic subjected to electric fields of up to ± 500 V/mm is investigated using scanning probe microscopy techniques. Atomic force microscopy (AFM) and Kelvin Probe Force Microscopy (KFM) are used to determine the crack opening displacement (COD) and the electrical potential difference across the crack, respectively. The electric field interior to the crack is calculated as the ratio of these quantities. Using this result the dielectric constant of the crack interior is determined for every remote electric field to evaluate whether the permittivity or a saturated electric field inside the crack is suitable as an electric boundary condition. To show the consequences for fracture the experimental results are used to calculate the corresponding crack tip stress and dielectric displacement intensity factors as well as the crack tip energy release rates. The results are discussed by means of a Griffith crack. Finally, dynamic measurements with a quickly varying electric field reveal a time dependence of the potential difference indicating that transient charges might be present on the crack face.

4:45 PM CC2.9
Mechanical Properties of Barium Titanate Measured by Scanning Probe Microscopy and Nanoindentation.
Gerold A. Schneider[1], Torben Scholz[1], Juan Munoz-Saldana[2], Mike V. Swain[3] and Frank Felten[1]; [1]Technische Keramik, Technical University Hamburg-Harburg, Hamburg, Germany; [2]CINVESTAV Unidad Queretaro, Queretaro, Mexico; [3]Faculty of Dentistry, Otago University, Dunedin, New Zealand.

Mechanical properties of single crystalline barium titanate were analyzed by nanoindentation with loads P from 0.25 mN to 10 mN using indenters with tip radii varying from 70nm to 2400nm. During loading, the penetration depth often shows a sudden additional penetration of the indenter at constant load, which is commonly denominated as pop-in effect. Three stages are identified through reproducible pop- in effects: purely elastic, elastic/plastic, and brittle fracture. Analyzing the elastic behaviour by using a Hertzian fit the aa-domain and ac-domain configurations in BaTiO3 revealed different indentation moduli. Additionally a hysteretic behaviour was found for a aa-domain configuration. A strong relaxation effect observed at the last portion of the unloading curve is correlated with domain wall movement. Domain structures around residual indentation marks before and after the mechanical testing were identified by piezoelectric force microscopy (PFM). The hardness in $BaTiO_3$ scales with the indentation radius as predicted by strain gradient plasticity. The length a of submicron cracks in the last stage of loading were analyzed with the AFM and the proportionally between P2/3 and a was verified.

SESSION CC3: Poster Session: Determination of Material Parameters
Tuesday Evening, March 29, 2005
8:00 PM
Salons 8-15 (Marriott)

CC3.1
Effective Medium Approach for Calculation of Linear and Nonlinear Properties of Porous Semiconductor Composites.
Vladimir Kochergin[2], Marc Christophersen[2] and Helmut Foell[1]; [1]Chair for General Materials Science, Faculty of Engineering, Christian-Albrechts-University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany; [2]Lake Shore Cryotronics, Inc., Columbus, Ohio.

Pore formation in semiconductors by means of electrochemical etching emerged as a promising technique to tailor the optical properties of these materials. Two and three dimensional photonic crystals uniformly etched into Si, optical filters, etc. can be mentioned in this regard. Considerable experimental efforts were devoted to investigations of linear and nonlinear optical properties of various porous semiconductors and composites, but a general theoretical approach is still missing. In this paper a general methodology for a detailed understanding of linear and nonlinear optical properties of nanoporous and nanostructured materials will be presented. First, a Maxwell-Garnett approach will be generalized for the case of porous semiconductor materials containing a number of differently oriented pore lattices. Specifically, the cases of electrochemically etched mesoporous silicon on (110)-oriented substrates and electrochemically etched porous InP and GaAs materials on (100) substrates will be considered and the observed optical anisotropy of mesoporous Si will be explained. A biaxial anisotropy of the porous InP or GaAs material with crystallographic pores is predicted for most of the material parameters. Next, a more accurate effective medium approach (based on the generalization of the Bruggeman method) will be presented for the case of the porous semiconductor material composed of a number of differently spatially oriented pore lattices. Theoretical results obtained by applying this theory to a composite material consisting of mesoporous Si on (110)-oriented substrate having pores filled with silver by, e.g., an electroplating process, will be presented. The theory permits a self-consistent determination of the effective dielectric permittivity tensor of such materials. It is shown that the optical anisotropy of such a composite can be greatly enhanced at some wavelength ranges. While this anisotropy is generally uniaxial as in non-metal-filled mesoporous Si etched on (110) substrate, the "sign" of the anisotropy (i.e., positive or negative) changes in some portions of the spectrum. The optimum material parameters for an experimental observation of the theoretically predicted effects are determined. At last, theoretical results, obtained by applying the modified effective medium theory to second harmonic generation (SHG) from a composite material, will be given. The theory presented permits a determination of the SGH tensor coefficients of such composites. It is shown that the SHG of such a composite can be greatly enhanced in some wavelength ranges due to the local electromagnetic field enhancement for surface plasmon resonance conditions of the metal-filled pores. Moreover, some peculiarities of SGH generation efficiency are predicted due to spectral peculiarities of the effective dielectric constant of such a composite. The optimum material parameters for an experimental observation of the theoretically predicted effects are determined.

CC3.2
Piezoelectric Coefficient by the Berlincourt Method: Experimental and FEA Modelling for Thin and Thick Discs.
Markys Cain, Mark Stewart and David A. Mendels; National Physical Laboratory, Teddington, United Kingdom.

The Berlincourt method has received wide acceptance by industry and academics because of its simplicity of operation and speed of obtaining data. However, research at NPL and other laboratories has identified anomalies in the values obtained following innapropriate application of the technique. In this presentation, a new Finite Element Model has been developed that incorporates the non-linear piezoelectric depolarisation that is observed in these materials when exposed to high point load stress. Results indicate that best practice may be achieved when preload is carefully controlled.

CC3.3
Finite Element Formulation of a Piezoelectric Continuum and Performance Studies of Laminar PZT-Patch-Modules.
Monika M. Gall[1], Baerbel Thielicke[1], Christophe Poizat[1] and Sven Klinkel[2]; [1]Fraunhofer-Institut fuer Werkstoffmechanik IWM, Freiburg, Germany; [2]Institut fuer Baustatik, Universitaet Karlsruhe (TH), Karlsruhe, Germany.

To make the use of piezoelectric sensors and actuators more attractive, it is of great interest to study the durability and life-span of such devices. Within the DFG (German Research Foundation) program "Adaptronics in Machine Tools" the failure behaviour of laminar piezoelectric patch-modules is investigated. For this purpose a combination of experimental and numerical methods is employed. In addition to using commercially available FE-codes, an FE-tool is developed within the research finite element code FEAP (Finite Element Analysis Program). This work describes the modelling of linear electro-mechanic coupling in a FEAP user element that is later to be used for the implementation of nonlinear material behaviour. In the finite element discretisation the differential equations of the mechanical balance of momentum and electric charge conservation laws are satisfied. The model renders an approximate solution for a finite deformation, isothermal, quasi-static electric boundary problem. The piezoelectric material properties are described by three-dimensional functional forms of high symmetry that determine the dependency of the piezoelectric modulus on the size and direction of a given material polarization vector. In sensor and actuator use the PZT-patch-modules have to withstand the operational demands of the structures on which they are applied. Testing conditions for the performance, durability and load limits of the modules should therefore be designed as closely as possible to the requirements in real applications. By conceiving and conducting the tests in interaction with finite-element simulation, a good transferability of the results to different module geometries and applications is achieved. To study the sensor function of the modules a 4-point bending test has been used that has a high relevance in practise. Also the electrical activation of free modules as well as specimen glued on a CFK-substrate has been tested. Results of FE-simulations are compared to the results of the experimental testing of the PZT-patch-modules under quasi-static and cyclic mechanical and electric loading.

SESSION CC4: Finite Element Methods
Chair: Marc Kamlah
Wednesday Morning, March 30, 2005
Room 2020 (Moscone West)

8:30 AM CC4.1
Constitutive Modelling and Finite Element Analysis of a Nonlinear Micropolar Continuum. Ingo Muench[1], Patrizio Neff[2] and Werner Wagner[1]; [1]Institute of Structural Analysis, Technische Universitaet, Karlsruhe, Germany; [2]Department of Mathematics, Technische Universitaet, Darmstadt, Germany.

Many materials show an inner structure, which will affect the mechanical behaviour. We investigate such effects for the static case and start with a purely elastic constitutive material model extended with a fundamental internal length. In order to incorporate this internal length into the continuum model we introduce an additional field of independent rotations defined in SO(3) which replace the continuum rotations. In this context we develop a geometrically nonlinear Cosserat continua of micropolar type, including an additional strain measure of second order (curvature), penalizing the inhomogeneity of the rotation field. The deformation gradient $\mathbf{F}$ and the micro-rotation field $\mathbf{R}$ are coupled through the non-symmetric strain measure of first order $\mathbf{U}$ with $\mathbf{U} = \mathbf{R}^T\mathbf{F}$. Besides the strain measure of first order (stretch), the curvature energy leads in our assumed form usually to comparatively small additional inner energy terms. On the positive side, the continuum model can benefit from the additional field $\mathbf{R}$ by a better description of lower energy modes. Depending on material constants, it is possible to simulate classical infinitesimal elasticity under small loads while length scale effects arise under higher loads. In the proposed framework the linearized Cauchy-stress tensor remain symmetric in contrast to traditional Cosserat-type models. This corresponds to setting the traditional Cosserat couple modulus to zero. This result is only possible in a nonlinear treatment, otherwise one would deal with linear elasticity. Boundary conditions for the micro-rotations at the clamped parts of the body induce inhomogeneous response also for homogeneous situations. This problem is circumvented by using a so called consistent coupling condition, introduced by Neff [1]. The condition requires the symmetry of the micropolar stretch $\mathbf{U}$ at the clamped boundary, which is realized by a simple penalty formulation in the finite element model. The mathematical well-posedness (existence of minimizers) has been shown by Neff [1]; notice that the problem is uniformly Legendre-Hadamard elliptic at prescribed rotations w.r.t.

the deformation. However, since we deal with an overall nonlinear, non-convex two-field problem, computed equilibrium solutions may loose their stability since a highly complicated energy landscape occur. The pseudo-homogenization achieved through the micropolar continuum theory does not represent a real physical material. By considering an imperfection field critical states of stability can be excluded. In our numerical tests we observe size effects. For the same internal length, great sample geometries behave weaker than small ones. The presented mechanical model offers weaker response than either the classical linear elastic model or the elastic model based on Neo-Hooke energy with similar elastic moduli when subjected to larger loads. [1] Preprint 2297: http://wwwbib.mathematik.tu-darmstadt.de/Math-Net/Preprints/Listen/pp03.html

8:45 AM CC4.2
Finite Element Modeling of the Ferroelectroelastic Material Behavior in Consideration of Domain Wall Motions.
Albrecht Charles Liskowsky[1], Artem Semenov[1], Herbert Balke[1] and Robert Maxwell McMeeking[2]; [1]IFKM, TU Dresden, Dresden, Germany; [2]Mechanical and Environmental Engineering, UCSB, Santa Barbara, California.

A simulation of the nonlinear electromechanical macroscopic behavior of ferroelectric materials by way of the finite element method is presented. A material point is depicted by a representative volume element, for which homogeneous boundary conditions are valid. The evolution of integral averages over the surface of the representative volume element is to homogenize the results. For this homogenization we favor a finite element model in which each Gauss Point represents exactly one single crystal. Their number of internal variables is limited to the lattice orientation and the volume fractions of the domains. The lattice orientations are randomly distributed in space. It is possible to calculate the material behavior for arbitrary coupled and nonlinear electromechanical loading cases, but it is not sufficient for the solution of boundary value problems for entire bodies.

9:00 AM CC4.3
A Computational Model for Switching in Ferroelectric Polycrystals. Robert M. McMeeking[1,2] and Amit Pathak[1]; [1]Mechanical Engineering, University of California, Santa Barbara, California; [2]Materials, University of California, Santa Barbara, California.

A single crystal constitutive law for ferroelectric switching due to the motion of domain walls has been developed. This model accounts for the effect of mechanical stress and electric field driving domain wall motion and uses resolved values of the stress and the field to determine the conditions in which the domain wall will move. The response is modeled as a rate dependent switching process in which the direction of switching and its rate are determined by the domain walls that are most strongly mobilized. The model also accounts for lock-up when the supply of switchable domains is exhausted and provides linear elastic, dielectric and piezoelectric response in addition to nonlinear switching. The model has been incorporated into a 3-dimensional finite element computer code to allow solution of the equations of mechanical equilibrium and Gauss's law while heterogeneous switching is taking place in a polycrystalline aggregate. Consequently, interactions among the grains in terms of mechanical constraint, clamping and depolarization fields are accounted for. Each single crystal is represented by one or more finite element and electric fields and mechanical stresses are applied as the electromechanical loading of the aggregate. Results are obtained for hysteresis and butterfly loops plus stress-strain curves for different realizations of the polycrystalline orientations. The results of these computational simulations are compared with experimental data.

9:15 AM CC4.4
Internal Stress Generation during Switching of Ferroelectrics.
Anja Haug, Patrick R. Onck and Erik Van der Giessen; Materials Science Center, University of Groningen, Groningen, Netherlands.

Ferroelectric ceramics are crystalline inorganic materials that can be made piezoelectric by poling. The poling is done by the reorientation of domains in each grain, which is a nonlinear process. The poled microstructure determines overall properties such as the linear elastic, dielectric and piezoelectric moduli. The latter are controlled by the electric field and by the inter- and intragranular stresses that develop as different domains in neighboring grains switch. A multi-grain finite element code for ferroelectrics is developed in which individual grains are modelled with their specific crystal orientation and switching system. Inside each grain, a fully coupled, nonlinear continuum model for piezoelectricity is adopted, due to Huber, Fleck, Landis and McMeeking*. Results will be given for a detailed mesh, in which a hexagonal grain consists of several elements and a simple mesh in which one element represents a grain. The switching behavior calculated with the detailed and simple mesh will be represented and compared. The inter-grain compatibility is investigated with the detailed mesh. The results demonstrate how this compatibility leads to the build-up of relatively large mechanical and electrical stress fluctuations. *Huber J.E., Fleck N.A.,Landis C.M., McMeeking R.M., A constitutive model for ferroelectric polycrystals, Journal of the Mechanics and Physics of Solids, 47 (1999) 1663-1697.

9:30 AM CC4.5
Micro-Mechanical Modeling of the Interaction between Defects and Domain Walls in Ferroelectric Materials.
Ralf Mueller and Dietmar Gross; Institute of Mechanics, Darmstadt University of Technology, Darmstadt, Germany.

Ferroelectric materials are nowadays widely used in sensor and actuator applications. Their applicability in cyclic loading however is limited by the so called 'electric fatigue' effect. Under this terminology various micro-mechanical phenomena are summarized. On the macroscopic level a reduction of the mechanical output for a fixed electric excitation is observed. One of suspected micro-mechanical mechanisms is the hindering and blocking of domain wall movement within the material. Possible sources of these blocking phenomena are point defects or volume defects in the material. The defects interact with the domain wall (inhomogeneity) and the external applied loads. Experimentally observations suggest that these point defects are oxygen vacancies. Their presence and characterization is however an experimentally difficult task. The intention of this presentation is to identify the driving forces also called material or configurational forces) acting on the domain wall. This is done for a general 3D case of a curved domain wall. The domain wall itself is described as a singular surface without material properties. The driving force acting on the domain wall depends on the solution of the field equations. In general the coupled field equation for the inhomogeneous case can only be solved numerically. A Finite Element Method is used to provide these solutions and in a post-processing step the driving forces on domain walls. A simple kinetic law that connects the driving force with the domain wall velocity is proposed. This kinetic law is based on experimental observations in a model system of Gadolinium molybdate. The defect free situation is used to calibrate this material law, which is of a visco-plastic type. The simulations will demonstrate the effect of defects on the movement of a domain wall. Surface and volume defects are considered, as some of them allow a comparison to experimental measurements. The simulation and the experiments show qualitative good agreement, although the simulations resort to the simplification of 2D calculations. Some quantitative agreement is found on the blocking capability of the defects.

9:45 AM CC4.6
Coupled Response of Piezoelectric Composite Materials. Ronit Kar-Gupta and T. A. Venkatesh; Mechanical Engineering, Tulane University, New Orleans, Louisiana.

Recognizing the potential for the use of piezoelectric materials in a number of applications as sensors and actuators, there has been a continuing research and development effort to synthesize monolithic materials with enhanced coupled properties. Because the sensing or actuating actions of monolithic piezoelectric materials are limited, the composite approach to piezoelectric materials provides a unique opportunity to access a new design space with optimal mechanical and coupled characteristics, hitherto inaccessible through monolithic materials. Through finite-element based numerical modeling, a systematic methodology for predicting a complete set of coupled properties of the piezoelectric composites as a function of the poling characteristics, size, shape, and distribution of the constituent phases is presented. Furthermore, a general method towards characterizing the coupled constitutive response of composite materials is also identified. Model predictions are compared with experimental results for select piezoelectric composites.

10:30 AM *CC4.7
Finite Element Modeling of Piezoelectric Actuators and Sensors: Local Analysis of the Ferroelectric and Ferroelastic Effects. Mourad Elhadrouz, Tarak Ben Zineb and Etienne Patoor; LPMM ENSAM, Metz Cedex 03, France.

Design of piezoelectric applications like sensors and actuators requires numerical simulation tools based on finite element method. This needs the use of electromechanical elements. The majority of the industrial FE codes propose such elements with a purely linear behaviour taking into account only the piezoelectric effect. Even if piezoelectric applications present globally a linear behaviour, it is noted that in certain local area, the electric field and stresses exceed the coercive values and activate the domain switching. Such an induced ferroelectric and/or ferroelsatic behaviour cannot be taken into account by these standard elements. We developed in the Abaqus FE code a new electromechanical element taking into account the ferroelectric and ferroelastic behaviour. It is a cubic element with eight nodes and linear interpolation. It is isoparametric and presents three mechanical d.o.f. and one electric d.o.f. (electric potential). The

Gauss integration method is adopted with a complete way for the deviatoric part and a reduced way for the hydrostatic part. In order to compute the electromechanical rigidity matrix of this element, we have developed a phenomenological ferroelectric and ferroelastic constitutive law. The developed phenomenological constitutive law is formulated within the thermodynamics of generalized standard materials. It is well adapted to a finite element formulation but it describes switching mechanisms in an average way. It has two internal variables. One corresponds to the remnant ferroelastic strain and the other to the remnant polarization. Two loading surfaces are introduced for the prediction of ferroelectricity and/or ferroelasticity. Saturation phenomena and depolarization under compression mechanical loading are taken into account in this behaviour model. In order to lead to a more physical description of ferroelectricity and ferroelsaticity, we also developed a micromechanical constitutive law describing such behaviour on the grain scale. It is derived from the expression of the Gibbs free energy. Internal variables for this law are volume fractions of the six possible domain orientations. The associated driving forces are obtained from the derivation of the Gibbs free energy expression with these internal variables. The consistency rule, combined with the piezoelectric behaviour, leads to the nonlinear electromechanical constitutive law on the grain scale. An interaction matrix is introduced in order to distinguish different interactions according to the domain orientations. Finally we studied, by In-situ mechanical tests, the evolution of domain structure in a Titanate Barium grain under a mechanical loading. This is in order to describe, on the best way, interactions between these domains.

11:00 AM CC4.8
Constitutive Theory and Numerical Simulation of Martensitic Phase Transitions in Shape Memory Alloys. Dirk Helm, Institute of Mechanics, Department of Mechanical Engineering, University of Kassel, Kassel, Germany.

The numerical simulation of structures based on shape memory materials is of increasing interest in different fields: e.g. the simulation of pipe connectors and medical devices like endoscopic instruments and stents is a challenge. In these practical applications the pseudoelastic effect as well as the one-way and two-way effect is applied. These material properties are caused by martensitic phase transitions between austenite and martensite. A thermomechanically consistent material model representing the multiaxial behavior of shape memory alloys is proposed in this lecture. The material model is formulated in the framework of continuum thermomechanics in form of a geometric linear theory. The model consists of a free energy function in order to represent the occurring energy storage and release effects. Furthermore, evolution equations for the inelastic strain tensor and the fraction of martensite are introduced. For the proposed system of constitutive equations, a stress algorithm is developed using a backward Euler method. In spite of the complexity of the constitutive theory, the development of an improved stress algorithm is successful. In this algorithm, the numerical integration of the constitutive theory requires only the solution of three nonlinear equations for three scalar-valued unknown variables. The thermomechanical behavior of structures is treated in the framework of an explicit finite element procedure. Numerical examples show the capability of the suggested model and the improved stress algorithm.

11:15 AM CC4.9
Fully Coupled 3-D Modelling of Ferroelectric Polycrystalline Behavior. Volkmar Mehling, Charalampos Tsakmakis and Dietmar Gross; Institute of Mechanics, Technical University Darmstadt, Darmstadt, Germany.

The electromechanical coupling effect shown by piezoelectric ceramics is used in a wide field for applications in actuation and sensoring. Piezoelectric materials with the capability of repolarization under high electrical or mechanical fields are called ferroelectrics. Their electromechanically coupled behavior is anisotropic and strongly nonlinear and therefore a challenge in constitutive modelling [1]. In this work a simple, macroscopic, fully coupled, three-dimensional model is presented, which is capable of reproducing all classical hysteresis effects of polycrystalline ferroelectric ceramics with tetragonal structure. Starting point is the additive decomposition of the strain tensor and the electric displacement into reversible and irreversible parts. For the piezoelectric part of the constitutive law an invariant formulation of the electric enthalpy function proposed by [3] is adopted and modified by the dependence on the magnitude of polarization. Following [1], irreversible strain and polarization are described as functions of a set of internal state variables. The choice of these variables is motivated by the assumption of a simple distribution function for the orientation of tetragonal unit cells within the polycrystal. By satisfying the second law of thermodynamics in the form of the Clausius-Duhem inequality, driving forces for the internal variables are derived. Using techniques from classical rate-independent metal plasticity theory a convex switching function combined with a normality rule is introduced. Saturation of strain and polarization is modelled by appropriately defined energy barrier functions [1,2] for the electromechanical enthalpy. The model has been implemented into a Matlab-based finite element code. Linear eight-node brick elements are used. Time-integration of evolution equations is performed by use of the implicit Euler-backwards integration. The constitutive equations are solved by the operator split method involving a piezoelectric predictor step and a ferroelectric general return algorithm. Numerical results show, that the model is able to reproduce the observed hysteretic behavior of ferroelectrics. [1] M.Kamlah. Ferroelectric and ferroelastic piezoceramics - modeling of electromechanical hysteresis phenomena. Continuum Mech. Thermodyn., 13(4):219–268, 2001. [2] C.M.Landis. Fully coupled, multi-axial, symmetric constitutive laws for polycrystalline ferroelectric ceramics. Journal of the Mechanics and Physics of Solids, 50:127-152, 2002. [3] J.Schroeder and D. Gross. Invariant formulation of the electromechanical enthalpy function of transversely isotropic piezoelectric materials. Archive of Appl. Mech., 73:533–552, 2004.

11:30 AM CC4.10
Simulation of Static Properties of Ferromagnetic Shape Memory Actuators in a Magnetic Field. Berthold Krevet and Manfred Kohl; IMT, Forschungszentrum Karlsruhe, Karlsruhe, Germany.

Smart materials like ferromagnetic shape memory alloys (SMA) allow the development of novel kinds of actuators, which perform complex operations with remarkable simple construction. As one application micromachined NiMnGa cantilevers have been developed which operate in an inhomogeneous magnetic field [1]. Static simulations of the mechanical response to an electrical heating current are an important prerequisite for design and optimization of such actuators. The simulation procedure is quite complex because the coupling of mechanical, electrical, thermal and magnetic properties has to be considered. In addition the results are influenced by mechanical and magnetic hysteresis effects. In the last years a simulation tool has been developed in IMT , which couples different kinds of FEM programs for calculation of hysteretic material behavior under multi field loading (electrical, thermal, mechanical) [2]. A two-phase shape memory model including history effects is implemented in the mechanical solver. The tool has already been used to calculate the behavior of conventional SMA microactuators loaded by heating with electrical currents [3]. In this work, we present simulations of the static properties of a cantilever in the inhomogeneous field of a permanent magnet as a function of heating current and compare it with experimental results. The ferromagnetic properties of the microactuator are taken into account by a magnetic field solver. The field of a permanent magnet is calculated along the trajectory of the microactuator, from which the magnetic forces and their gradients are derived with help of the material characteristics of NiMnGa. Thus, static force equilibrium can be defined allowing the position analysis of the actuator. For NiMnGa shows magnetic history effect, a magnetic hysteresis model, which describes the field dependent remanent magnetization is included. We show how the simulation tool will reveal the combined effect of magnetic and mechanical history. Extension possibilities to a time dependent analysis of the coupled problems for a full simulation of the dynamic behavior of the scanner are discussed. [1] M. Kohl, D. Brugger, M. Ohtsuka, T. Takagi, A novel actuation mechanism on the basis of ferromagnetic SMA thin films, Sensors and Actuators A 114 (2004) 445-450. [2] Krevet, B. and Kaboth, W., Coupling of FEM programs for simulation of complex systems, Proc. MSM 98, Santa Clara (1998), pp. 320-324. [3] Krevet, B. and Kohl, M., Finite element simulation of SMA microactuators with large deflection, J. Phys. IV France 115 (2004) 365-373.

11:45 AM CC4.11
Finite Element Analysis of the Non Linear Behavior of a Multilayer Piezoelectric Actuator. Mourad Elhadrouz, Tarak Benzineb and Etienne Patoor; LPMM UMR CNRS 7554, ENSAM, Metz, France.

Ferroelasticity and ferroelectricity are the non linear behaviours exhibited by piezoceramics, especially in the case of high electric field or stress. Many studies have focused on the role of ferroelastic and ferroelectric switching in fracture of actuators. However, engineering reliability analyses are carried out with tools like finite element software that do not take into account these non linear phenomena. To overcome such a problem, a simplified phenomenological constitutive law has been developed and describe the hysteresis effect of piezoceramics. It is time-independent and relies on the introduction of remnant polarization and remnant strain as internal variables. Two loading surfaces, similar to the ones used in plasticity, provide the evolution laws for the internal variables. Besides, polarization-induced anisotropy in the piezoelectric tensor is taken into account. That constitutive law has been implemented in the commercial software ABAQUS. It has been necessary to develop a finite element with electrical and mechanical degrees of freedom: it is an eight node hexahedron. The stiffness matrix integrates the constitutive law from the four tangent operators given by the constitutive law. The non linear problem is solved by the Newton method. This finite element tool is used to study the effects of applied voltage on the electroelastic field concentrations ahead of electrodes in a multilayer piezoelectric actuator. The study lies on the experimental observations made by Shindo et al. [1]. Electroelastic analysis on piezoceramics with surface electrode showed that high values of stress and electric displacement arose in the neighbourhood of the electrode tip. Thus, the strain, stress and electric displacement concentrations were calculated and the numerical results showed that ferroelectric switching arose in the area of the electrode tip, causing a change in remnant polarization and remnant strain. [1] Y. Shindo, M. Yoshida, F. Narita, K. Horiguchi, J. Mech. Phys. Solids, 52, 1109 1124, 2004.

SESSION CC5: Micro and Nano Modeling
Chair: Robert M. McMeeking
Wednesday Afternoon, March 30, 2005
Room 2020 (Moscone West)

1:30 PM *CC5.1
L. Eric Cross

Abstract Not Available

2:00 PM CC5.2
Micromechanical Modelling of Ferroelectric Films. John Huber, Engineering, University of Cambridge, Cambridge, United Kingdom.

Ferroelectric films are growing in significance as non-volatile memory devices, sensors and micro-actuators. The stress state of the film, induced by processing or constraints such as the substrate, strongly affects device behaviour. Thus it is important to be able to model the coupled and constrained behaviour of film material. This work presents a preliminary study of the application of micromechanical modelling to ferroelectric films. A self-consistent micromechanics model of ferroelectric behaviour has worked well for modelling bulk materials. What (if anything) can this approach contribute to understanding thin films? At first sight, the micromechanics model, which has no length scale, cannot distinguish bulk from thin film behaviour. However, by incorporating features such as grain structure, mechanical clamping by the substrate, residual stresses, and crystallographic orientation of the film, behaviour particular to films can be reproduced. Preliminary results are compared with the observed behaviour of films, and future directions in modelling are identified.

2:15 PM CC5.3
A Macroscopic Model for the Strain Dependence of the Ferromagnetic Critical Temperature in Manganites. Paolo Cermelli and Paolo Podio Guidugli; Mathematics, University of Torino, Torino, Italy.

Many rare-earth perovskite manganites of the form ReAMnO3, with Re a rare earth and A an alkali element such as Sr or Ca, are ferromagnetic metals at low temperature and paramagnetic insulators at high temperature. Their applicative interest lies in the fact that they exhibit 'colossal' magnetoresistance in the vicinity of the Curie temperature. It has been experimentally proved that these materials show a strong dependence of the critical temperature on strain, both when the material is chemically deformed by substituting the rare earth with elements with different atomic radii, [1] or by biaxial epitaxial strain [2]. Indeed, the effect of epitaxial strain is known to have dramatic consequences on the critical temperature of other perovskites, such as high-Tc superconductors [3]. In this work we propose a model for the epitaxial strain dependence of the ferromagnetic critical temperature of the perovskite manganites using the approach developed previously by us to describe the strain dependence of Tc in LaSrCO [4]. We use Born's approach to quantify the dependence of the interatomic distances within the perovskite unit cell on the macroscopic epitaxial strain, and this allows to study the variation of the critical temperature using a modified Ginzburg-Landau functional. [1] H. Y. Hwang, S-W. Cheong, P. G. Radaelli, M. Marezio and B. Batlogg, Lattice Effects on the Magnetoresistance in Doped LaMnO3, Phys. Rev. Lett. 75, 914-917 (1995) [2] A. J. Millis, T. Darling and A. Migliori, Quantifying strain dependence in "colossal" magnetoresistance manganites, Journal of Applied Physics, 83, 1588-1591, 1998 [3] J.-P., Locquet, J. Perret, J. Fompeyrine, E. Maechler, J.W. Seo, G. Van Tendeloo, Doubling the critical temperature of La1.9Sr0.1CuO4 using epitaxial strain. Nature, 394, 453, 1998 [4] P. Cermelli and P. Podio Guidugli, Modeling deformation effects on Tc in epitaxial films of La1.9Sr0.1CuO4, Physica C, 371, 117-128 (2002)

2:30 PM CC5.4
Effect of Texture Distribution on Electromechanical Behavior of Barium Titanate. Jennifer Lynn Ruglovsky, Kaushik Bhattacharya and Harry A. Atwater; California Institute of Technology, Pasadena, California.

The ability to comprehensively model and realize ferroelectric thin film devices requires a detailed consideration of both microscopic structure and phenomena on many length scales. In this paper, we consider the effect of the grain-scale mosaic spread in the crystallographic texture and in-plane orientation on the device-scale piezoeoelectric displacement achievable in thin film electromechanical devices. Our method enables the effective piezoelectric displacement to be obtained for a polycrystalline film. The grain orientations in a ferroelectric polycrystal can be described by rotations by Euler angles relative to a single crystal. The grain orientation distribution is assumed to be described by a Gaussian distribution when considered at the device scale, with texture ranging from that of a single-crystal to completely isotropic polycrystalline film. The effective electromechanical properties, characteristic of piezoelectric materials and governed by constitutive equations for stress and electric displacement of such an aggregate of grains, can be modeled using a self-consistent approach. The essence of the self-consistent approach is to use the electromechanical field for a single grain embedded in a matrix -with yet-to-be-determined uniform effective moduli- to simulate the electromechanical field in a grain at a particular orientation in the film. The total effective properties are found via numerical iteration over all grain orientations.[1] Our investigation focuses on application of the above-mentioned method to polycrystalline barium titanate (BTO) characterized by Gaussian distributed in-plane texture and out-of plane texture. Thus there are four microstructure states that serve as reference points for relating film microstructure to electromechanical device behavior - - 1. a single crystal thin film, 2. a biaxially textured thin film, 3. a fiber textured thin film, and 4. a randomly-oriented (nearly isotropic but still piezoelectric) thin film. For example, a film with random in-plane orientation and a 60^o full-width-half-max distribution in out-of-plane grain orientation (state 3) shows a 10% increase in the piezoelectric constant d_{33}, as compared to the single crystal case. Quantitative experimental measurements of texture of BTO films have been obtained using reflective high energy electron diffraction (RHEED) and a RHEED-based software analysis program.[2] This experimental method enables grain orientation distribution measurements that can be fitted to the model. The device-scale displacement behavior of thin film cantilever devices will be discussed and related to film grain orientation distribution. Ultimately using a combined theory/experiment approach, knowledge of thin film crystallographic structure can be used to predict device-scale electromechanical performance. 1. Li, MechMat 36, (2004) 949-958 2. Hartman et al., JAP 92, 9 (2002) 5133-5139

2:45 PM CC5.5
Multiscale Study of Ferroelectrics with Advanced Diffraction Techniques. Ersan Ustundag[1], Robert Rogan[1,2], Maziar Motahari[1,2], Nobumichi Tamura[3], Lawrence Margulies[4], Henning Poulsen[4], Ulrich Lienert[5] and Mark Daymond[6]; [1]Ames Laboratory and Department of Materials Science and Engineering, Iowa State University, Ames, Iowa; [2]Materials Science, California Institute of Technology, Pasadena, California; [3]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California; [4]Materials Research Department, Riso National Laboratory, Roskilde, Denmark; [5]Advanced Photon Source, Argonne National Laboratory, Argonne, California; [6]Mechanical and Materials Engineering, Queens University, Kingston, Ontario, Canada.

Ferroelectric materials exhibit a complicated behavior in response to both electrical and mechanical loads which produce large internal stresses that eventually lead to failure. While many measurements have been conducted on the macroscopic response of single-crystals or polycrystals, multiaxial (and multiscale) data about the in-situ internal strain and texture response of these materials are lacking. Yet this information is critical to the development of accurate models, and diffraction techniques which directly measure internal lattice strains and material texture are aptly suited to supply it. A neutron diffraction technique was employed for the simultaneous measurement of material texture and lattice strains in directions parallel and transverse to an applied mechanical load. By comparing the behaviors of various Pb(Zr,Ti)O3 or PZT compositions, information concerning the bulk, macroscopic behavior was inferred. To probe the multiaxial constitutive behavior, a high-energy X-ray diffraction technique was also employed. Using transmission geometry and a two-dimensional detector, multiple directions of sample response were measured simultaneously. At a smaller scale, a novel XRD technique (called '3-D XRD') was used to probe the mesoscale constitutive behavior of single, embedded grains of BaTiO3 within a polycrystalline matrix. Finally, polychromatic scanning X-ray microdiffraction was used to investigate the microscale three-dimensional strain tensor in single crystals at the domain level. We present an example experiment which recorded the domain switching mechanisms activated to accommodate indentation-induced fracture stresses in single crystal BaTiO3. The novel experimental methods presented in this talk provide access to two- and three-dimensional multiaxial constitutive behavior in ferroelectrics for each of the microscopic, mesoscopic, and macroscopic length scales ranging from sub-?m to cm. Results from each of these length scales yield critical data for mechanics model validation.

3:30 PM *CC5.6
Continuum Level Modeling of Linear Ferroelectro-magnetic Materials. Greg P. Carman, MAE, UCLA, Los Angeles, California.

Since the discovery of piezoelectricity and magnetostriction over a century ago, the use of these materials has become pervasive throughout society (e.g. sonar, lighters, accelerometers). Such use has been predicated primarily upon the transduction ability of these materials, and has proceeded to the sub-continuum levels in the research community. More recently single-phase materials capable of responding mechanically to either an electric or magnetic stimulus, so called ferroelectro-magnets, have generated excitement within the scientific community. While applications for ferroelectro-magnetic materials include those of both the parent ferroelectric and ferromagnetic materials (e.g. signal transduction, actuation, damping, energy harvesting, etc.), a whole new range of uses can be envisaged through the extra degree of freedom provided by the coupling between polarization and magnetization. This paper presents the governing equations for the continuum mechanics of electro-magneto-elastically coupled materials along with a criterion for establishing the uniqueness of their solutions. General relations are given for the individual coupling coefficients encountered in the present study. An analytical solution for the case of a two-dimensional beam experiencing simultaneous field and mechanical loadings is subsequently provided. From this result an equivalent theory is drawn for describing the ability of ferroelectro-magnets to convert and store input energy or energies and highlight the candidacy of ferroelectro-magnets for specific applications.

4:00 PM CC5.7
Effective Piezoelectric Constants of Epitaxial Ferroelectric Films as MEMS Transducers. Jun Ouyang[1], Ramamoorth Ramesh[2,1] and Alexander Roytburd[1]; [1]Materials Research and Science Engineering Center, Dept. of Materials Science and Engineering, University of Maryland, College Park, Maryland; [2]Dept. of Materials Science and Engineering, University of California, Berkeley, California.

The effective converse and direct piezoelectric constants of an epitaxial ferroelectric film are generally formulated, which can help to predict and optimize the performance of MEMS transducers (sensors and actuators) made by ferroelectric thin films. Based on available experiment data, numerical results are obtained for lead zirconate titanate and lead titanate-relaxor solid solution ferroelectric films.

4:15 PM CC5.8
First-principles Theory of Interfacial Electronic Structures and Energy Barriers in Electroceramic Thin-film Devices. Christian Elsaesser[1], Matous Mrovec[1], Jan-Michael Albina[1] and Bernd Meyer[2]; [1]Fraunhofer-Institut fuer Werkstoffmechanik, Freiburg, Germany; [2]Lehrstuhl fuer Theoretische Chemie, Ruhr-Universitaet Bochum, Bochum, Germany.

Nanostructured thin-film devices on the basis of electroceramic perovskite-type oxides have very promising structural, physical and chemical properties for highly integrated functional components, e.g., in computer technology, like high-density dynamic random access memory (RAM) devices made of (Ba,Sr)TiO3, or novel non-volatile ferroelectric Pb(Zr,Ti)O3 RAM devices. Critical issues in such systems are the interfacial structure, adhesion and electrical barriers at the contacts of the electroceramic thin films to conducting metallic electrodes (e.g., Pt, SrRuO3), and to insulating inorganic substrates (e.g., SrTiO3, LaAlO3). First-principles electronic-structure calculations, by density functional theory and the mixed-basis pseudopotential method, were carried out to analyse interfacial Schottky barriers and band offsets at planar and coherent perovskite/metal and perovskite/perovskite contacts. Influences of different electrode materials, varying chemical film compositions and interface terminations on the interfacial energy barriers will be discussed. This work is supported by the German Research Foundation (DFG) within the Priority Program "Integrated electroceramic functional structures".

4:30 PM CC5.9
Atomistic Simulations of Barium Titanate: Phases, Domain Walls and Oxygen Vacancies. Qingsong Zhang, Tahir Cagin and William A. Goddard; California Institute of Technology, Pasadena, California.

We present the Polarizable Charge Equilibration (P-QEq) force field to include self-consistent atomic polarization and charge transfer in molecular dynamics of materials. The short-range Pauli repulsion effects are described by two body potentials without exclusions. A linear self-consistent field solution to the charge transfer is proposed for charge transfer in large systems. The P-QEq is parameterized for BaTiO3 based on quantum mechanics calculations (DFT with GGA) and applied to the study of the phase transitions, domain walls and oxygen vacancies. Frozen phonon analysis reveals that the three high-temperature BaTiO3 phases in the displacive model are unstable. Within their corresponding macroscopic phase symmetries, the smallest stable phase structures are achieved by antiferroelectric distortions from unstable phonons at the Brillouin zone boundaries. The antiferroelectric distortions soften phonons, reduce zero point energies and increase vibrational entropies. A correct BaTiO3 phase transition sequence and comparable transition temperatures are obtained by free energy calculations. The inelastic coherent scattering functions of these phases agree with X-ray diffraction experiments. BaTiO3 180 degree domain wall is Ba-centered with abrupt polarization switching across the wall. The center of BaTiO3 90 degree domain wall is close to its orthogonal phase. There are transition layers from the wall centers to the internal domains in the types of domain walls. Polarization variation in these transition layers induces polarization charge and free charge transfer. This effect causes a strong bipolar electric field in BaTiO3 90 degree domain wall. Oxygen vacancies are frozen at room temperature, and mobile near the Curie temperature. In the tetragonal phase, the broken Ti-O chains are frozen, reducing switchable polarization. Due to charge redistribution and local relaxation, oxygen vacancy interaction is short-range and anisotropic. Two oxygen vacancies can form a stable pair state, where two broken Ti-O chains are aligned parallel. Oxygen vacancy clusters can form dendritic structures as a result of local relaxation and charge interaction.

4:45 PM CC5.10
Phase Diagrams of Epitaxial BaTiO3 Ultrathin Films from First Principles. Bo-Kuai Lai, Physics, U of Arkansas, Fayetteville, Arkansas.

In the past two decades, the potential of ferroelectric thin films for applications such as next generation dynamic random access memories (DRAM), nonvolatile ferroelectric random access memories (FeRAM) and integrated radio-frequency and microwave devices has attracted a lot of research interest. To incorporate ferroelectric thin films into current semiconductor processing technology, one has to choose suitable substrates, electrodes, buffer layers and a thermal processing to deposit high-quality films ranging from several micrometers down to several monolayers. The use of substrates and thermal processing inevitably introduces strains into films, which can significantly affect their properties. For instance, paraelectric-to-ferroelectric transition temperatures that are higher than the one of the corresponding bulk material have been reported for epitaxial thin films under some tensile and compressive strains. Furthermore, uncompensated depolarization field also occurs inside a thin film when the screening of polarization-induced charges at the electrode/film and/or buffer layer/film interface is only partially accomplished. Such internal field can dramatically affect properties of ferroelectric thin films too, and has been a major issue for controlling polarization behavior in ferroelectric memory field-effect transistors. In fact, many other factors (e.g., thickness, surface termination, interface roughness, charge transfer at the free surface and interface) have also been associated with the decrease in dimensionality when going from bulk to thin films. However, the experimental evaluation of the effect of each factor on physical properties is extremely difficult, because the properties of real thin films are a combined result of these factors. Theoretical study is, thus, important to untangle these factors and can provide fundamental insights into thin films. A first-principles-based scheme is used to investigate effects of surface/interface, thickness and electrical boundary conditions on the temperature-misfit strain phase diagrams of epitaxial (001) BaTiO3 ultrathin films. In addition to provide detailed quantitative predictions, our calculations also yield three main qualitative results. Under ideal short-circuit (SC) conditions, (1) the existence of a surface/interface results in a asymmetric phase diagram and (2) increasing the film thickness leads to a decrease of such asymmetry. (3) Under non-ideal SC conditions, phase transitions leading to the activation of an out-of-plane component of the polarization occur at lower temperatures. Our calculation approach can also be applied to PZT and BST ultrathin films. The former is used in its ferroelectric phase for FeRAM applications while the later is used in their paraelectric phase for DRAM and RF applications. Both films requires strict processing control of strain, temperature and interface/surface to achieve desired properties.

SESSION CC6: Design of Smart Materials
Chair: Greg P. Carman
Thursday Morning, March 31, 2005
Room 2020 (Moscone West)

8:30 AM CC6.1
Transferred to CC4.1

8:45 AM CC6.2
Phase Field Simulations of Domain Structures in Epitaxial Nanostructured Ferroelectrics with Different Sizes. Jie Wang and Tong-Yi Zhang; Department of Mechanical Engineering, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China.

Epitaxially ferroelectric islands and thin films at the nanometer scale are attracting considerable attention due to the potential migration of microelectronics to nanoelectronics. The ferroelectric properties of nanostructured ferroelectrics substantially deviate from their bulk counterparts. The size-dependent properties are stemmed from the size-dependent domain structures. In the present work, we use a phase field model that incorporates the long-range elastic and electrostatic interactions to investigate the size-dependent domain structures and the polarization instability in a two-dimensional epitaxially ferroelectric island, which shape is represented by its width and thickness. The island can be approximately treated as a film if its width is much larger than its thickness. The spatial distributions of polarizations are simulated for the epitaxial ferroelectrics with different sizes and different thickness-to-width ratios. There is a critical thickness, at which a ferroelectric inland changes from a multi-domain structure to a single-domain state, and the critical thickness is dependent on the thickness-to-width ratio. Different kinds of domain walls are formed due to the elastic constraint of the substrate and the depolarization field with varying thickness-to-width ratio.

9:00 AM *CC6.3
Manufacture of Shape Memory Alloy Honeycombs by Transient-Liquid Reactive Joining. John Shaw[1], David Grummon[2] and John Foltz[2]; [1]Aerospace Engineering, University of Michigan, Ann Arbor, Michigan; [2]Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan.

A method is presented to construct light-weight, cellular structures from simple commercially-available, wrought, NiTi-based (Nitinol) shape memory alloy (SMA) elements. The method consists of a reactive-brazing process that can be used to create a robust metallurgical bond between Nitinol and itself, or between Nitinol and some other metals and ceramics. This process facilitates the fabrication of a variety of sparse built-up structures, including cellular SMAs, meshes, and space frames. The internal structure can be designed and tailored to the needs of the application and can be made arbitrarily light-weight. So far, prototype honeycombs have been fabricated and demonstrated. Such structures can be designed to be less than 10% dense, for example, yet retain the adaptive properties of the underlying SMA material (shape memory effect and superelasticity). The combination of the sparse topology of a cellular solid and the adaptive properties of an SMA represents a new class of materials that can be used as light-weight passive or adaptive structural elements that respond to changes in external loads and temperature. In addition, the sparse topology should lead to an order of magnitude improvement in thermal response time and recoverable strain capability as compared to monolithic (100% dense) Nitinol. Potential applications include reusable energy absorbing structures, highly resilient structures, light-weight armor, thermal actuation materials, vibration isolation, and biomedical implants, to name a few. These materials have potential broad application in the aerospace, automotive, energy, and biomedical industries.

9:30 AM *CC6.4
Magneto-Electric Coupling in Self-Assembled Complex Oxide Films. Florin Zavaliche[1,2], H. Zheng[1,3], Y. Qi[3], L. Mohaddes-Ardabili[1,3], D. G. Schlom[5] and R. Ramesh[1,4]; [1]Materials Science and Engineering, University of California, Berkeley, California; [2]Materials Research Science and Engineering Center, University of Maryland, College Park, Maryland; [3]Materials Science and Engineering, University of Maryland, College Park, Maryland; [4]Physics, University of California, Berkeley, California; [5]Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania.

Multiferroics are materials which show multiple order parameters, associated with the presence of a rich spectrum of functional responses including ferroelectricity and magnetism. A recent development has been the discovery of the formation of spontaneously assembled nanostructures consisting of a $CoFe_2O_4$ ferrimagnetic phase embedded in a $BiFeO_3$ ferroelectric matrix. This involves 3-dimensional heteroepitaxy between the substrate, the matrix perovskite phase, and the spinel phase that is embedded as an array of single crystalline pillars in this matrix. This epitaxial coupling leads to the coexistence of ferroelectricity and magnetism in the same material, and a strong magneto-electric coupling mediated by the lattice elastic strain is expected. Indeed, our experimental observations point at a strong coupling between the matrix ferroelectric order and pillars magnetization. By a combined piezoelectric – magnetic force microscopy technique we were able to observe reversible magnetization switching in the $CoFe_2O_4$ pillars at ambient conditions solely as the result of changing the polarization in the ferroelectric $BiFeO_3$ matrix. Conversely, changes of the dielectric constant were measured by microwave microscopy upon the application of an ac magnetic field. We conclude that the 3D epitaxial growth of self-assembled ferrimagnetic and ferroelectric phases leads to a strong coupling between the order parameters of the two phases. This work has been supported in part by the U. of Maryland NSF-MRSEC under grant #DMR 00-80008, and by the ONR under a MURI program.

10:30 AM *CC6.5
Magnetic Tweed Contrast in Ferromagnetic Shape Memory Alloys. Marc De Graef, Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania.

Recent advances in high resolution imaging of magnetic patterns (domains and microstructure) such as magnetic force microscopy (MFM) and Lorentz microscopy have revealed fascinating modulated magnetic patterns both above and below the Curie temperature in certain magnetic alloys. They can be termed "magnetic tweed", in analogy with structural tweed familiar so far in the context of some ferroelastic transitions. Based on experimental observations of modulated magnetic patterns in a $Co_{0.5}Ni_{0.205}Ga_{0.295}$ alloy, we propose a model to describe (purely) magnetic tweed and a magnetoelastic tweed. The former arises above the Curie (or Néel) temperature due to magnetic disorder. The latter results from compositional fluctuations coupling to strain and then to magnetism through the magnetoelastic interaction above the structural transition temperature. We discuss the origin of purely magnetic and magnetoelastic precursor modulations and their experimental thermodynamic signatures. We will present experimental evidence for the existence of magnetoelastic tweed in the form of Lorentz transmission electron microscopy images.

11:00 AM *CC6.6
A Way to Search for New Smart Materials with "Unlikely" Combinations of Physical Properties. Richard D. James[1], Zhiyong Zhang[1] and Jun Cui[2]; [1]Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, Minnesota; [2]Materials Science and Engineering, University of Maryland, College Park, Maryland.

Recent first principles' studies give a clear understanding of why the simultaneous occurrence of ferromagnetism and ferroelectricity is unlikely. While these studies usually do not consider the possibility of a phase transformation, there is a lot of indirect evidence that, if the lattice parameters are allowed to change a little, then one might have co-existence of "incompatible properties" like ferromagnetism and ferroelectricity. Thus, one could try the following: seek a reversible first order phase transformation, necessarily also involving a distortion, from, say, ferroelectric to ferromagnetic phases. If it were highly reversible, there would be the interesting additional possibility of controlling the volume fraction of phases with fields or stress. The key point is reversibility. Even big first order phase changes can be highly reversible (liquid water to ice, some shape memory materials), and we argue that it is the nature of the shape change that is critical. We suggest, based on a close examination of measured hysteresis loops in various martensitic systems, that reversibility is governed by the presence of certain special relations among lattice parameters. We give a example of the systematic use of these relations to discover new low hysteresis shape memory materials. Besides ferroelectricity – ferromagnetism, there are many potential property pairs that exhibit lattice parameter sensitivity and are candidates for the proposed strategy: soluability for hydrogen, optical nonlinearity, high band gap – low band gap semiconductors, insulator – conductor (electrical or thermal), opaque – transparent (at various wavelengths), high – low index of refraction, luminescent – nonluminescent, and new kinds of thermoelectric and thermomagnetic material.

11:30 AM *CC6.7
Magnetoelectric Composite Materials Promising High Magnetic Field Sensitivity and High Voltage Gain. Shuxiang Dong, Junyi Zhai, Feiming Bai, Zhengping Xing, Naigang Wang, Li Yan and Jie-Fang Li; Materials Science & Engineering, Virginia Tech, Blacksburg, Virginia.

We have found that laminates of longitudinally-magnetized magnetostrictive Terfenol-D and Fe-Ga layers and longitudinally-poled piezoelectric $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ crystal and $Pb(Zr,Ti)O_3$ ceramic have giant magnetoelectric voltage coefficients of up to 550 mV/Oe under low magnetic bias. That will gramatically increase to the maximum value of up to 60V/Oe, when they operate at resonance frequency points. In resonance frequency points, these laminates also presented a strong voltage gain effect. In addition, an ultrahigh magnetic field sensitivity of near 10^{-12} Tesla has been observed at room temperature.