

2ND SEMINAR ON FERROIC FUNCTIONAL MATERIALS

AND

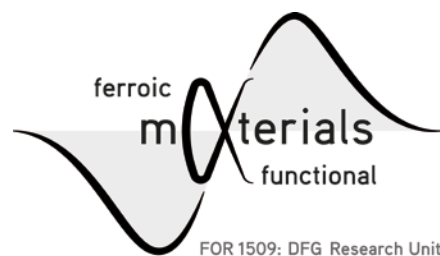
**12TH INTERNATIONAL WORKSHOP ON DIRECT AND INVERSE PROBLEMS IN
PIEZOELECTRICITY**

OCTOBER 4 - 6, 2016

**FRIEDRICH-ALEXANDER-UNIVERSITÄT
ERLANGEN-NÜRNBERG, GERMANY**

PROGRAM AND BOOK OF ABSTRACTS

ORGANIZED BY: P. STEINMANN, D.C. LUPASCU, F. ENDRES



PREFACE

The joint seminar is dedicated to the diverse fields of ferroic materials including ferroelectricity, ferromagnetism and combined multiferroic materials. It covers mathematical modeling, experimental methods and industrial applications of ferroic materials and devices.

Aim of the combined seminar is to contribute to open problems in:

- numerical simulation (direct and inverse analysis)
- advanced material characterization
- discussion of fatigue, damage, cracks and reliability
- manufacturing processes and
- performance of piezoelectric devices

The overall intention of the workshop is to bring together experts from different fields of research such as engineering, applied mathematics, and materials science, as well as from the industrial sector.

The 2nd Seminar on Ferroic Functional Materials and the 12th International Workshop on Direct and Inverse Problems in Piezoelectricity will continue the previous workshops/ seminars that were animated by lively discussions from numerous participants.

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Bai-Xiang Xu (TU Darmstadt)

LOCATIONS

The seminar/ workshop will be held at the Technical Faculty of the University of Erlangen-Nuremberg in Erlangen. Erlangen is easy to reach by plane via Nuremberg-Airport or by train. Tickets for the free usage of the public transport in Erlangen are included in the conference fee.

The registration and the coffee breaks are at the LTM seminar room:

SR TM –Seminar room LTM

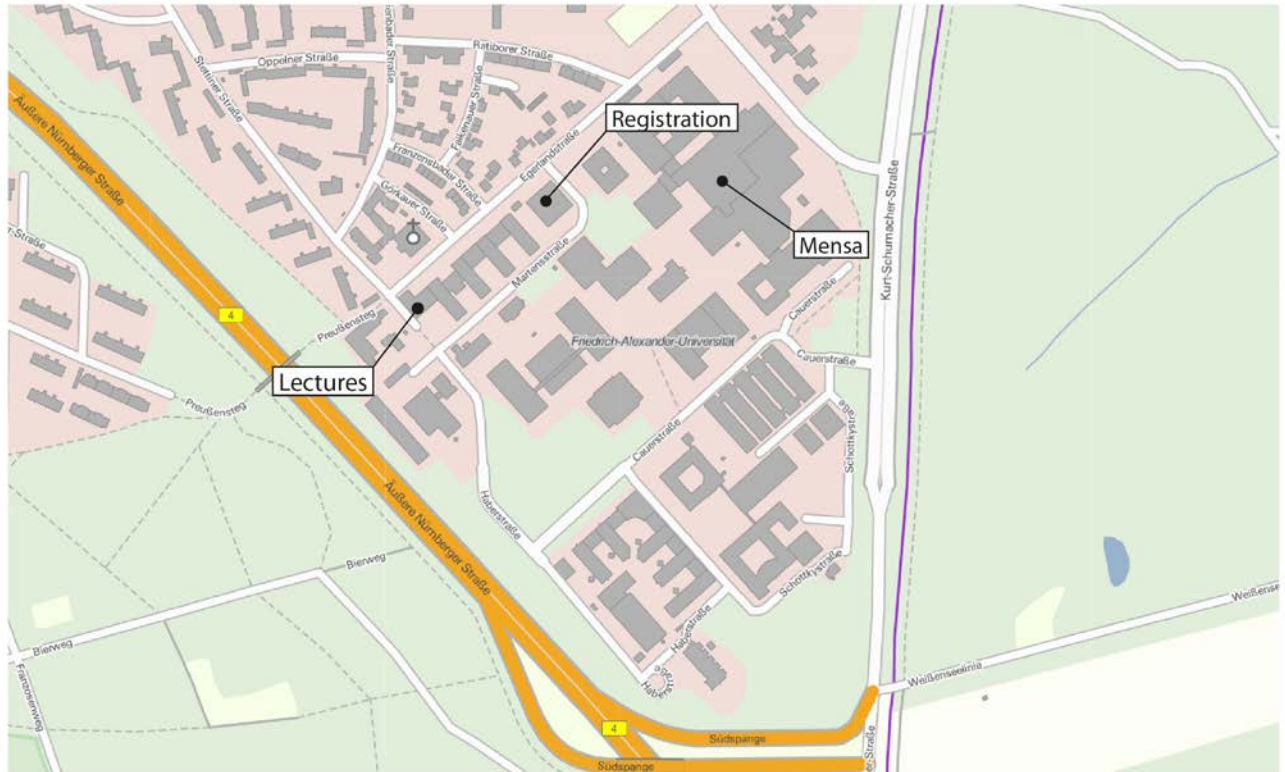
Room: 0.044

Egerlandstraße 5, 91058 Erlangen



The lectures are at the lecture room H17:

H17 Maschinenbau
Hörsaal Maschinenbau
Haberstraße 1, 91058, Erlangen



The Conference Dinner takes place at the Steinbach Brauerei:

Steinbach Bräu
Vierzigmannstr. 4 , 91054 Erlangen



PROGRAM

	Tuesday 4 th October	Wednesday 5 th October	Thursday 6 th October
08:30		Manuel Weiß	Paul Dunst
08:45			
09:00		S.S. Nanthakumar	Neamul Khansur
09:15			
09:30		Vishal Boddu	Heiko Wende
09:45			
10:00		Coffee Break	Coffee Break
10:15			
10:30		Dinesh Dusthakar	Bai-Xiang Xu
10:45			
11:00	Registration	Karsten Buckmann	Min Yi
11:15			
11:30		Stephan Lange	Marius Wingen
11:45			
12:00			
12:15	Coffee Break	Lunch Break	Lunch Break
12:30			
12:45	Welcome		
13:00	Keynote: Meinhard Kuna	Keynote: Andrew Bell	Barbara Kaeswurm
13:15			
13:30			
13:45	Sergii Kozinov		Benjamin Jurgelucks
14:00			
14:15	Artjom Avakian	Harsh Trivedi	
14:30			Michael Nierla
14:45	Michael Wünsche	Di Chen	
15:00			Closing
15:15	Coffee Break	Coffee Break	
15:30			
15:45	Hans-Dieter Alber	Jan Sladek	
16:00			
16:15	Ashish Sridhar	Matthias Labusch	
16:30			
16:45	Shuai Wang	Matthias Rambašek	
17:00			
17:15	David Schrade		
17:30			
17:45			
18:00		Social Program Guided City Tour: Erlangen	
18:15			
18:30			
18:45			
19:00		Conference Dinner Steinbach Bräu (open end)	
19:15			
19:30			
19:45			
20:00			
20:15			

Location:

Registration	SR TM -Seminar room LTM Room: 0.044 Egerlandstraße 5, 91058 Erlangen
Coffee Break	

↕ 3 minutes walking distance

Welcome	H17 Maschinenbau Hörsaal Maschinenbau Haberstraße 1, 91058 Erlangen
Keynote Lectures	
Talks	

Tuesday 4th October

13:00 - 13:45 **Fracture mechanics modeling of ferroelectric materials**
Meinhard Kuna

13:45 - 14:15 **Failure simulation of ferroelectric ceramics under cyclic electromechanical loading**
Sergii Kozinov, Meinhard Kuna

14:15 - 14:45 **Numerical simulation of magnetoelectric coupling including damage in multiferroic composites applying phenomenologically and physically motivated constitutive models**
Artjom Avakian, Andreas Ricoeur

14:45 - 15:15 **Investigations of dynamic crack problems in functionally graded piezoelectric materials by a TDBEM**
M. Wünsche, J. Sladek, V. Sladek, Ch. Zhang

15:15 - 15:45 *Coffee Break*

15:45 - 16:15 **A study of different phase field models for the evolution of phase interfaces in solids by numerical computations**
Hans-Dieter Alber

16:15 - 16:45 **A Phase field Approach For Large Deformation Magneto-Mechanically Coupled Material Response**
A. Sridhar, M.-A. Keip, C. Miehe

16:45 - 17:15 **Phase field simulation of layered relaxor/ferroelectric composite with diffusive interface**
Shuai Wang, Bai-Xiang Xu

17:15 - 17:45 **Phase field simulations of ferroelectric/ferromagnetic heterostructures**
David Schrade

Wednesday 5th October

08:30 - 09:00 **Simulation-based homogenization and characterization of piezoelectric actuators**
Manuel Weiß, Stefan J. Rupitsch, Reinhard Lerch

09:00 - 09:30 **Topology Optimization of Piezoelectric Nanostructures**
S.S. Nanthakumar, Xiaoying Zhunag, Harold S. Park, Tom Lahmer, Timon Rabczuk

09:30 - 10:00 **Molecular dynamics simulations of domain wall movement in BaTiO₃ single crystals**
Vishal Boddu, Florian Endres, Paul Steinmann

10:00 - 10:30 *Coffee Break*

10:30 - 11:00	External stress-dependent response of ferroelectric materials based on a sequential laminate approach <u>D.K. Dusthakar</u> , A. Menzel, B. Svendsen
11:00 - 11:30	A Micromagnetics Inspired Approach for the Macroscale Finite Element Analysis of Magnetostrictive Materials <u>Karsten Buckmann</u> , Björn Kiefer, Thorsten Bartel, Andreas Menzel
11:30 - 12:00	A condensed micromagneto-electromechanical approach to model the constitutive behavior of ferroelectric, ferromagnetic and multiferroic materials <u>Stephan Lange</u> , Andreas Ricoeur
12:00 - 13:30	<i>Lunch Break</i>
13:30 - 14:15	The Evolution of a New Piezoelectric Material <u>Andrew Bell</u>
14:15 - 14:45	Microscopic perspective of magnetoelectric effect in multiferroic composites <u>Harsh Trivedi</u> , Vladimir V. Shvartsman, Doru C. Lupascu, Robert C. Pullar, Andrei Kholkin, Pavel Zelanovskiy, Vladimir Shur
14:45 - 15:15	Magnetostrictive-piezoelectric coupling of COFe₂O₄ nanopillars embedded in a BaTiO₃ matrix <u>Heiko Wende</u>
15:15 - 15:45	<i>Coffee Break</i>
15:45 - 16:15	Analyses of coated fibrous composites with piezoelectric and piezomagnetic phases <u>Jan Sladek</u> , Vladimir Sladek, Chuanzeng Zhang, Michael Wünsche
16:15 - 16:45	A multiscale homogenization approach for the characterization of nonlinear magneto-electric composites <u>M. Labusch</u> , J. Schröder
16:45 - 17:15	Magnetorheological elastomers: from multiscale characterization towards macroscopic devices <u>Matthias Rambauser</u> , Marc André Keip
Thursday 6th October	
08:30 - 09:00	Numerical and Experimental Investigation of Pre-Stress in Ultrasound Transducers <u>Paul Dunst</u> , Tobias Hemsel, Walter Sextro
09:00 - 09:30	Contrasting strain mechanisms in lead-free piezoelectric ceramics <u>Neamul H. Khansur</u> , Kylie G. Webber, John E. Daniels

09:30 - 10:00	<p>Experimental Investigation of Stain Distributions in Lead-based and Lead-free Ferroelectrics by Digital Image Correlation</p> <p><u>Di Chen</u>, Azatuhi Ayrikyan, Kyle G. Webber, Marc Kamlah</p>
10:00 - 10:30	<i>Coffee Break</i>
10:30 - 11:00	<p>Monte Carlo simulations of relaxor ferroelectrics based on Ginzburg-Landau type effective Hamiltonian</p> <p><u>Bai-Xiang Xu</u>, Yang-Bin Ma, Karsten Albe</p>
11:00 - 11:30	<p>Charge-mediated magnetoelectric coupling for 180 degree switching in nanomagnets: a multiscale study</p> <p><u>Min Yi</u>, Bai-Xiang Xu</p>
11:30 - 12:00	<p>Temperature changes in ferroelectric materials due to domain switching and their influence on mechanical fields</p> <p><u>Marius Wingen</u>, Andreas Ricoeur</p>
12:00 - 13:30	<i>Lunch Break</i>
13:30 - 14:00	<p>Mechanically induced ferroelectric long range order in relaxor ferroelectrics</p> <p><u>B. Kaeswurm</u>, F.H. Schader, K.G. Webber</p>
14:00 - 14:30	<p>Increasing the sensitivity of impedance with respect to material parameters of triple-ring electrode piezoelectric transducers using algorithmic differentiation</p> <p><u>Benjamin Jurgelucks</u>, Leander Claes</p>
14:30 - 15:00	<p>Stageless evaluation of a vector Preisach model on the basis of rotational operators</p> <p><u>M. Nierla</u>, A. Sutor, S.J. Rupitsch, M. Kaltenbacher</p>

ABSTRACTS

A study of different phase field models for the evolution of phase interfaces in solids

Hans-Dieter Alber^{a,*}

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Abstract

We present the results of numerical computations based on different models for the evolution of phase interfaces in solids in some simple, but critical model situations [1].

References

- [1] Hans-Dieter Alber. Asymptotics and numerical efficiency of the allen-cahn model for phase interfaces with low energy in solids. *arXiv preprint arXiv:1505.05442*, 2015.

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Numerical simulation of magnetoelectric coupling including damage in multiferroic composites applying phenomenologically and physically motivated constitutive models

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Abstract

The coupling of magnetic and electric fields due to the constitutive behavior of a material is commonly denoted as magnetoelectric effect. The latter is only observed in a few crystal classes exhibiting a very weak coupling, mostly at low temperatures, which can hardly be exploited for technical applications. Much larger coupling coefficients are obtained at room temperature in composite materials with ferroelectric and ferromagnetic constituents. The magnetoelectric effect is then induced by the strain of matrix and inclusions converting electrical and magnetic energies based on the piezoelectric and magnetostrictive effects.

In this paper, the constitutive modeling of nonlinear multifield behavior as well as the finite element implementation are presented [1, 2]. Nonlinear material models describing the magneto-ferroelectric or electro-ferromagnetic behaviors are presented. Both physically and phenomenologically motivated constitutive models have been developed for the numerical calculation of principally different nonlinear magnetostrictive behaviors. Further, the nonlinear ferroelectric behavior is based on a physically motivated constitutive model. On this basis, the polarization in the ferroelectric and magnetization in the ferromagnetic and magnetostrictive phases, respectively, are simulated and the resulting effects analyzed. Additionally, the ferroelectric model accounts for damage due to microcrack growth. Numerical simulations focus on the calculation of magnetoelectric coupling and on the prediction of local domain orientations as well as damage processes going along with the poling process, thus supplying information on favorable electric-magnetic loading sequences.

References

- [1] A. Avakian, R. Gellmann, and A. Ricoeur. Nonlinear modeling and finite element simulation of magnetoelectric coupling and residual stress in multiferroic composites. *Acta Mechanica*, 226:2789–2806, 2015.
- [2] A. Avakian and A. Ricoeur. Constitutive modeling of nonlinear reversible and irreversible ferromagnetic behaviors and application to multiferroic composites. *Journal of Intelligent Material Systems and Structures*, 2016.

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The Evolution of a New Piezoelectric Material

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Abstract

The commercial introduction of a completely new piezoelectric material is a relatively rare event, understandably so, given the excellence of the existing materials. Notwithstanding the continuing efforts to identify lead-free alternatives to market leader PZT, there are numerous applications for which PZT does not meet the performance requirements. Perhaps first amongst those is operation at temperatures above 200°C. This presentation will recount the 10 year scientific development of a family of higher operating temperature piezoelectric ceramics based on BiFeO₃. Just as in PZT, proximity to a morphotropic phase boundary provides the largest charge coefficients. However, maximising domain wall contributions, through optimising spontaneous strain, needs to be achieved whilst avoiding the onset of relaxor behaviour. Inevitably the inclusion of lead, in the form of a PbTiO₃ component cannot be avoided, if acceptable performance is to be achieved. The demand for high temperature ultrasound transducers for applications, such as continuous structural health monitoring, has provided a ready route to market for the material and some of the issues of modifying known device technologies for higher temperature operation will be addressed. Finally, scale up to even moderate batch sizes is shown to be challenging, especially the control of stoichiometry in a ternary solid solution containing three relatively volatile cations.

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Molecular dynamics simulations of domain wall movement in BaTiO₃ single crystals

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Abstract

Ferroelectric functional materials are used in a countless number of applications due to the electro-mechanical coupling properties of such materials. Therefore, ferroelectrics have been studied for several decades and the macroscopic material behavior can be accurately predicted by continuum models. Due to recent advancements in manufacturing technologies the simulation of the material behavior of ferroelectrics at the nano scale is of significant importance not only to predict the material behavior but also to understand the material behavior in general. For example the simulation of domain switching in advanced ferroelectric random access memories at the nanoscale is of great importance in order to optimize such electronic parts [4]. Quantum mechanical models could observe the material behavior very detailed. However, even by utilizing sophisticated DFT algorithms the time and length scales of domain wall movement are too large for such *ab initio* approaches due to the enormous computational costs.

In order to investigate size effects of domain walls in BaTiO₃ we apply the core shell model [2] in a molecular dynamics algorithm. We study how domain sizes and the strength of an external electric field affect the domain wall speed of uncharged 180° domain walls. The results are compared with previous numerical and experimental studies [1, 3]. Furthermore, we discuss how these simulations may be used in order to improve macroscopic continuum modeling.

References

- [1] Gustau Catalan, J Seidel, R Ramesh, and James F Scott. Domain wall nanoelectronics. *Reviews of Modern Physics*, 84(1):119, 2012.
- [2] Mohamed T Ghoneim and Muhammad Mustafa Hussain. Study of harsh environment operation of flexible ferroelectric memory integrated with pzt and silicon fabric. *Applied Physics Letters*, 107(5):052904, 2015.
- [3] HL Stadler and PJ Zachmanidis. Nucleation and growth of ferroelectric domains in batio3 at fields from 2 to 450 kv/cm. *Journal of Applied Physics*, 34(11):3255–3260, 1963.
- [4] Jason M Vielma and Guenter Schneider. Shell model of batio3 derived from ab-initio total energy calculations. *Journal of Applied Physics*, 114(17):174108, 2013.

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A Micromagnetics Inspired Approach for the Macroscale Finite Element Analysis of Magnetostrictive Materials

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Abstract

In earlier work we proposed an energy relaxation based material model for magnetic shape memory alloys (MSMA), which is capable of predicting all of their key response features [2]. This microstructure evolution-driven behavior is characterized by a nonlinear, anisotropic, hysteretic, and highly stress level dependent strain and magnetization behavior under complex magnetomechanical loading. The material model is motivated by the constrained theory of magnetoelasticity [1], but additionally incorporates elastic deformations, deviations from magnetic easy axes, and dissipation in variant reorientation. These microstructural mechanisms are captured by a set of internal state variables, whose evolution is determined by the constrained minimization of a total incremental potential. The influence of nonlocal magnetostatic self-fields, which cause even simple experiments to record system responses—instead of purely constitutive responses—was captured by predetermined demagnetization tensors for spatially homogeneous problems. With the goal of simulating the response of arbitrarily shaped samples on the macroscopic scale—without sacrificing the physical motivation of microscale mechanisms—we present a micromagnetics inspired finite element framework, in which energy relaxation based constitutive models can be implemented. Note that in contrast to classical micromagnetics, an energetic penalization of magnetization gradients is neglected on the considered scale in the sense of the large body limit. Moreover, to capture physically meaningful boundary conditions, magnetostatic self-fields are spatially resolved within the respective magnetostrictive sample geometries as well as sufficiently large surrounding free space boxes. First results demonstrate the effect of the sample shape dependence and anisotropy for single-crystalline magnetostrictive materials under magnetomechanical loading.

References

- [1] A. DeSimone and R. D. James. A constrained theory of magnetoelasticity. *Journal of Mechanics and Physics of Solids*, 50(2):283–320, 2002.
- [2] B. Kiefer, K. Buckmann, and T. Bartel. Numerical energy relaxation to model microstructure evolution in functional magnetic materials. *GAMM-Mitteilungen*, 38(1):171–196, 2015.

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Experimental Investigation of Strain Distributions in Lead-based and Lead-free Ferroelectrics by Digital Image Correlation

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Abstract

Ferroelectric piezoceramics, have many excellent characteristics that are attractive for sensor and actuator applications [1]. These materials on the market are now categorized into two groups, mainly: lead-based, e.g. PIC151 lead zirconate titanate (PZT) and lead-free piezoceramics, e.g. PIC700 modified bismuth-sodium-titanate (BNT) [2]. In order to move these lead-based and lead-free piezo-materials into real applications, the deformation behavior under stimulations needs to be understood. In this work, digital image correlation (DIC) method was employed to measure the strains on the PZT under both the electric field and compressive loadings, independently. The DIC method was validated and the accuracy of the measurement was discussed. Under the mechanical compressive load, shear strains can be observed on the bottom region of the specimen which indicates this region is not at a purely uniaxial stress state. To get a desired stress-strain curve, the area on which the measurement is focused should be carefully considered. The electric field-induced strains on 0.93(Na_{1/2}Bi_{1/2})TiO₃-0.07BaTiO₃ (NBT-7BT) and 0.91(Na_{1/2}Bi_{1/2})TiO₃-0.06BaTiO₃-0.03K_{0.5}Na_{0.5}NbO₃ (NBT-6BT-3KNN) were also measured by using this method. Especially, the deformation of the lead-free ceramic/ceramic (NBT-7BT/NBT-6BT-3KNN) bilayer composite was monitored. The strain states were demonstrated by focusing on each layer which provides a better understanding of the mechanism of those composite effects.

References

- [1] Gene H Haertling. Ferroelectric ceramics: history and technology. *Journal of the American Ceramic Society*, 82(4):797–818, 1999.
- [2] PI Ceramic GmbH. Pi ceramic material data.

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Numerical and Experimental Investigation of Pre-Stress in Ultrasound Transducers

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Abstract

Nowadays, pre-stressed sandwich-type ultrasound transducers, also named “bolted Langevin transducers”, are standard parts for various ultrasound applications like sonar, cleaning, welding or machining. They consist of piezoceramics clamped between metal parts, which help reducing the amount of expensive piezoceramics in the setup and make it easier to adapt the transducer to the process. Compressional stress is applied to the piezoceramics to avoid tensional stress, which may lead to crack damage during operation. The application of pre-stress is also very important for the performance of the transducer as too high or too low pre-stress will result in low performance or even failure. Thus, pre-stress should be applied systematically and should be uniformly distributed across the contact area, which demands proper mechanical design and manufacture. Conventionally, the “optimum” pre-stress is found by testing several prototypes with varying pre-stress, which is quantified by the tightening torque or a voltage generated by the piezoceramics during assembly. This quantification is subject to several uncertainties making it difficult to produce several transducers with consistent characteristics. To improve the manufacturing process, more knowledge about the pre-stress remaining in the piezoceramics after manufacture and during operation is needed. In this contribution results of finite element calculations will show that the distribution of pre-stress within the contact areas is considerably affected by friction. Furthermore, different methods to estimate or measure pre-stress in the contact areas are discussed and first experimental results are presented.

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External stress-dependent response of ferroelectric materials based on a sequential laminate approach

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Abstract

Under pure electrical loading conditions, the hysteretic material response of ferroelectric solids is dependent on the rate of applied electric field. In addition to this rate-dependent behaviour, the shape of butterfly and dielectric hystereses are further dependent on the magnitude of external compressive stress acting along the direction of electrical loading. Experimental investigations on poly-crystal ferroelectric ceramic reveals that, along with alternating electric field, increasing magnitudes of applied constant compressive pre-stress results in decreasing macroscopic strain and polarisation values. This corresponds to a reduction in area of the obtained butterfly and dielectric hysteresis curves, e.g. [3]. Single-crystal ferroelectric materials, on the other hand shows contrasting response when subjected to combined electromechanical loading. With increase of compressive stress magnitudes, in addition to the electrical field on a tetragonal BaTiO₃ single-crystal, the actuation strain obtained along the loading direction also shows an increase. This is mainly due to the enhancement of stress-activated 90° domain switching, e.g. [2].

This contribution deals with the sequential laminate-based modelling of both single- and poly-crystal tetragonal ferroelectric materials, barium titanate in particular. The laminate model, established for single crystal BaTiO₃ in [1], is extended to capture the electrical rate- and external stress-dependent response of poly-crystal BaTiO₃.

References

- [1] D. K. Dusthakar, A. Menzel, and B. Svendsen. A laminate-based modelling approach for rate-dependent switching in ferroelectric materials. *Proceedings in Applied Mathematics and Mechanics*, 15(1):3–6, 2015.
- [2] J.-H. Yen, Y.-C. Shu, J. Shieh, and J.-H. Yeh. A study of electromechanical switching in ferroelectric single crystals. *Journal of the Mechanics and Physics of Solids*, 56(6):2117–2135, 2008.
- [3] D. Zhou, M. Kamlah, and D. Munz. Effects of uniaxial prestress on the ferroelectric hysteretic response of soft PZT. *Journal of the European Ceramic Society*, 25(4):425–432, 2005.

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Increasing the sensitivity of impedance with respect to material parameters of triple-ring electrode piezoelectric transducers using algorithmic differentiation

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Abstract

For efficient solving of the inverse problem characterizing material parameters of piezoelectric ceramics via impedance measurements, a high sensitivity of the impedance with respect to the material parameters is required. In [3] it was shown that the sensitivity could be increased by using ceramic discs with three ring-shaped electrodes as specimens. Furthermore, the sensitivity depends on the geometry of the triple-ring electrodes. This leads to the optimization problem of increasing the sensitivity of impedance with regard to material parameters by varying the electrode geometry. However, this could not be solved to fullest satisfaction.

The authors have implemented the algorithmic differentiation [1] tool ADOL-C into the simulation software CFS++ [2] used for the simulation of piezoelectric ceramics and revisit the optimization problem in [3] substituting occurring finite differences with precise derivatives given by algorithmic differentiation and demonstrate the improvements this method makes towards increased sensitivity of impedance with respect to material parameters.

References

- [1] Andreas Griewank and Andrea Walther. *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*. Society for Industrial Mathematics, 2nd edition, November 2008.
- [2] M. Kaltenbacher. Advanced simulation tool for the design of sensors and actuators. *Procedia Engineering*, 5:597 – 600, 2010. Eurosensor XXIV Conference.
- [3] K. Kulshreshtha, B. Jurgelucks, F. Bause, J. Rautenberg, and C. Unverzagt. Increasing the sensitivity of electrical impedance to piezoelectric material parameters with non-uniform electrical excitation. *Journal of Sensors and Sensor Systems*, 4:217–227, 2015.

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Mechanically induced ferroelectric long range order in relaxor ferroelectrics

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Abstract

A transition from a relaxor ferroelectric state to a long-range ferroelectric order can be induced by means of electric field and manifests itself by an anomaly in the dielectric temperature dependence [1-3]. An external uniaxial mechanical stress can also induce long-range ferroelectric order in relaxor ferroelectrics as shown in lead-free relaxors ((Na_{1/2}Bi_{1/2})TiO₃-0.06BaTiO₃) [4]. We developed a novel characterisation technique allowing us to measure the piezoelectric and dielectric properties simultaneously as a function of temperature, frequency and mechanical load. We show the influence of stress on the relaxor to ferroelectric transition in lead free and lead containing model systems. Temperature and load dependent measurements of the longitudinal piezoelectric coefficient d_{33} and electrical permittivity are presented. The dielectric and piezoelectric properties are discussed in the context of a stress-temperature phase diagram.

References

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Contrasting strain mechanisms in lead-free piezoelectric ceramics

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Abstract

Piezoelectric ceramics find a wide range of applications in advanced technological fields. Most of the currently used electro-active ceramics contain lead (Pb). Environmental concerns and limitations in high temperature performances of lead based compositions have spurred the field of lead-free electroceramics research. Compositions based on bismuth sodium titanate (NBT), sodium potassium niobate (NKN), bismuth ferrite (BF) and barium titanate (BT) have long been considered as candidates to replace lead based electroceramics. Although lead-free compositions based on these systems exhibit piezoelectric properties for potential device application, further enhancement is required. To improve their properties, extensive knowledge of structure-property relationships, especially during the field-on condition is essential. Diffraction is a useful technique to highlight structure-property relationships. To understand the microscopic origin of strain in lead-free electroceramics several compositions based on NBT, NKN, BF and BT have been studied using in situ high energy (87 keV) x-ray diffraction. Their microscopic strain response has been elucidated under electric field. Both the intrinsic (lattice) and extrinsic (domain switching and/or phase transformation) strain contributions have been analysed for each system and have been correlated with their macroscopic properties. This comparative study of their strain responses will enable us to focus on some important aspects that are essential to improve electro-mechanical properties in future lead-free systems.

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Failure simulation of ferroelectric ceramics under cyclic electromechanical loading

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Abstract

The reliability of smart-structures is essentially reduced by the crack formation at the grain boundaries under the action of external electrical and/or mechanical loading. Severe operating conditions, as for example high electrical fields or local stress concentrations, make it necessary to avoid and correctly predict failure of smart devices. Detailed reviews about cracking of ferroelectric ceramics can be found in [1].

The aim of the current research is a finite element method (FEM) modeling of intergranular fracture in polycrystalline ferroelectric structures.

The non-linear behavior of ferroelectric bulk ceramics is taken into account by means of the micromechanical single crystal model of 3D tetragonal domain switching. A coupled electromechanical cohesive zone model with electrical degree of freedom, allowing damage accumulation under cyclic loading of constant amplitude, [2] was used in order to simulate initiation and evolution of damage and cracking along interfaces in polycrystalline ceramics.

Cyclic electric and/or mechanical loading are applied to simple test examples, an initially polarized piezoelectric mesostructure and a ferroelectric mesostructure with randomly distributed grain orientations taking into account the poling process.

A significant influence of the poling process on ceramics' fracture due to domain reorientation is found. Intergranular fracture under external cyclic loading is visualized together with the domain switching in the grains.

It is the first numerical analysis of ferroelectric mesostructure taking into account domain switching inside the grains of ceramics combined with cohesive zone modeling of delamination/intergranular fracture. Such simulations lead to deeper understanding of the electromechanical processes going on at the micro- and meso- scales in the ceramics.

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Fracture mechanics modeling of ferroelectric materials

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Abstract

Nowadays, piezo- and ferroelectric ceramic materials cover widespread applications as sensors or actuators in mechatronics, adaptive structures and smart composites. Under in-service conditions, these brittle materials are exposed to severe static and cyclic electrical and mechanical loading, which may cause crack formation and final failure. In order to ensure reliability of ferroelectric devices fracture mechanical concepts have to be applied. While *linear fracture mechanics of piezoelectric materials* has been investigated rather intensively in the last decades, *non-linear fracture phenomena* in ferroelectric materials are a subject of intensive current research [1].

The presentation will attempt to review the state-of-the-art in this growing research field. Firstly, an introduction is given into the electromechanical field theory of non-linear ferroelectric behavior, manifested by the macroscopic polarization- and associated strain-hysteresis. Various modern approaches are discussed to capture the problem either on the macro-scale by phenomenological constitutive models, on the meso-scale by domain-switching simulations or on the micro-scale by phase field theory. Pros and cons of these methods are discussed in connection with non-linear FEM-realizations.

Secondly, the existing fracture mechanical criteria and concepts for cracks in ferroelectric materials are discussed. The high electromechanical field concentrations around cracks lead to intensive non-linear ferroelectric behavior due to domain switching processes. This results in irreversible polarization, strain and stress states that affect the loading situation in the fracture process zone. Several experimental and numerical investigations made evident that these switching processes are crucial for understanding fracture and fatigue. The concept of configurational forces or adopted J-integral formulations are presented [2], which offer an promising approach for ferroelectric fracture mechanics.

Thirdly, a cyclic electromechanical cohesive zone model is suggested to simulate subcritical fatigue crack growth [3]. These cohesive elements are able to model the evolution of damage and microcracks at grain boundaries in polycrystals or interfaces, whereas in the ferroelectric bulk material the domain-switching model is used.

Fourthly, as an application, the evolution of damage and fatigue cracking in a multi-layer PZT actuator is simulated during poling process and subsequent in-service alternating electric field.

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A multiscale homogenization approach for the characterization of nonlinear magneto-electric composites

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Abstract

Multiferroic materials combine two or more ferroic characteristics and can exhibit an interaction between electric and magnetic fields. This magneto-electric (ME) coupling can find applications in sensor technology or in electric field-controlled magnetic data storage devices [5]. Since most ME single-phase materials show an interaction between electric polarization and magnetization far below room temperature and therefore outside of a technical relevant temperature range, the manufacturing of two-phase composites, consisting of a ferroelectric matrix with magnetostrictive inclusions, becomes important. They generate the ME coupling at room temperature as a result of the interaction of their constituents. Hence, the ME coupling of composite materials significantly depends on the material behavior of both phases. In order to determine the effective properties with respect to both aspects, a finite element (FE²) homogenization approach is performed, which combines via a scale bridging the macro- and microscopic level meanwhile the microscopic morphology of a representative volume element is considered [4, 3]. Furthermore, the nonlinear properties of both phases are approximated with appropriate material models. On the one hand, the switching behavior of spontaneous polarizations of barium titanate unit cells are taken into account [1], which reproduces after a homogenization step the typical dielectric and butterfly hysteresis loops of the ferroelectric matrix material. On the other hand, the nonlinear remanent magnetizations of the magnetostrictive inclusions are described with a Preisach operator [2]. Both models affect the strain-induced coupling, such that we obtain a nonlinear behavior of the ME coefficient.

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A condensed micromagnetoelctromechanical approach to model the constitutive behavior of ferroelectric, ferromagnetic and multiferroic materials

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Abstract

Ferroelectric as well as ferromagnetic materials are widely used in smart structures and devices as actuators, sensors etc. To model their nonlinear behavior, a variety of models has been published in the past decades. Most of the models that have been developed were implemented within the framework of the Finite Element Method (FEM), e.g. [1]. The implementation of a discretization scheme is going along with a high computational effort and the solution of the boundary value problem (BVP) requires high computational costs. Most investigations, however, are restricted to simple BVP under uniaxial loading and their goal is the calculation of hysteresis loops. In [2] the so-called condensed method (CM) is introduced to investigate the macroscopic polycrystalline material behavior at a global material point without any kind of discretization scheme. Based on the condensed theory, a high cycle fatigue model to predict the life time of piezoelectrics under combined electromechanical loading is introduced in [3]. Besides classical ferroelectrics, other fields of application of the CM have been exploited, e.g. ferromagnets, ferroelectric-ferromagnetic composites or ferroelectrics with phase transition. Two possible fields of application are presented: On the one hand, the CM is extended to ferromagnetic material behavior to investigate the magnetoelectric coupling in a composite. On the other hand, rhombohedral unit cells are implemented within the framework of the CM to examine the morphotropic phase boundary (MPB).

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Topology Optimization of Piezoelectric Nanostructures

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Abstract

We present an extended finite element formulation for piezoelectric nanobeams and nanoplates that is coupled with topology optimization to study the energy harvesting potential of piezoelectric nanostructures. The finite element model for the nanoplates is based on the Kirchoff plate model, with a linear through the thickness distribution of electric potential. Based on the topology optimization, the largest enhancements in energy harvesting are found for closed circuit boundary conditions, though significant gains are also found for open circuit boundary conditions. Most interestingly, our results demonstrate the competition between surface elasticity, which reduces the energy conversion efficiency, and surface piezoelectricity, which enhances the energy conversion efficiency, in governing the energy harvesting potential of piezoelectric nanostructures[1].

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Stageless evaluation of a vector Preisach model on the basis of rotational operators

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Abstract

Preisach hysteresis models are oftentimes used to describe and compute the nonlinear and hysteretic behavior of ferroelectric and piezoelectric materials. The common scalar Preisach model approximates hysteresis in form of a weighted sum of rectangular loops [1],[2]. Thereby, each loop is defined by a pair α, β which describes the switching thresholds for the rising and falling edges. A standard implementation of this model uses two triangular matrices of N rows and columns. Each element of these matrices corresponds to one rectangular loop and stores the current switching state as well as a material specific weighting \wp , respectively. In order to capture vector hysteresis, Sutor et al. [3] extended the scalar model by an additional rotational operator. This rotational operator assigns a direction to each of the rectangular loops and can be represented analogously by a matrix of vector entries. The classical matrix-based implementation has the major drawback that it is only able to resolve input variations of $2/N$ of the saturation value. Scalar models often treat this issue by utilizing the so-called Everett function. This function allows a stageless — i.e., independent from the discretization N — reproduction of the switching states of the loops from a list of non-wiped out input minima and maxima. In our contribution, we present a stageless evaluation scheme for the extended Preisach model based on rotational operators. It exploits nested lists to exactly reproduce both the state of the rotational operator and the corresponding switching state.

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Magnetorheological elastomers: from multiscale characterization towards macroscopic devices

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Abstract

Magnetorheological elastomers (MREs) are magneto-active composites which consist of an elastomer matrix with magnetic inclusions. The inherently heterogeneous micro-structure of MREs drastically complicates the determination of their effective properties. One approach is to employ computational homogenization schemes for the determination of the effective properties [3]. However, the resulting multiscale simulation approaches require considerable computational effort. Therefore, purely macroscopic descriptions of MREs are of great interest. For this purpose, the parameters of a macroscopic constitutive law need to be fitted against experimental data [1]. However, in the case of MREs it is extremely difficult to obtain effective material properties via experiments. In fact, because of the well-known shape effects of MRE specimens [2], the observed response is *always* a product of *material and structural* properties. Following these considerations, our goal is to close the gap between computational homogenization of MREs and experimental observations [4]. This talk focuses on the important distinction of material and structural contributions to the macroscopic response of MREs. For this purpose, we employ a multiscale simulation framework to mimic experiments found in literature. We critically analyze our results and compare them to published data and analytical considerations.

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Phase field simulations of ferroelectric/ferromagnetic heterostructures

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Abstract

Multiferroic heterostructures consist of different ferroic materials combined to form a layer structure with well-defined interfaces. In recent years there have been attempts to utilize ferroelectric/ferromagnetic (FE/FM) heterostructures to switch a magnetization by the application of an electric field [1]. The coupling in such FE/FM heterostructures is via the strain mismatch between the different layers. This strain mismatch depends on the direction of magnetization/polarization, and by switching the latter it is possible to alter the former.

The presentation will introduce two phase field models for ferroelectric [2] and ferromagnetic [3] microstructure evolution. Numerical simulations will illustrate the effect of strain coupling on the evolution of the ferroelectric/ferromagnetic microstructures.

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Analyses of coated fibrous composites with piezoelectric and piezomagnetic phases

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Abstract

It is well-known that some composite materials can provide superior properties as compared to their virgin monolithic constituent materials (Ryu et al., 2002). Remarkably larger magnetoelectric (ME) effect is observed in composites as compared to those in either composite constituents (Nan, 1994). The ME coefficient is defined as the ratio between the magnetic (electrical) field output over the electrical (magnetic) input. The ME effect is intensively studied to utilize it for energy conversion between the magnetic and the electric fields, ME memory elements, smart sensors and transducers. Pan and Wang (2009) investigated bilayer multiferroic composite, where an applied magnetic field induces strains in the magnetostrictive constituent and these are passed on to the piezoelectric constituent. The strains in the piezoelectric layer induce an electric polarization. The thickness ratio of the piezomagnetic and piezoelectric layers has influence on the ME effect (Laletin et al., 2008). The ME coefficient can be enhanced in fiber composites too. Kuo and Wang (2012) proposed a method to optimize the effective ME voltage coefficient of fibrous composites made of piezoelectric and piezomagnetic phases. They showed that the effective in-plane ME voltage coefficient and the out-of-plane coefficient can be enhanced manifold at the optimal orientation compared to those at normal orientation. Surface coating of a base material plays an important role in various engineering applications. The subject of piezoelectric/piezomagnetic fibrous composites with multicoated circular/elliptic fibres is rarely analyzed in literature. These composites are analyzed only under anti-plane shear deformation (Kuo, 2011, Kuo and Pan 2011). In the present paper the influence of the coating layer on the ME coefficient in fibrous composites with piezoelectric and piezomagnetic phases is investigated. The effective material parameters are computed based on the homogenization techniques performed on the representative volume element (RVE). The solution of the general boundary value problems for coupled multi-field problems requires advanced numerical methods due to the high mathematical complexity. Such a multi-field problem is described by a system of partial differential equations because of the interactions among the magnetic, electric and mechanical fields involved in the constitutive equations. The finite element method (FEM) is applied to solve the corresponding boundary value problems.

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A Phase field Approach For Large Deformation Magneto-Mechanically Coupled Material Response

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Abstract

Magneto-Rheological Elastomers (MREs) have received significant attention in recent years. MREs contain micron-sized ferromagnetic particles that are embedded in an elastomeric matrix material. The behavior of such materials under the effect of an external applied field is a complex phenomenon that spans multiple scales. The interaction between the magnetic and elastic forces gives rise to the reversible actuation effects and the variable stiffness behavior, seen on the macro-scale. In order to accurately predict the behavior of these materials we need a model that consistently takes into account the micro-scale response of such materials. To this end we propose a *large deformation micro-magnetic framework*, where the magnetization vector acts as the order parameter. A large deformation description of the *Landau-Lifshitz-Gilbert* equation gives the temporal evolution of the magnetization vectors. A *penalty solution scheme* is used to satisfy the unity constraint of the magnetization vectors. Appropriate numerical examples are presented that showcase the capability of the framework to determine the domain wall motion in ferromagnetic materials, and in turn determine the effect of particle shape and volume fraction in the macroscopic behavior of MREs.

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Analyses of coated fibrous composites with piezoelectric and piezomagnetic phases

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Abstract

Multiferroic composites, which have emerged as an ideal solution for room temperature magnetoelectricity, involve a large class of materials where strain mediates the effective coupling. Hence, it becomes evident to explore the coupling mechanism from a micromechanical perspective. Very recently, attempts have been made to construct robust models for understanding the strain mediated magnetoelectric effect in composites with various morphologies. However, such models lack the necessary experimental support. In general, there is a lack of proper understanding about the behavior of the strain mediation in the vicinity of the interface between the constituent phases. In this study we demonstrate the potential of various cantilever based microscopic techniques like Piezoresponse Force Microscopy (PFM), Magnetic Force Microscopy (MFM), Kelvin Probe Force Microscopy (KPFM) etc. in studying the local manifestations of the strain mediated magnetoelectric effect in various classical composite systems like Co/NiFe₂O₄ – BaTiO₃ and Ba/SrFe_{1.2}O_{1.9} – BaTiO₃. The outcomes not only present an opportunity to gauge the magnitude of the effect locally, but also reveal interesting phenomena that could be rationalized by a synergistic support from modeling.

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Phase field simulation of layered relaxor/ferroelectric composite with diffusive interface

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Abstract

Piezoelectric materials have received considerable attention in both industry and academia due to the electromechanical effect. Large-signal response d_{33}^* is one of the most important parameters for actuator applications. In the past decades, great efforts have been made in developing lead-free piezoceramics in view of environmental issues. Ever since a large strain was reported on a BNT-BT-KNN ceramics, different approaches are attempted in BNT-BT system to obtain the enhanced piezoelectric effect. For instance, BNT-BT-AN layered composite shows the enhanced d_{33}^* at a FE volume content of 30%. [2] The coupling effect between different layers is believed to be the origin for this phenomenon. The interface between layers also affects the composite property, especially for BNKT-BA.

In this presentation, a phase field model is established to simulate the layered RE/FE composite. The relaxor model is based on our previous work, in which a Gaussian distributed random field is introduced to represent the chemical disorder.[1] For the case of the sharp interface (BNT-BT-KNN), the enhancement of d_{33}^* is observed at a FE volume content of 10%. Different coupling mechanism is found between serial and parallel structure. For the case of the diffusive interface, the properties of the material, such as random field, are assumed to linearly change in the direction that is perpendicular to the interface. The large signal response is compared between the two types of interfaces. The simulation results can favor the design of the future FE/RE composite.

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Simulation-based homogenization and characterization of piezoelectric actuators

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Abstract

Piezoelectric actuators (e. g., piezoelectric stack actuators, piezoelectric patch transducers) are employed in a wide field of applications due to their good mechanical properties (i. e., force, displacement). To predict the mechanical and electrical performance of such actuators, commonly, numerical simulations are utilized. Piezoelectric actuators consist, however, of various materials and show a complex structure, which requires a detailed knowledge regarding internal structure of the actuator as well as precise material parameters of all involved materials.

In this contribution, we show a novel and efficient method to homogenize complex piezoelectric actuators by an uniform model with only one fictive piezoelectric material. The effective small signal parameter set of this fictive material is determined by the simulation-based inverse method [1, 2]. The inverse method iteratively adapts the material parameters through an optimization algorithm in order to match numerical simulation results to measurements (i. e., frequency-resolved electrical impedance, mechanical displacement).

We will present the homogenization approach, the principle of the adapted inverse method, measurement setups and exemplary material parameters of commercially available piezoelectric actuators. Furthermore, we show advantages, challenges but also limitations associated with this approach.

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Magnetostrictive-piezoelectric coupling of CoFe_2O_4 nanopillars embedded in a BaTiO_3 matrix

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Abstract

Multiferroic materials showing both magnetic and electric ordering allow an additional degree of freedom in the design of actuators, transducers and storage devices and thus have attracted scientific interest from the technological perspective as well as from basic research. Because the choice of single-phase multiferroic materials being suitable at room temperature is limited, the use of magnetoelectric two-phase composites has proven to be more promising [2]. Here we study ferrimagnetic CoFe_2O_4 (CFO) nanopillars embedded in a ferroelectric BaTiO_3 (BTO) matrix. They operate at room temperature and are free of any resource-critical rare-earth element, which makes them interesting for potential applications. Prior studies succeeded in showing strain-mediated coupling between the two subsystems. In particular, the electric properties can be tuned by magnetic fields and the magnetic properties by electric fields. Here we take the analysis of the coupling to a new level utilizing soft X-ray absorption spectroscopy and its associated linear dichroism [1]. We demonstrate that an in-plane magnetic field breaks the tetragonal symmetry of the (1,3)-type $\text{CoFe}_2\text{O}_4/\text{BaTiO}_3$ structures and discuss it in terms of off-diagonal magnetostrictive-piezoelectric coupling. This coupling creates staggered in-plane components of the electric polarization, which are stable even at magnetic remanence due to hysteretic behaviour of structural changes in the BaTiO_3 matrix. The competing mechanisms of clamping and relaxation effects are discussed in detail. The effect in the electric in-plane polarization of BTO obtained in this work extends over a large area. Under the constraint of completely regular arrays of CFO nanopillars, one might even envisage data-storage concepts by encoding the local polarization patterns of single nanopillars via external current-controlled local magnetic fields.

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Temperature changes in ferroelectric materials due to domain switching and their influence on mechanical fields

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Abstract

Due to their special electromechanical properties, nowadays ferroelectric materials are widely used in many technical applications, mostly as actuators or sensors. Advantages compared to other smart devices are their extremely fast reaction times in a range of $\mu m - ms$ and large actuation forces. In the past, temperature changes inside the material were rather disturbing during the investigation and usage of these materials and were mostly neglected in numerical models, although they may have a non-negligible impact on issues like phase transitions, domain wall motion or reliability and lifetime.

In this paper, the theoretical background and a Finite Element (FE) solution of a micromechanically and physically based constitutive model is presented. The model considers the mutual nonlinear coupling of thermal and electromechanical fields. Numerical calculations show the effects of temperature on the electromechanical field quantities and vice versa. They also reveal switching processes in ferroelectrics and associated heating or cooling.

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Investigations of dynamic crack problems in functionally graded piezoelectric materials by a TDBEM

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Abstract

Modern piezoelectric structures offer certain performance advantages over conventional ones due to their capability of converting electrical energy into mechanical energy and vice versa. Important applications of piezoelectric materials are layered or laminated composites because they can be optimized to satisfy the high-performance requirements according to different in-service conditions. In recent years composites with a continuously change of the material properties are getting increasing attention in advanced engineering applications. An important advantage over conventional laminates is that interfaces and stress discontinuities are avoided. Piezoelectric composites are very brittle and have a low fracture toughness. Since they are often applied under time-dependent loadings, the dynamic crack analysis is of special importance. The analysis of functionally graded materials (FGMs) is mathematically very complex and analytical solutions are possible only for very simple geometry and loading conditions. Therefore, efficient numerical methods are needed to solve more general problems.

In this paper, static and dynamic crack analysis in two-dimensional (2D) functionally graded piezoelectric composites is presented. For this purpose, a time-domain boundary element method (BEM) is developed. The collocation method is used for the spatial discretization of the time-domain boundary integral equations (BIEs), while the convolution quadrature is adopted for temporal discretization. Since fundamental solutions for piezoelectric FGMs are not available, a boundary-domain integral formulation is derived. The Laplace transformed fundamental solutions for homogeneous piezoelectric materials are applied. Special regularization techniques based on a suitable change of variables are used to deal with the singular boundary integrals. The radial integration method is adopted to compute the resulting domain integrals. Adjacent the crack-tips are square-root elements implemented to capture the local square-root-behaviour of the generalized crack-opening-displacements properly. An explicit time-stepping scheme is obtained to compute the unknown boundary data. Numerical examples will be presented and discussed to show the influences of the material gradation, poling direction and the dynamic loadings on the intensity factors.

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Monte Carlo simulations of relaxor ferroelectrics based on a Ginzburg-Landau type effective Hamiltonian

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Abstract

Relaxor ferroelectrics have attracted considerable research interests in the last decades due to their large electromechanical coupling and promising electrocaloric effect (ECE). Despite the existing body of work on relaxors, the origin for the relaxor behavior is still controversially discussed, and there exist various models, such as the concept of polar nanoregions, the dipole-glass model, the random field model, and the spherical random bond - random field model. In this work the domain structure and the ECE of several types of relaxor materials are investigated by using lattice-based Monte Carlo simulations based on Ginzburg-Landau type effective Hamiltonian. It allows us to consider different mechanisms which may lead to relaxor properties. Compared with DFT-calculations based effective Hamiltonian, the Ginzburg-Landau type Hamiltonian is more effective and permits flexible study on parameters of domain structure, such as domain wall thickness and domain wall thickness. Another advantage is that the combined canonical and micro-canonical MC algorithm allows us to evaluate the ECE directly without using the Maxwell relations.

Through simulations it will be revealed that depending on the material type, different governing mechanisms of relaxors can be dominant. For instance, for the PMN system the generic study by including random electric fields is important, while in the BZT system defect dipole model can be used to explain the relaxor behavior and the ferroelectric-relaxor transition. Moreover, results show that defect dipoles can have a significant influence on the domain structure and thus ECE. Particularly, a positive-negative ECE transition is observed, which can be explained domain structures and revealed by interplay between the internal field of defect dipoles and the external field.

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Charge-mediated magnetoelectric coupling for 180 degree switching in nanomagnets: a multiscale study

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Abstract

For revolutionizing spintronic devices, 180 degree switching purely with a voltage via the magnetoelectric (ME) coupling has deemed as a potential way to revolutionize the spintronic devices, in terms of low-power consumption, fast response, low loss, and device minimization. Many efforts have been devoted to achieving magnetization switching via ME coupling induced by the piezoelectric strain. Intrinsically, this is a mechanical strain assisted switching process [1, 2, 3]. However, in thin film multiferroic heterostructures, due to the substrate clamping effect the strain-mediated ME coupling is often limited.

In this presentation, we demonstrate the charge-mediated ME coupling for voltage-driven 180° switching in nanomagnets by multiscale simulations combining first-principles calculations and magnetization dynamics. We focus on the ME coupling in metal-magnet-insulator nanoheterostructures. Taking the Pt-FePt-MgO nanoheterostructure as a model system where FePt is an attractive magnet for memory and logic devices, we firstly apply first-principles calculations to determine the relationship between magnetic anisotropy energy (MAE) and the electric field (E). MAE change of the system is shown to be attributed to the electric field induced charge in the FePt-MgO interface. The dependence of the MAE-E relationship on the layer number of FePt and the lattice variation of the system is also studied. Then the MAE-E relationship is input to the magnetization dynamics analysis of a single-domain nanomagnet in the shape of an elliptical cylinder. The switching dynamics are studied in terms of different ramp rates, pulse widths, amplitudes of the voltage, in order to find the conditions for a fast and deterministic 180° switching. Finally the finite temperature induced thermal fluctuation effect is considered.

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