Karlsruhe Institute of Technology

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Microscopically motivated modeling of ferroelectric materials

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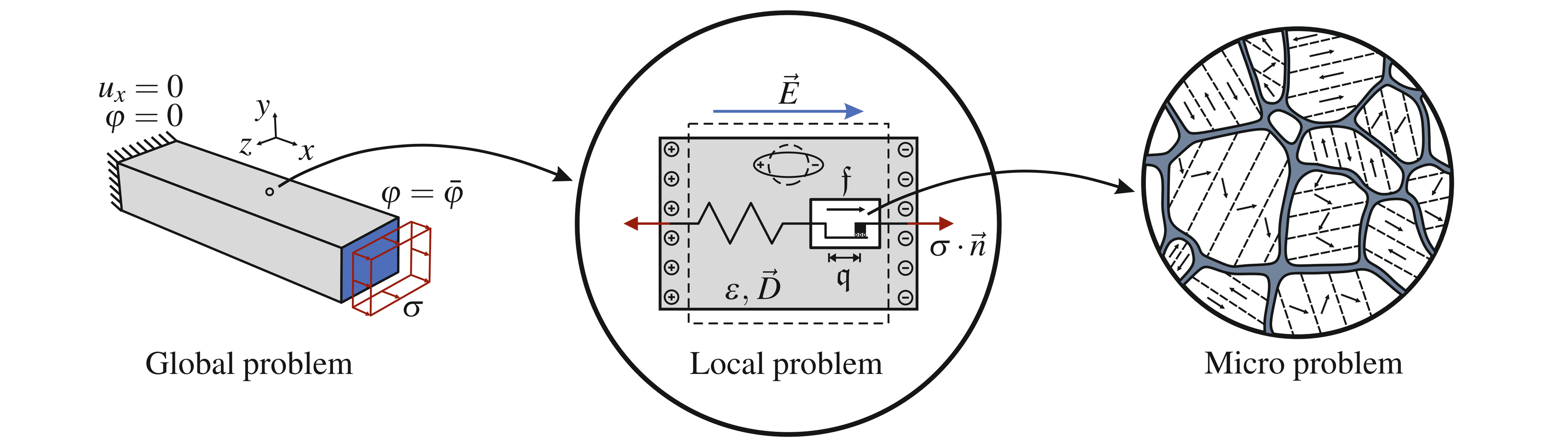
Keynotes:

- Variational formulation of a thermodynamically consistent continuum theory for electro-mechanically coupled problems
- Representation of domain switching effects by microscopically motivated internal state variables inside a phenomenological material theory
- Capability to reproduce experimentally measured macroscopic material behavior of PZT ceramics

Variational modeling framework

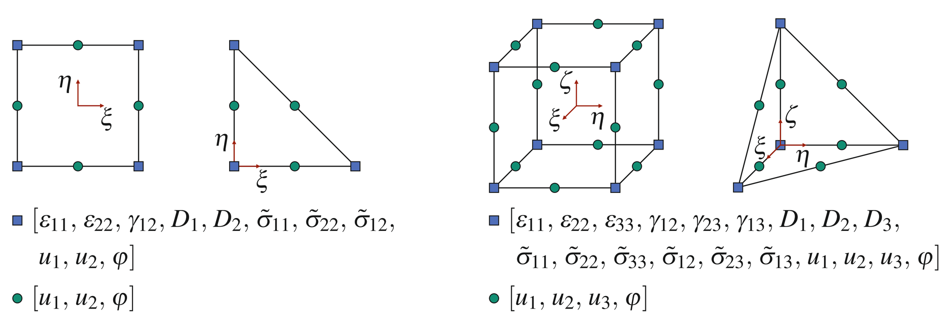
Modeling levels under consideration



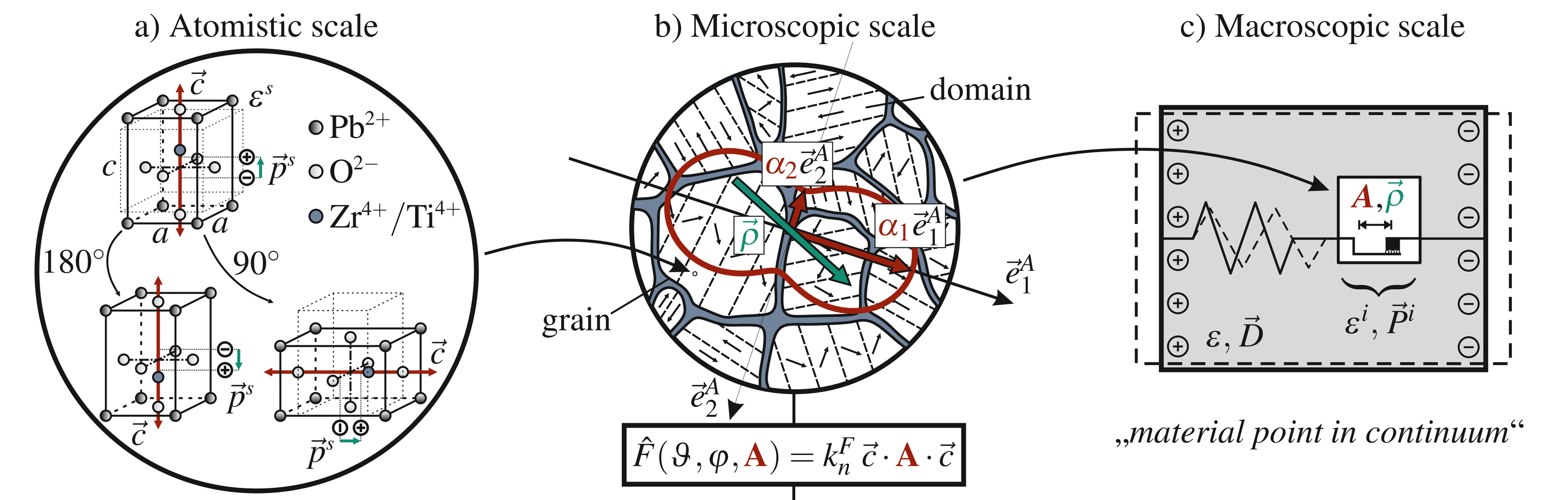
- Electro-mechanically coupled boundary value problem
- Solved by five-field finite element formulation
- Local material point element
- Phenomenological approach for representation of reversible and dissipative material behavior
- Polycristalline microstructure
- Grains subdivided in domains with intrinsic polarization state
- Switchability of domains caused by external electric fields or mechanical stresses

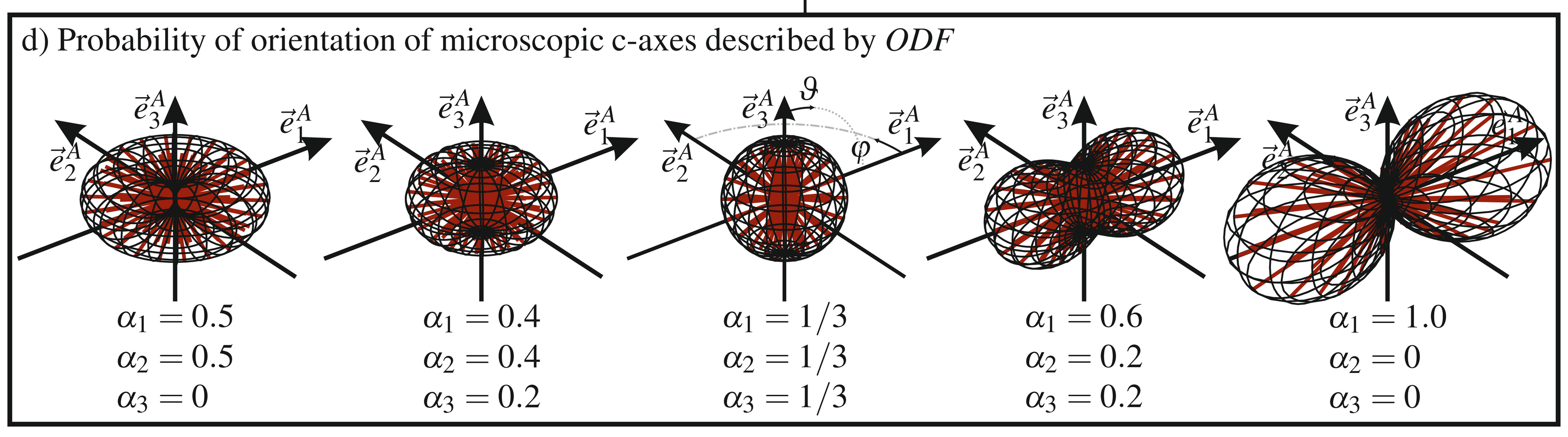
Variational formulation of the global boundary value problem and FEM

$$\hat{\Pi}^{HW}\left(\varepsilon,\vec{D},\boldsymbol{\sigma},\vec{u},\varphi\right)=\int_{\mathcal{B}} W\left(\varepsilon,\vec{D}\right)\,dV+\int_{\mathcal{B}}\nabla\varphi\cdot\vec{D}\,dV+\int_{\mathcal{B}}\boldsymbol{\sigma}:\left(\nabla^{s}\vec{u}-\varepsilon\right)\,dV+\Pi^{ext}(\vec{u},\varphi)$$

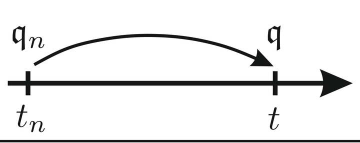


Microscopically motivated internal state variables [1]





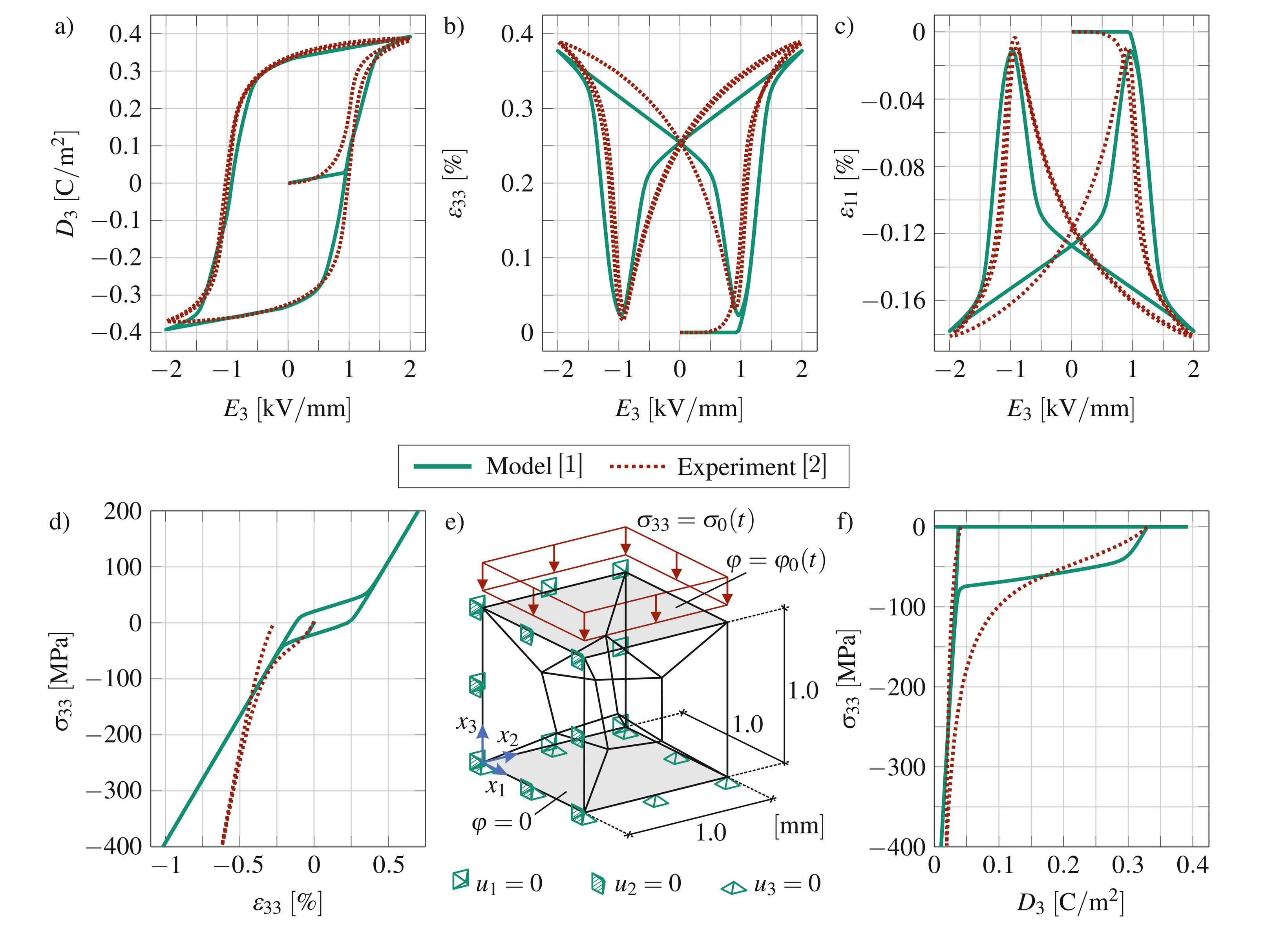
Incremental variational update of the internal state variables



$$\mathfrak{q}=\mathrm{Arg}\left\{\inf_{\mathfrak{q}}\left\{\psi(\varepsilon,\vec{D},\mathfrak{q})-\psi_n(\varepsilon_n,\vec{D}_n,\mathfrak{q}_n)+\underbrace{\sup_{\mathfrak{f}^{\mathfrak{q}},\gamma}\{\mathfrak{f}^{\mathfrak{q}}\cdot(\mathfrak{q}-\mathfrak{q}_n)-\gamma(f(\mathfrak{f}^{\mathfrak{q}})-f_c)\}}_{\Delta t\phi((\mathfrak{q}-\mathfrak{q}_n)/\Delta t)}\right\}\right\}$$

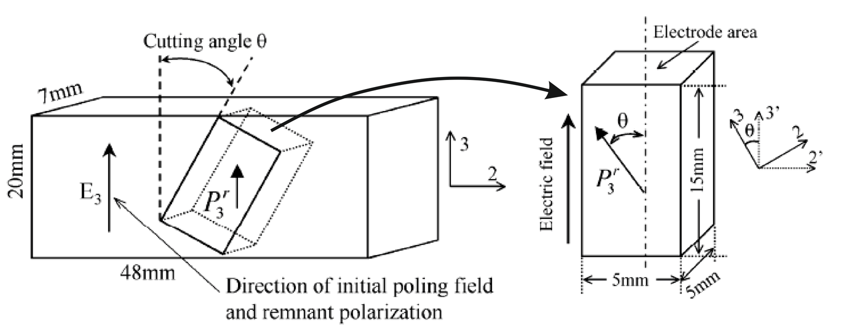
Numerical results and comparison to experiments

Characteristic hystereses of PZT

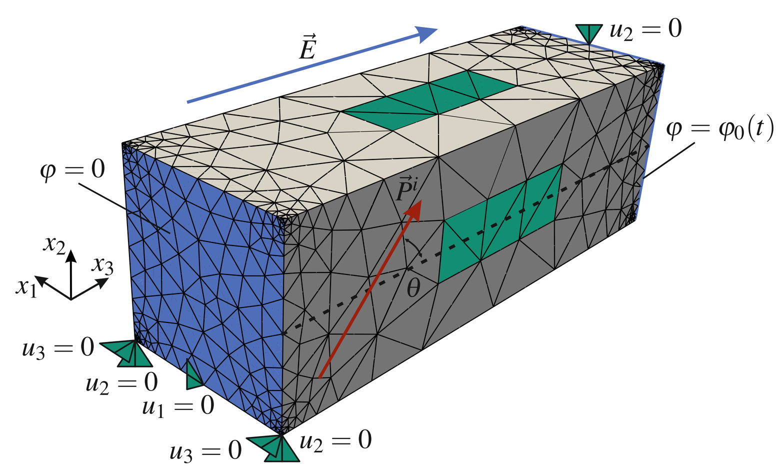


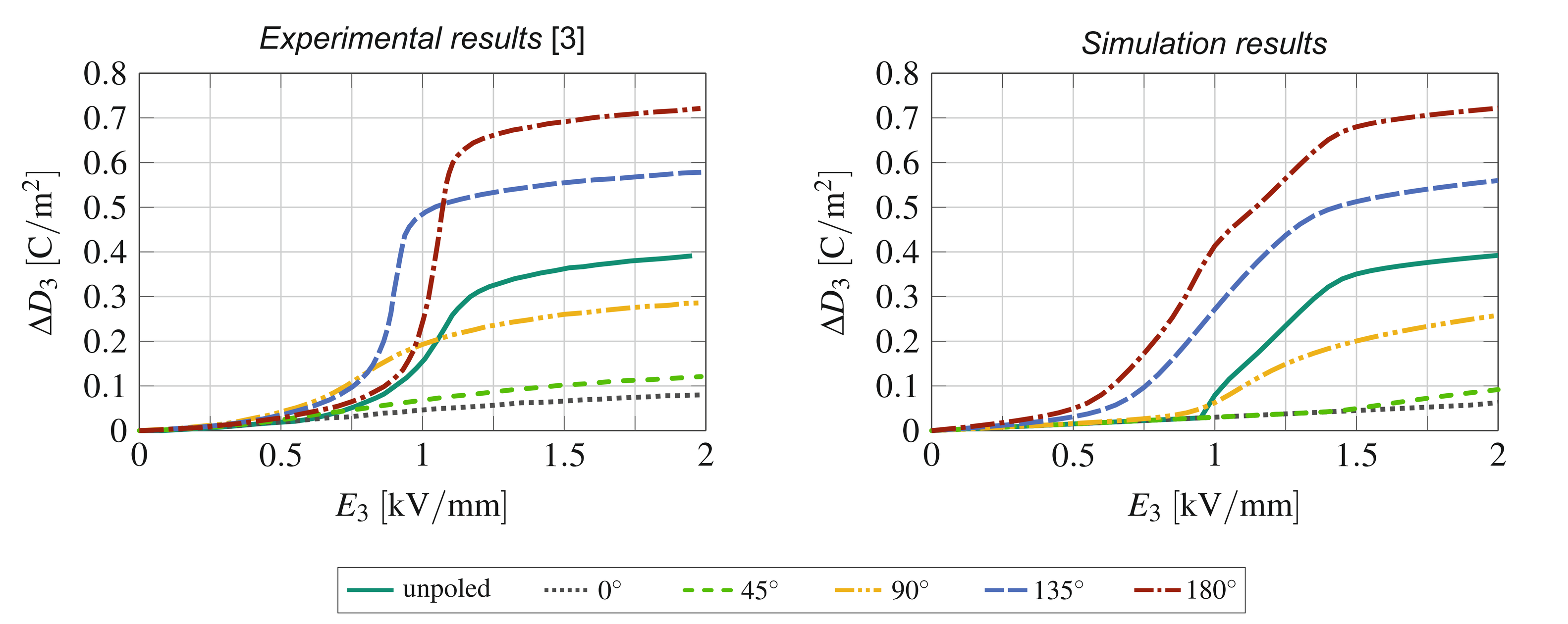
Polarization rotation test

- Specimen preparation before the experiment [3]:



- Finite element model:





Summary

- Numerically stable methods were developed and implemented in an in-house finite element code in MATLAB
- The model is able to reproduce the characteristic material behavior of PZT ceramics, even under complex loading scenarios
- Realistic simulations of the initial poling processes of piezoceramics can make a decisive contribution to the development of fail-safe actuator systems

Next steps

- Incorporation of the effect of flexoelectricity into the variational modeling framework
- Numerical investigations to the influence of the flexoelectric effect on the poling process in ferroelectric materials
- Gaining insights into the design rules of electrode layouts in order to to take advantage of the flexoelectric effect technically

[1] V. Mehling, C. Tsakmakis, D. Gross: Phenomenological model for the macroscopical material behavior of ferroelectric ceramics, J. Mech. Phys. Solids 55 (10) (2007) 2106-2141.
[2] D. Zhou: Experimental investigation of non-linear constitutive behavior of PZT piezoceramics, PhD Thesis, FZ Karlsruhe, 2003
[3] D. Zhou, M. Kamlah, B. Laskewitz: Multi-axial non-proportional polarization rotation tests of soft PZT piezoceramics under electric field loading, Proc. SPIE 6170, Smart Structures and Materials, 2006

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