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UNIVERSITÀ DEL SALENTO

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Scientific Program - Timetable

Sunday 22	Time	Monday 23	Tuesday 24	Wednesday 25	Thursday 26	Friday 27
	9:15		Contributed sessions (15 in parallel)	Plenary Lecture Moritz Diehl	Contributed sessions (15 in parallel)	Contributed sessions (14 in parallel)
	9:30					
	9:45					
	10:15	Registration		von Mises prize lecture		
	10:30					
	10:45					
	11:15		Coffee Break	Coffee Break	Coffee Break	Coffee Break
	11:30					
	11:45					
	12:15		Plenary Lecture Thomas Böhlke	General Assembly	Plenary Lecture Ferdinando Auricchio	Contributed sessions (11 in parallel)
	12:30					
	12:45					
	13:15	Opening	Lunch	Lunch	Lunch	
	13:30					
	13:45	Univ. Chorus Performance				Closing
	14:15	Prandtl Lecture Keith Moffatt	Plenary Lecture Enrique Zuazua	Contributed sessions (15 in parallel)	Plenary Lecture Daniel Kressner	
	14:30					
	14:45					
	15:15	Plenary Lecture Giovanni Galdi	Plenary Lecture Nikolaus Adams		Plenary Lecture Stanislaw Stupkiewicz	
	15:30					
	15:45					
Registration pre-opening	16:15	Coffee Break	Coffee Break Poster session	Coffee Break	Coffee Break Poster session	
	16:30	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	16:45					
	17:15					
	17:30					
	17:45					
	18:15		Public lecture Francesco D'Andria			
	18:30					
	18:45					
	19:15	Opening reception at Castle of Charles V				
	19:30					
	19:45					
	20:15			Conference dinner at Hotel Tiziano		
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MS1: Multi-Scale Modeling of Ferroic Functional Materials

In the minisymposium, latest developments related to two central aspects of multi-scale modeling of ferroic functional materials will be discussed, namely techniques for the modeling at different scales, e.g. discrete atomistic (MD) simulations, phase-field approaches, energy relaxation techniques, and scale-bridging techniques, e.g. micro-mechanics and direct micro- macro transitions through numerical homogenization. Such tools allow the computation of effective properties for multi-functional composites, as well as advanced multi-scale analyses of critical constitutive mechanisms related, for instance, to micro- and domain structure evolution, fracture, damage or fatigue, in a physically well-motivated manner.

Multiscale mechanical behaviour of nematic elastomers

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Phase transforming materials have been used as actuator materials for some time already. They are typically made of hard materials but, more recently, interest has grown on soft materials, which are capable of responding to external stimuli with large deformations. Nematic elastomers provide one example in which spontaneous deformations can be induced by temperature changes, applied electric fields, or irradiation with light.

We will discuss the mechanical multiscale behaviour of nematic elastomers and speculate on their possible applications in the field of soft robotics.

A laminate-based modelling approach for rate-dependent switching in ferroelectric materials

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Ferroelectric materials, both single- and polycrystals, exhibit characteristic hysteric behaviour when subjected to a sufficiently high macroscopic cyclic electric field. Moreover, related butterfly curves and hysteresis loops depend on the rate of electrical loading; cf. Zhou et al. [1]. Experimental studies show that the shape of such hysteresis curves additionally depends on the magnitude of external compressive stresses acting along the direction of the applied electrical field; cf. Li et al. [2], Zhou et al. [3], Shieh et al. [4].

This work focuses on the modelling and simulation of ferroelectric single- and polycrystalline materials based on a laminate-based mixture-type theory, wherein several phases or rather variants are considered; cf. Yen et al. [6] and references cited therein. By considering compatibility between ferroelectric domains, this formulation rests upon the framework of sequential lamination to generate so-called engineered domain microstructures in ferroelectric materials. Furthermore, the formulation is governed by an energy-enthalpy function in terms of the total strains, the electric field and a set of internal variables, namely the multi-rank laminate volume fractions. The evolution of these volume fractions is determined by the dissipation potential introduced. Based on a previously established micromechanically motivated and rate-dependent laminate-based approach for the modelling of single crystal ferroelectrics, see Dusthakar et al. [5], this work extends that formulation to computationally capture polycrystalline ferroelectric material behaviour under the influence of external stresses and at different loading rates. The proposed laminate-based approach accounts for a limited number of material parameters and, at the same time, remains computationally efficient.

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Variational Structural and Material Stability Analysis in Finite Electro-Magneto-Mechanics of Active Materials

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Materials like electro-active polymers (EAPs) and magneto-rheological elastomers (MREs) exhibit coupled electro- and magneto-mechanical behavior at large strains. They respond by a deformation to an applied electric or magnetic field and are used in advanced industrial environments as sensors and actuators, for example in robotics, biomimetics and smart structures. In field-activated or electronic EAPs, the electric activation is driven by Coulomb-type electrostatic forces, resulting in Maxwell stresses. MREs are composites consisting of a polymer matrix with embedded magnetizable iron particles, which allow a change of mechanical properties by application of magnetic fields. Polymer-based magneto-electric composites (MECs) are a new class of tailor-made materials with promising future in industrial applications. The ME effect is the phenomenon of inducing electric polarization by applying an external magnetic field or vice versa.

However, these types of composite materials suffer from different types of instabilities. This concerns structural instabilities, such as buckling and wrinkling of EAP and MRE devices, as well as material instabilities, such as limit- and bifurcation-points in the constitutive response which induce snap-through and fine scale localization of local states.

In this work, we outline variational-based definitions for structural and material stability of MRCs, and design algorithms for accompanying stability checks in typical finite element computations of composites. The formulation starts from stability criteria for a canonical energy minimization principle of electro-magneto-elasto-statics, and then shifts them over to representations related to an enthalpy-based saddle point principle that is considered as the most convenient setting for numerical implementation. Here, global structural stability is analysed based on a perturbation of the total electro-magneto-mechanical energy, and related to statements of positive definiteness of incremental finite element tangent arrays. We base the local material stability on an incremental quasi-convexity condition of the electro-magneto-mechanical energy, inducing the positive definiteness of both the incremental electro-magneto-mechanical moduli as well as a generalized acoustic tensor. It is shown that the incremental arrays to be analysed in the stability criteria appear within the enthalpy-based setting in a distinct diagonal form, with mechanical, electric and magnetic partitions. Applications of accompanying stability analyses in finite element computations are demonstrated by means of representative model problems.

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Simulation of Size Effects in Ferroelectric Materials using a Phase Field Model

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Ferroelectric materials couple mechanical and electrical fields. Crucial for the coupling is the material microstructure which consists of different domains separated by domain walls. A domain is an area of almost constant polarization. The application of mechanical or electrical fields causes a temporal change of the domain structure which establishes a time dependent material behavior. In this presentation a phase field model based on the remanent polarization as order parameter is proposed, see [1]. The evolving anisotropy is considered by using a formulation of the electric enthalpy based on invariant theory, see [2]. This approach can capture the polarization dependent material properties quite well, as is demonstrated by the example of barium titanate. The invariant formulation allows for a straight forward application of the model in two and three dimensions. In order to analyse size effects the boundary conditions on the order parameter (polarization) are discussed and recast into a Robin-type boundary condition. Numerical simulations using finite elements demonstrate size effects in nano dots and thin films, see [3]. The presentation also addresses the evolution of volume fractions of different domain orientations within a polycrystalline aggregate. In polycrystalline settings the grain boundaries require a special treatment of the order parameter. As additional jump conditions for the order parameter are required from a mathematical point of view, which cannot be derived from physical arguments based on balance relations, two limit cases are analyzed by virtue of numerical simulations. In the first case, a continuity of the order parameter across the grain boundary is assumed, resulting into a strong interaction of the grains. In a second approach, the order parameters are decoupled on the grain boundary, resulting in a communication of different grains only via the electrical and mechanical jump conditions on the grain boundary and thus a weak coupling. Again the size effect is studied by simulation of hysteresis loops for different grain sizes of a polycrystalline microstructure.

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On molecular statics simulations of ferroelectric functional materials

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Smart materials, such as ferroelectric functional materials are of great interest for technological and scientific reasons and various material models and simulation algorithms are available in order to predict material behaviour on different length scales. On the macroscopic, mesoscopic and sub-monocrystal length scale continuum mechanics models, e.g. phase field models can accurately calculate phenomena like polarization switching or the change of polarization due to mechanical stress. However, most material models used for continuum mechanics do not fit the material behaviour of ferroelectric materials on the length scale of a few nanometers whereas simulation models and algorithms on the atomistic level are required.

Today it is possible to fabricate ferroelectric nanocomponents like ferroelectric nanofilms with less than 5 nanometers in thickness due to rapid developments in manufacturing technologies [1]. Therefore, also simulations on the atomistic length scale are becoming more important to predict and understand material behaviour.

Methods like the density functional theory can accurately calculate the ground state of atomistic systems [2]. However, the system sizes of quantum energy models and methods are restricted due to the significant computational costs of such approaches. In order to analyze size effects of ferroelectric nanofilms or nanowires several thousand atoms have to be considered. Molecular dynamics (MD) methods are able to calculate large ferroelectric atomistic systems using the core-shell model [3]. Nevertheless the computational costs for the simulation of electromechanical problems are still significant due to long range Coulomb interactions. Furthermore the coupling of MD approaches with continuum mechanics is a challenging task.

To overcome the disadvantages of the mentioned methods an extended molecular statics algorithm has been developed which efficiently calculates the ferroelectric behaviour of large discrete particle systems [4]. The proposed algorithm is able to compute efficiently the continuum deformation of a discrete particle system caused by an external electrical field in analogy to the Parrinello-Rahman method [5]. Therefore, the proposed algorithm is able to not only calculate the piezoelectric effect but also the converse piezoelectric effect which is still a limitation for other atomistic simulation algorithms of ferroelectric materials.

The aim of this talk is to present the developed extended molecular statics algorithm and the applied core-shell model for the simulation of ferroelectric materials and discuss the possibilities of the coupling of molecular statics and continuum mechanics.

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