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Book of Abstracts - Extract

2015

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					
	16:45	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	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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YRMS2: Phase Field Modeling in Mechanics and Applied Mathematics

The coupling of phase field equations to solid or fluid mechanics offers a wide range of possibilities in the modeling of e.g. ferroelectric solids. The mechanically inclined talks focus on the modeling and numerical simulation of phase field models for piezoelectric and ferroelectric materials. Theoretical aspects like the well-posedness of the coupled PDEs of phase field models, stability issues, and conservation properties of the numerical schemes are addressed in the mathematically inclined contributions.

On numerical schemes for phase-field models for electrowetting with electrolyte solutions

Stefan Metzger
Friedrich-Alexander-Universität Erlangen-Nürnberg

We present an energy-stable, decoupled discrete scheme for a recent model (see [1]) supposed to describe electrokinetic phenomena in two-phase flow with general mass densities. This model couples momentum and Cahn–Hilliard type phase-field equations with Nernst–Planck equations for ion density evolution and an elliptic transmission problem for the electrostatic potential.
The transport velocities in our scheme are based on the old velocity field updated via a discrete time integration of the force densities. This allows to split the equations into three blocks which can be treated sequentially: The phase-field equation, the equations for ion transport and electrostatic potential, and the Navier–Stokes type equations. By establishing a discrete counterpart of the continuous energy estimate, we are able to prove the existence of discrete solutions. Finally, we shall present numerical simulations of lab-on-a-chip applications to underline the full practicality of this approach.

References

[1] E. Campillo-Funolet, G. Grün, F. Klingbeil. On Modeling and Simulation of Electrokinetic Phenomena in Two-Phase Flow with General Mass Densities. SIAM Journal on Applied Mathematics, Society for Industrial and Applied Mathematics 72 (2012), 1899–1925.

On elastic Cahn-Hilliard systems coupled with evolution inclusions for damage processes

Christian Heinemann, Christiane Kraus
Weierstrass Institute

In elastically stressed alloys different physical processes such as separation of chemical substances and propagation of micro-cracks/micro-voids are shaping the micro-structure simultaneously. These processes are usually modeled independently by adapting phase-field approaches in context of Cahn-Hilliard systems and gradient-of-damage models. However, especially in modern materials, the interaction of damage and phase separation cannot be neglected for a realistic description. For instance, as indicated by experiments and numerical simulations, the long-term behavior of solder joints significantly depends on the interplay of both processes.

The aim of this talk is to present a system of partial differential equations coupling two phase field models in order to describe damage phenomena and phase separation in elastic media in one unifying model. The system reads as

$$\left.\begin{aligned}
&c_t = \operatorname{div}(m(c,z)\nabla\mu),\\
&\mu = -\Delta c + \Psi'(c) - \mathbf{C}(c,z)(\varepsilon(\mathbf{u}) - \varepsilon^*(c)) : (\varepsilon^*)'(c)\\
&\qquad +\tfrac{1}{2}\mathbf{C}_{,c}(c,z)(\varepsilon(\mathbf{u}) - \varepsilon^*(c)) : (\varepsilon(\mathbf{u}) - \varepsilon^*(c)),\\
&\lambda\mathbf{u}_{tt} - \operatorname{div}\big(\mathbf{C}(c,z)(\varepsilon(\mathbf{u}) - \varepsilon^*(c))\big) = \ell,\\
&z_t - \operatorname{div}\big(|\nabla z|^{p-2}\nabla z\big) + f'(z) + \xi + \varphi\\
&\qquad +\tfrac{1}{2}\mathbf{C}_{,z}(c,z)(\varepsilon(\mathbf{u}) - \varepsilon^*(c)) : (\varepsilon(\mathbf{u}) - \varepsilon^*(c)) = 0,\\
&\xi \in \partial I_{(-\infty,0]}(z_t),\\
&\varphi \in \partial I_{[0,1]}(z).
\end{aligned}\right\} \tag{1}$$

The order parameter z modeling the damage process is not only constrained to the unit interval but also has to obey an irreversibility condition. Because of this highly nonsmooth evolution, the possible nonsmoothness of the underlying domain and the mixed boundary condition for the elastic deformation field, a new notion of weak solutions had to be devised.

To this end, a notion which reformulates the double inclusion for these kind of systems by a variational approach in combination with a total energy-dissipation inequality was introduced in [2] and extended to further cases in [1, 3]. Global-in-time existence of weak solutions for various types of system (1) are provided. Our contribution includes cases where the mechanical forces are assumed to be in a quasi-static equilibrium ($\lambda = 0$) and cases where inertia terms are taken into account ($\lambda > 0$).

References

[1] C. Heinemann, C. Kraus. Existence of weak solutions for a PDE system describing phase separation and damage processes including inertial effects. Discrete Contin. Dyn. Syst. Ser. A (to appear)

[2] C. Heinemann, C. Kraus. Existence of weak solutions for Cahn-Hilliard systems coupled with elasticity and damage. Adv. Math. Sci. Appl. 21 (2011), 321–359.

[3] C. Heinemann, E. Rocca. Damage processes in thermoviscoelastic materials with damage-dependent thermal expansion coefficients. Math. Methods Appl. Sci. (to appear)

Phase field modeling of ferroelectric materials with defects

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The phase field method is known as a powerful tool for the simulation of microstructure evolution in various materials, as it was revealed in the review article [1]. Recently it has become also successful for the study of polarization switching in ferroelectric materials, e.g. [2, 3]. Piezoelectrics/ferroelectrics are widely used materials for sensor and actuator applications, and are known to suffer from aging and fatigue. The degradation mechanism is closely related to defects in the materials. Therefore, it is of importance to study the domain structure in the presence of defects. In this work the phase field approach is applied to study the influence of defects on the domain structures in ferroelectrics.

By a continuum phase field model implemented with the finite element method various effects of the defects in ferroelectrics, such as space charge contribution and defect dipole, are taken into account [4, 5]. The evolution of the phase field variables is governed by the Ginzburg-Landau type evolution equation. The space charge contribution of defects are considered by formulating a volume charge density according to the semiconducting theory, while the defect dipole was treated through a static eigen-polarization. Energetically unfavorable head-to-head domain structures can be stabilized by space charges induced by defects.

In addition, the abnormal behavior of relaxor ferroelectrics is simulated by applying the phase field potential to Lattice-based Monte Carlo simulations. Results show that random local electric fields can be used to explain the characteristic behavior of relaxor ferroelectrics, such as the double loop dielectric hysteresis and diffusive phase transitions.

References

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[4] Y. Zuo, Y.A. Genenko, B.X. Xu, Charge compensation of head-to-head and tail-to-tail domain walls in barium titanate and its influence on conductivity. J. Appl. Phys. 116 (2014) 044109

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Simulation of Atomic Force Microscopy for investigating $BaTiO_3$ and $LiMn_2O_4$ nanostructures based on Phase Field Approach

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Atomic force microscopy (AFM) probes the surface features of specimens using an extremely sharp tip scanning the sample surface, AFM is widely used for investigating the electrically non-conductive materials by applying an electric potential on the tip [1]. Piezoresponse Force Microscopy (PFM) and Electrochemical Strain Microscopy (ESM) are variants of AFM for different materials. Both PFM and ESM signals are obtained by observing the displacement of the tip when applying electric fields during the scanning process. The PFM technique is based on converse piezoelectric effect of ferroelectrics [2] and the ESM technique is based on electrochemical coupling in solid ionic conductors [3]. In this talk, two continuum-mechanical formulations for simulation of PFM and ESM are discussed.

In the first model, for PFM simulation, a phase field approach based on the Allen-Cahn equation for non-conserved order parameters is employed for ferroelectrics [4]. Here, the polarization vector is chosen as order parameter. Since ferroelectrics have highly anisotropic properties, this model accounts for transversely isotropic symmetry using an invariant formulation. The polarization switching behavior under the applicant of the electric field will be discussed with some numerical examples.

In the simulation of ESM, we employ a constitutive model based on the work of Bohn et. al. [5] for the modeling Lithium manganese dioxide $LiMn_2O_4$ (LMO). The model is similar to phase field approach based on Cahn-Hilliard equation where the concentration of Lithium is order parameter. It simulates the deformation of the LMO particle according to the applying voltage and the evolution of Lithium concentration after removing an DC pulse. The modeling results are compared to experimental data of ESM.

References

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