On the Formulation and Numerical Implementation of Dissipative Electro-Mechanics at Large Strains

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• Variational Formulation of Ferroelectricity

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SISSA, Trieste, October 19-21, 2009

Motivation and Overview

Background

- Electromagnetic field matter interactions in deformable continua

  Hutter et al [2006], Pao et al [1978], Maugin [1988], Eringen and Maugin [1990] ....

- Constitutive equations of electroelastic solids undergoing large deformations

  Dorfmann and Ogden [2005], Bustamante et al. [2006], Bustamante et al. [2009] ...

- Numerical modeling of non-linear electroelasticity

  Vu, Steinmann and Possart, [2007], Vu and Steinmann [2007], Klinkel [2007] ...

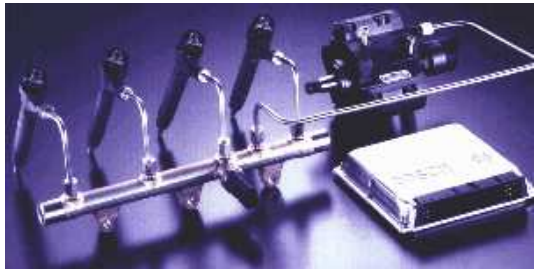
- Modeling of dissipative effects of ferroelectricity for small strains

  Kamlah [2001], Landis [2002], McMeeking and Landis [2002], Schröder and Romanowski [2005], Klinkel [2006], Miehe and Rosato [2009] ...

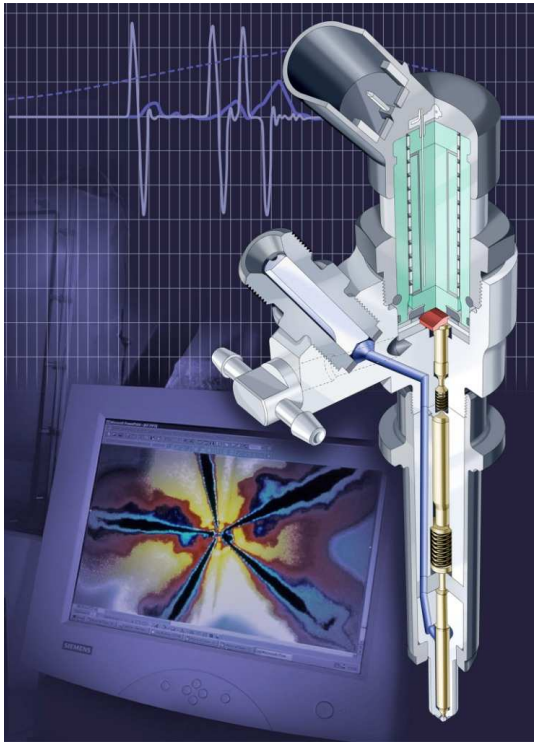
Goal of Development

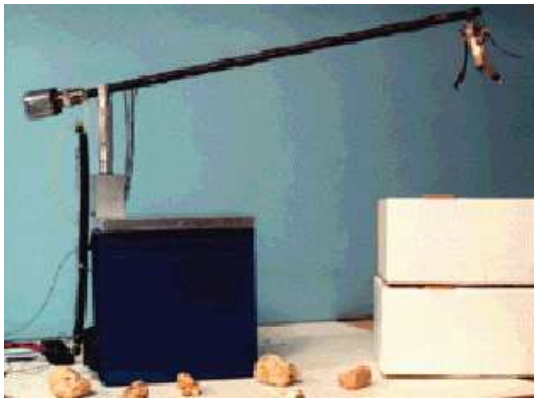
- Geometrical aspects of non-dissipative electromechanics with representations in Eulerian and Lagrangian setting
- Element of constitutive formulation of dissipative electromechanics (ferroelectricity) at large strains
- Constitutive updates and finite element formulations based on incremental variational principles

Motivation and Overview

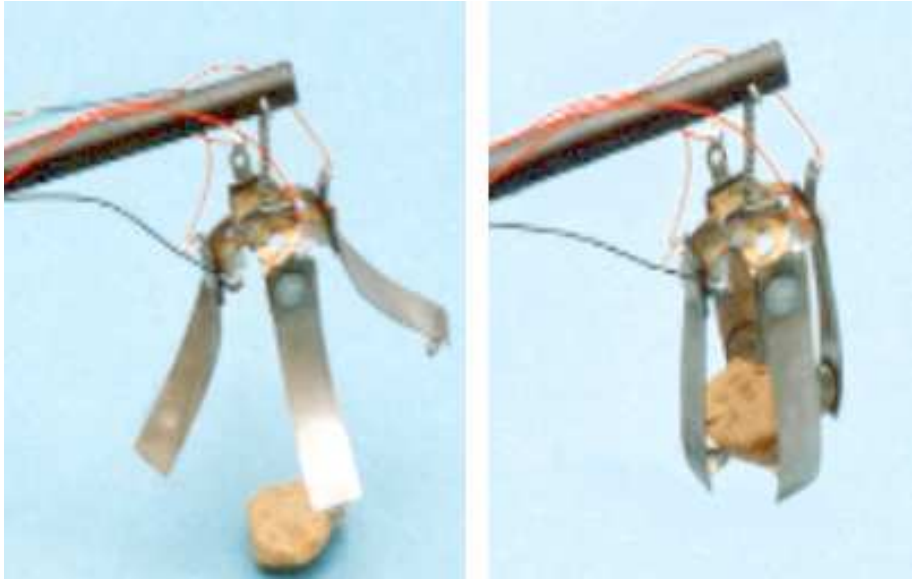


Bosch piezo inline injector
(http://www.bosch.com)

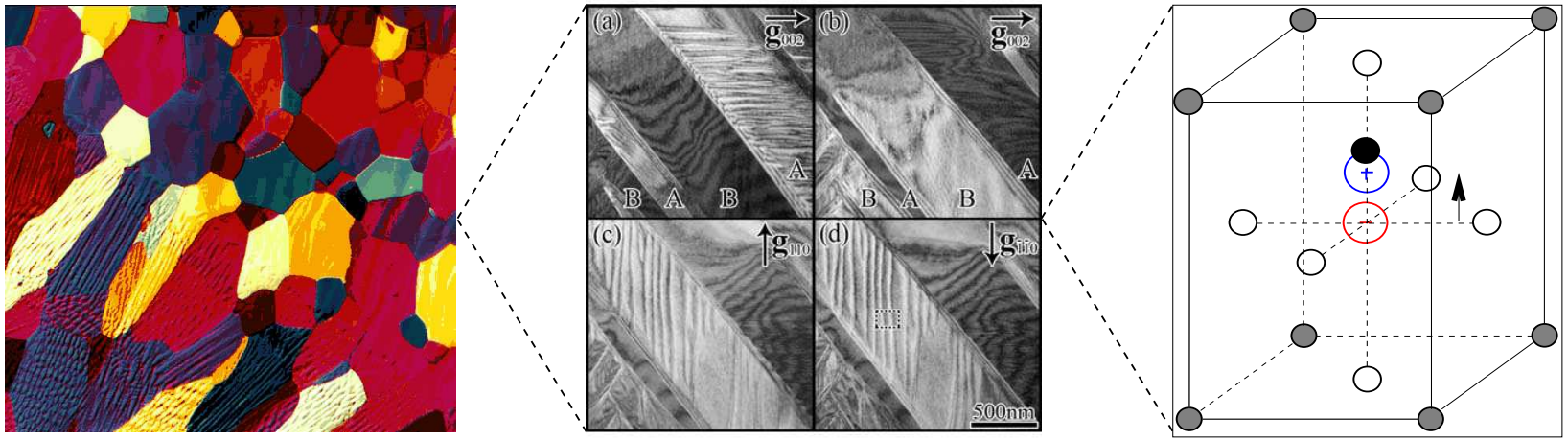




Robotic arm with 4-finger EAP gripper
(http://ndeaa.jpl.nasa.gov)



Scale Bridging of Piezoceramics

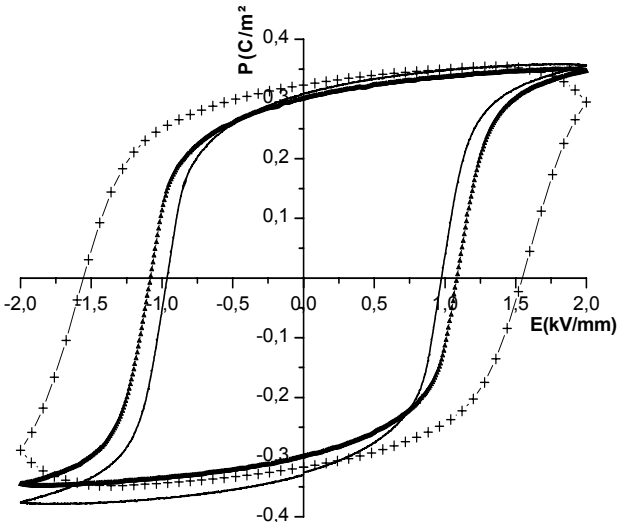


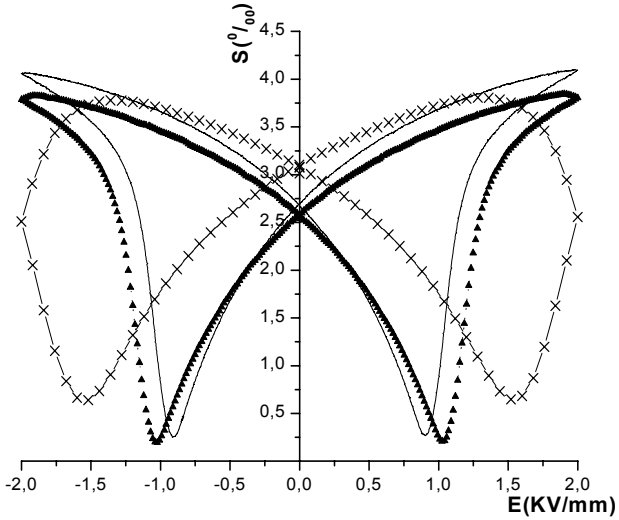
Mesoscale Microscale Nanooscale

- The typical material with piezoelectric features is a polycrystal as a result of ceramic processing techniques
- Piezoceramics are typically aggregates of several grains with differently oriented crystal lattices
- Each grain may consist of substructures, domains, regions of unit cells with equal spontaneous polarization
- The randomly distributed spontaneous polarizations cancel each other, resulting in a thermally depoled state
- The unit cell consists of a structure of positively and negatively charged ions typical of the specific material

Motivation and Overview

Time-Dependent Hysteretical Behaviour of Piezoceramics, Zhou, Kamlah & Munz [2001]

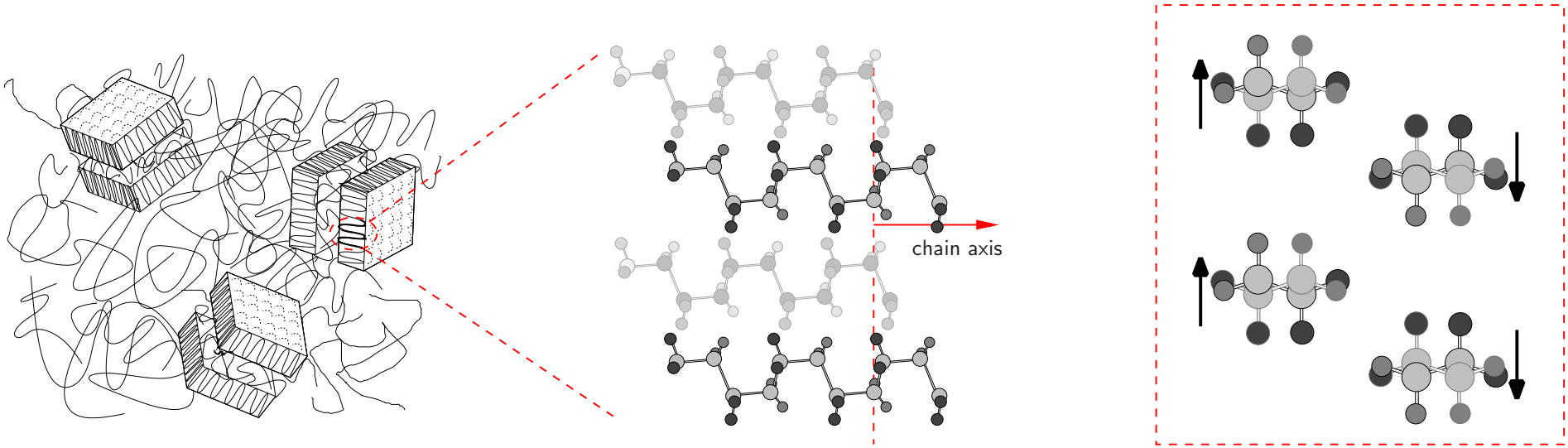




- Application of an electric field of magnitude above coercive field e_c will switch unit cells by $90\,^\circ$ or $180\,^\circ$
- After unloading, there exists a remanent macroscopic polarization, restricted by saturation polarization p_s
- After unloading, a remanent strain induced by alignment of c-axes appears, restricted by saturation strain ε_s
- Symmetry of the butterfly curves because of independence of switching strain from orientation of polarization
- Poling process leads to a transversely isotropic material with axis of anisotropy in the direction of the remnant polarization vector and an accompanying linear piezoelectric behavior

Ferroelectricity in Polymers

Microstructure of Polyvinilidene Fluoride (PVDF) demonstrating polarization mechanism



- A ferroelectric polymer is a polymer possessing unit cells in the microstructure with a spontaneous polarization
- Ferroelectric polymer encontered in a semicrystalline form with crystallites embedded in an amorphous matrix
- When prepared using the melt crystallization or solution cast, in most cases PVDF form α–pase
- In the α–pase adjacent phases are packed such that dipole moments are perpendicular to the chain and canceling one other out. Thus the α–pase is not a polar phase

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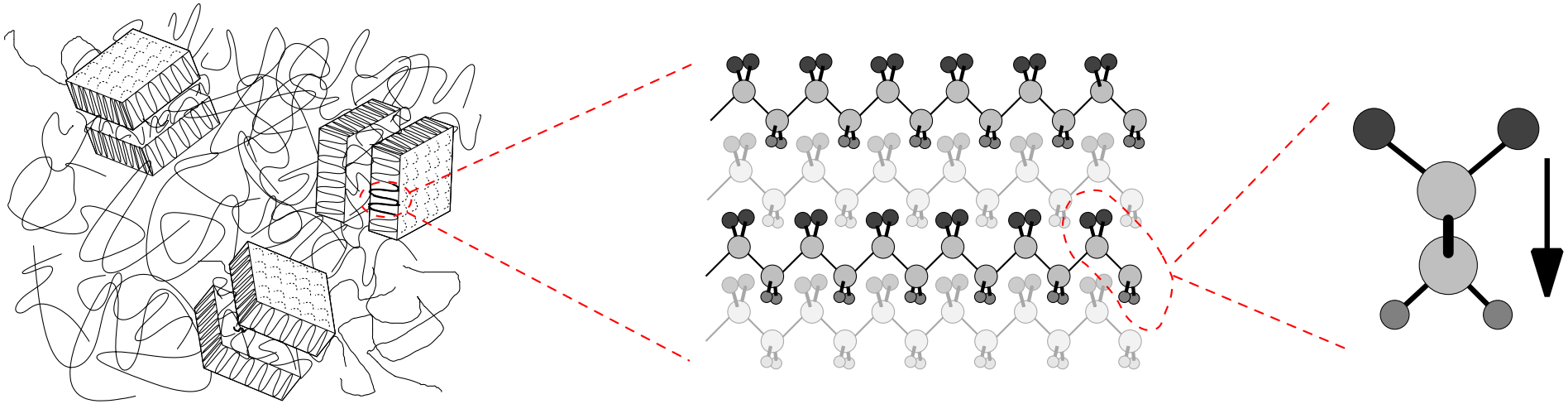
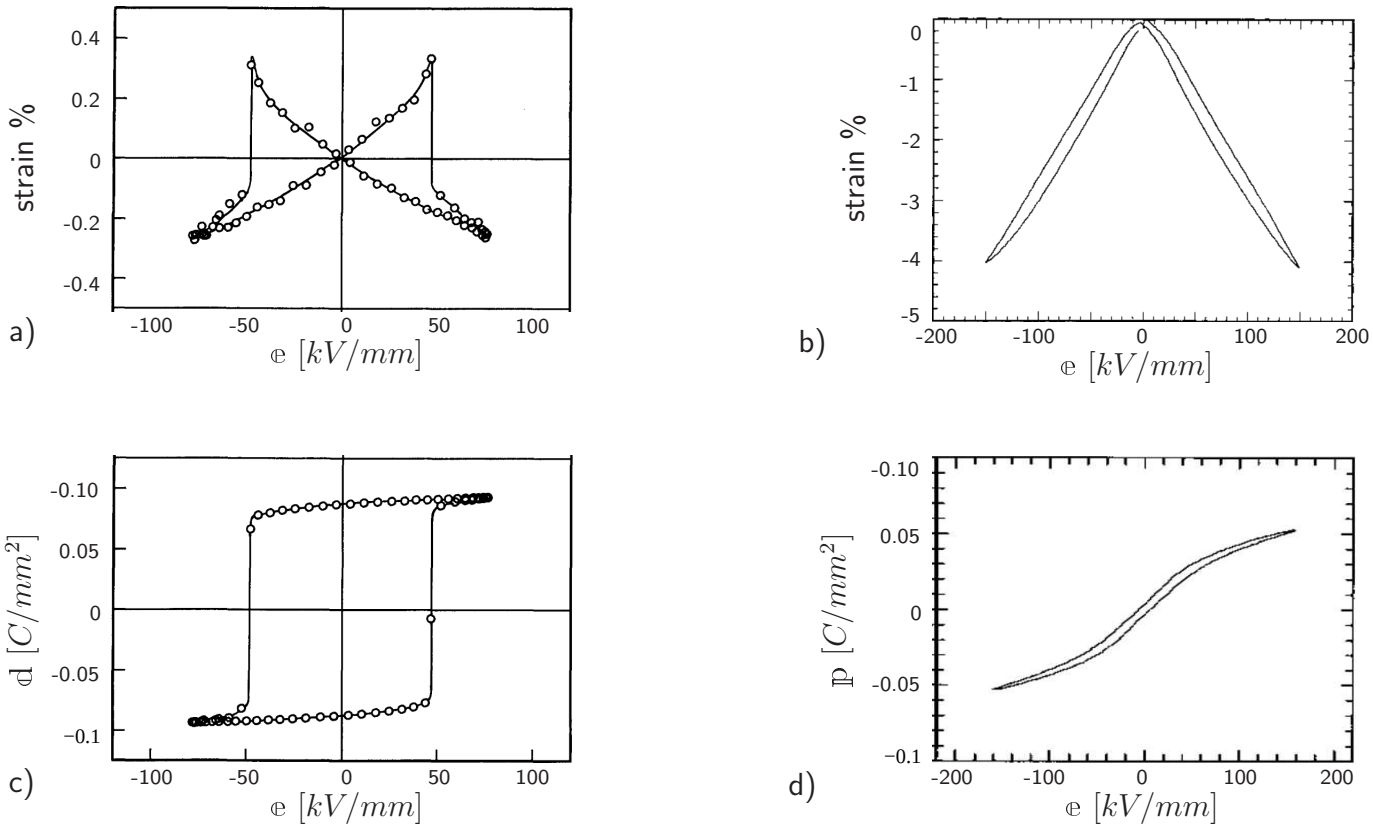


- Mechanical stretching is often used to convert the non-polar α–phase into the polar β–phase
- Copolymers of PVDF with trifluorethylene (TrFE) with VDF less than 85 mol% form directly the β–phase
- In the β–phase the fluorine and hydrogene atoms are positione on opposite sides of the chains resulting in a net dipole moment. Thus the β–phase is a polar phase

Dissipative Material Response of Ferroelectric Polymers

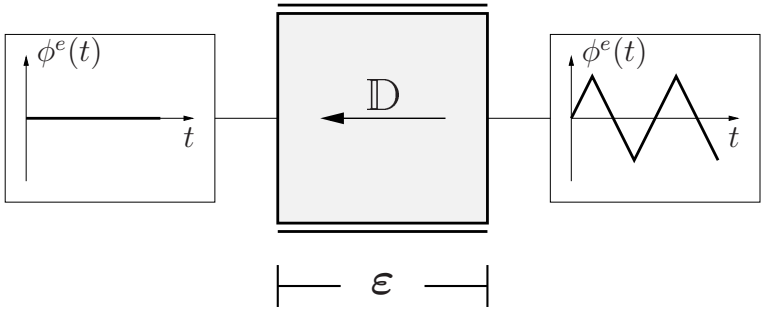
Experimental dielectric hysteresis and butterfly

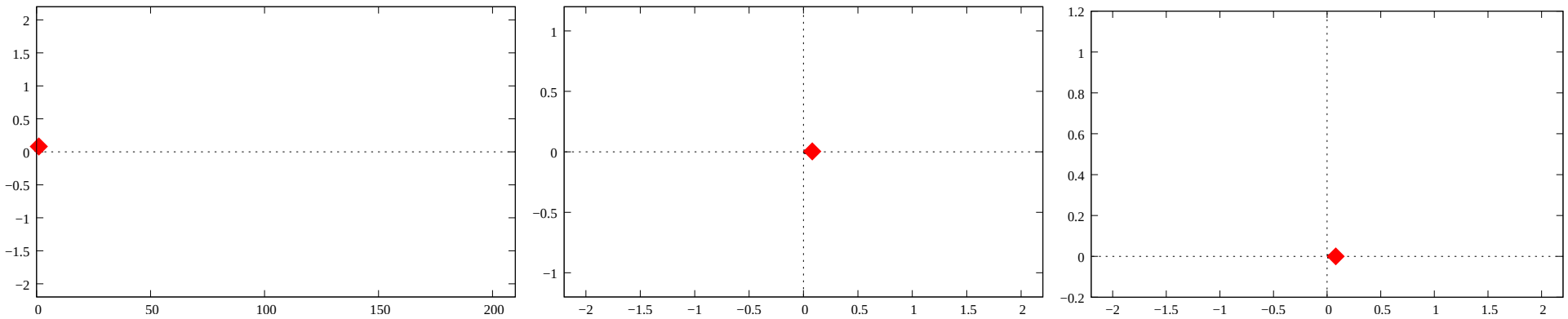


- Measured on VDF–TrFE (65/35) copolymer in natural state, a) butterfly curve, c) dielectric hysteresis
- Measured on VDF–TrFE (50/50) copolymer in irradiated state, b) butterfly curve, d) dielectric hysteresis
- Basis for simulations are Zhang, Bharti & Zhao [1998] and Furukawa & Seo [1990]

Dissipative Material Response of Piezoceramics

Time-dependent dielectric hysteresis and butterfly curves





$\mathbb{E}$ vs t $\qquad$ $\mathbb{D}$ vs $\mathbb{E}$ $\qquad$ ε vs $\mathbb{E}$

- Orientation of the microscopic unit cells produces an hysteretical behaviour
- Different time frequencies are consider to exploit the time-dependent behavior of the piezoceramics
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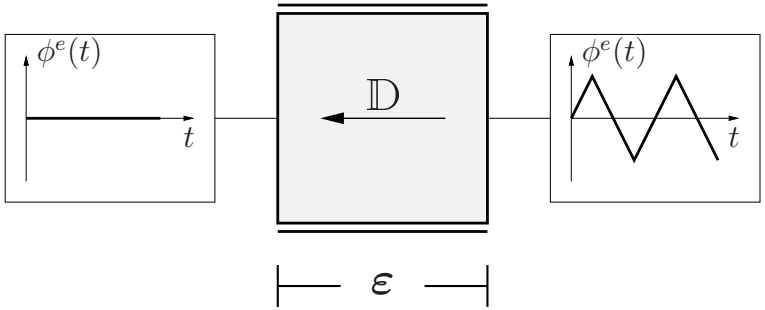

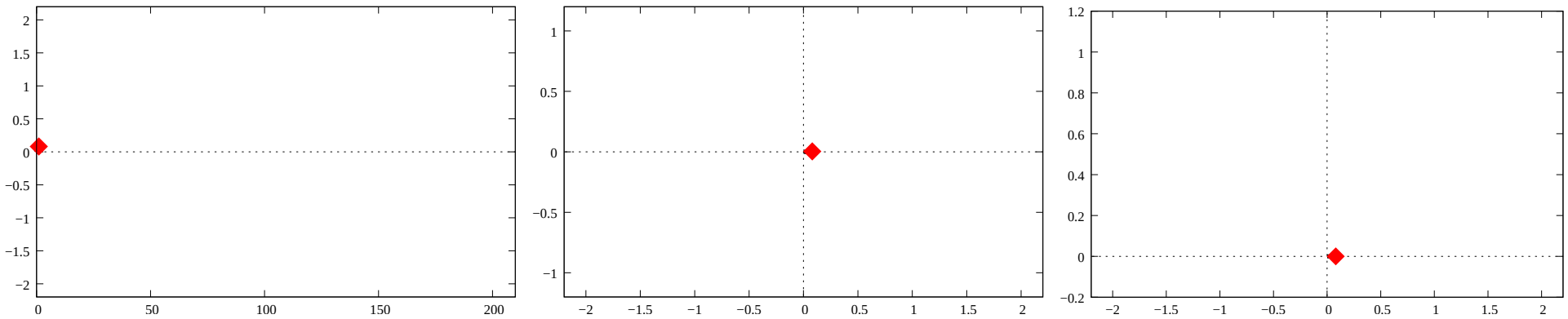

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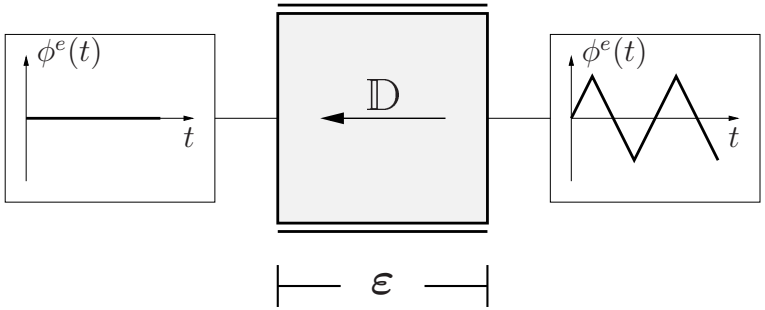

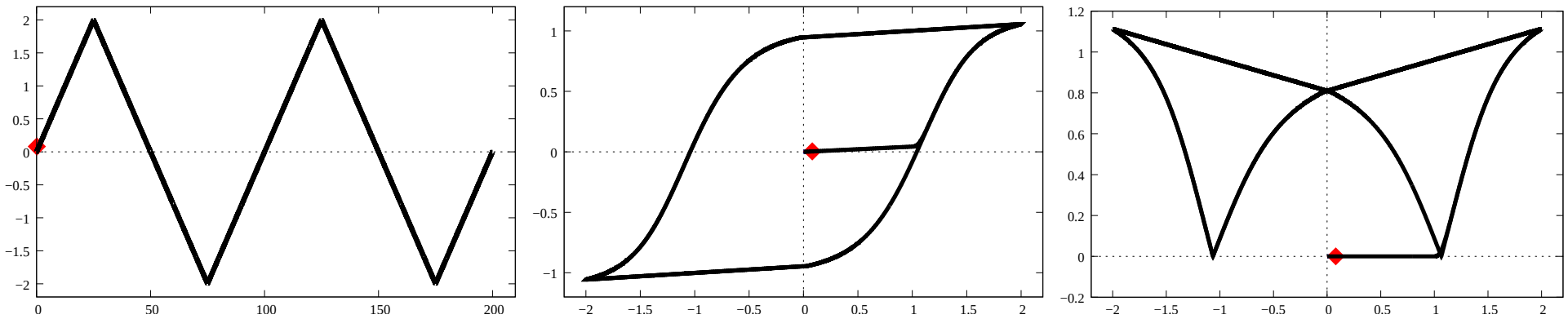

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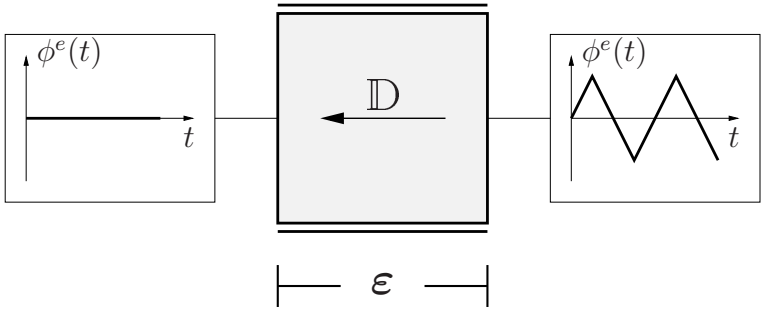

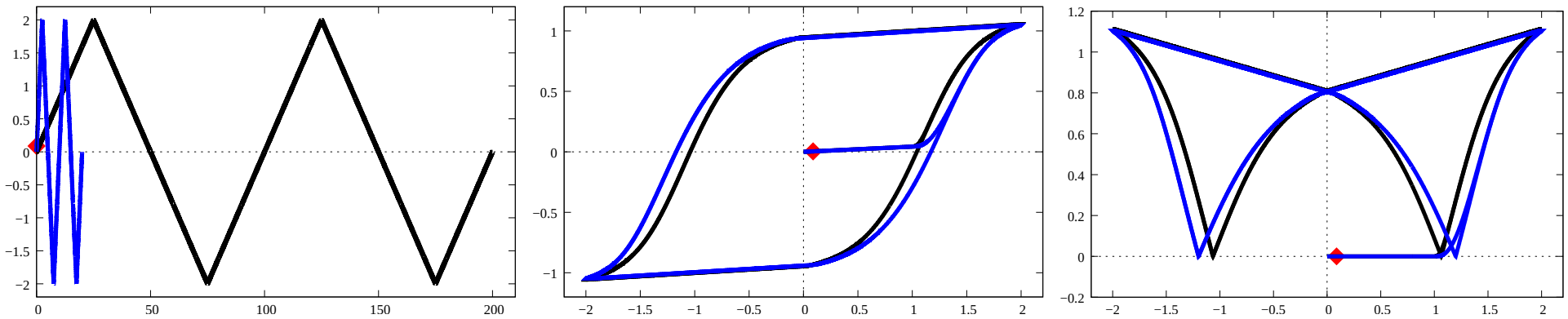

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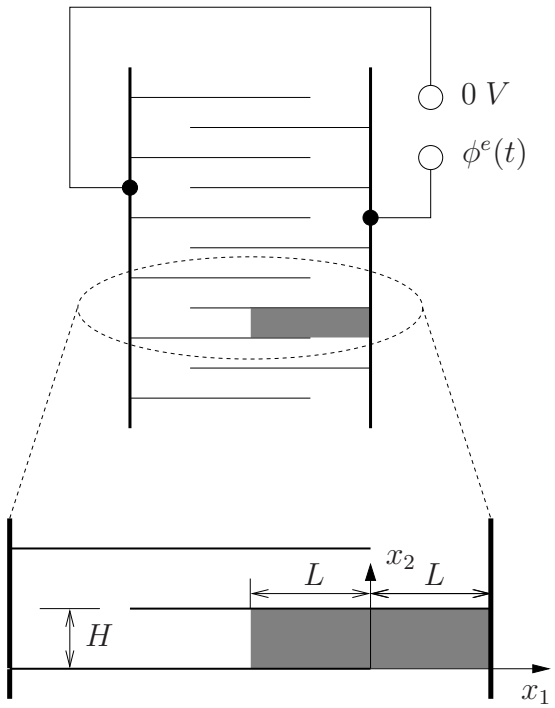
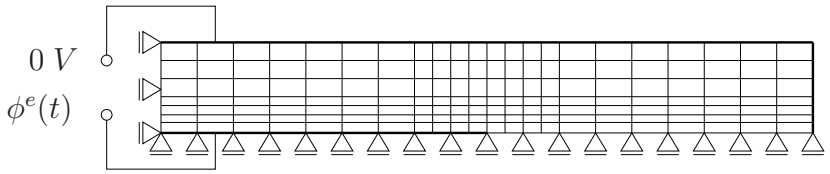
Numerical Example: Multilayer Actuator

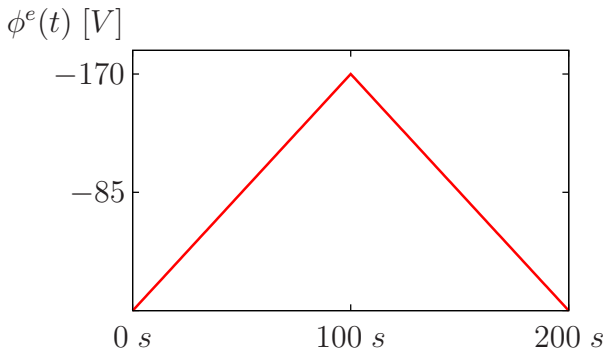
Kamlah [2001]

Schematic Representation



FEM Mesh and Loading function

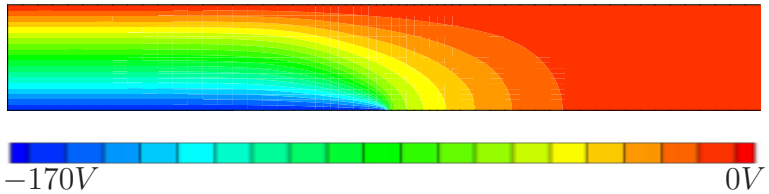


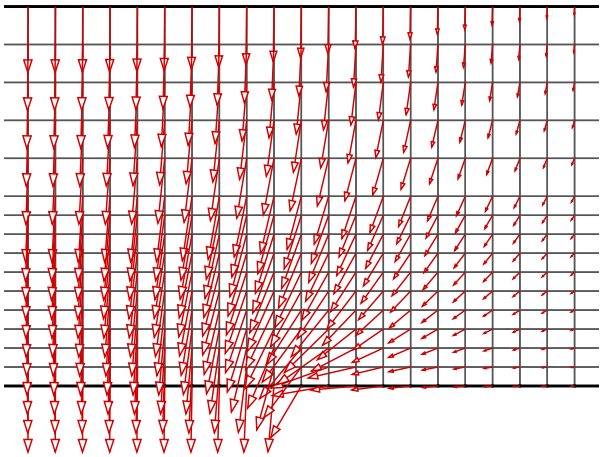


- The multilayer actuator is a typical technical application of the piezoceramics materials
- The poling process is simulated by applying a triangular-type electric potential
- Between the electrodes the coercive field $\mathbb{e}_c$ is reached and a full poling is guaranteed

Numerical Example: Multilayer Actuator

$t = 100\ s$





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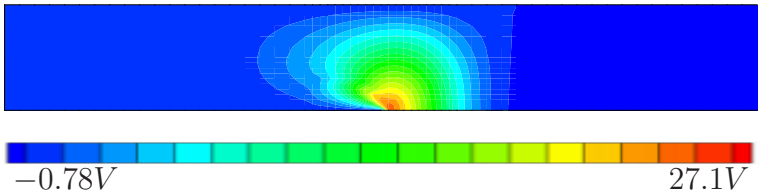
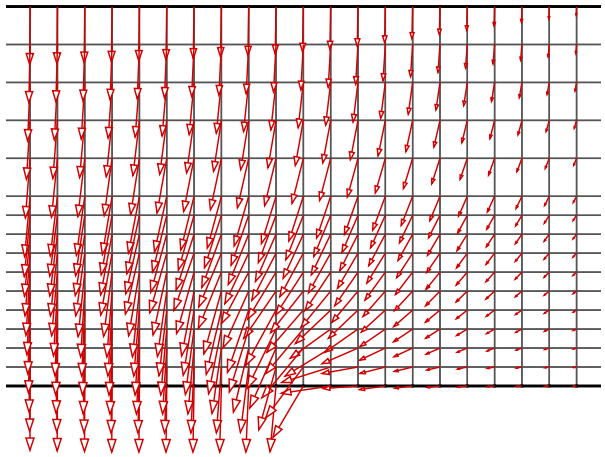
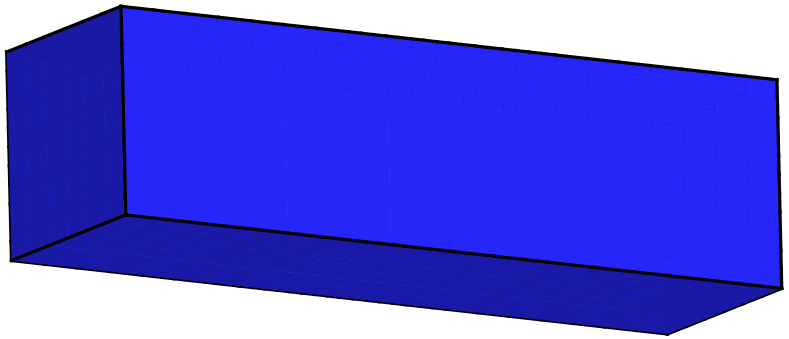
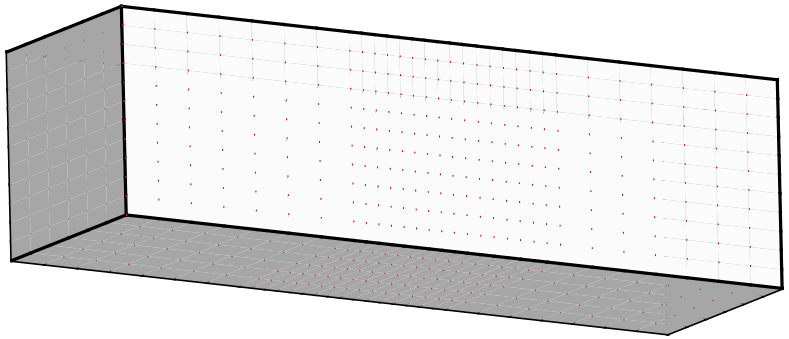




- Electric potential at $t = 100\ s$ (max applied electric potential) and at $t = 200\ s$ (zero applied electric potential)
- Uniform polarization between the electrodes in the region not closed to the electrode tip
- Distortion of the polarization in the neighborhood of the electrode tip

Numerical Example: Multilayer Actuator





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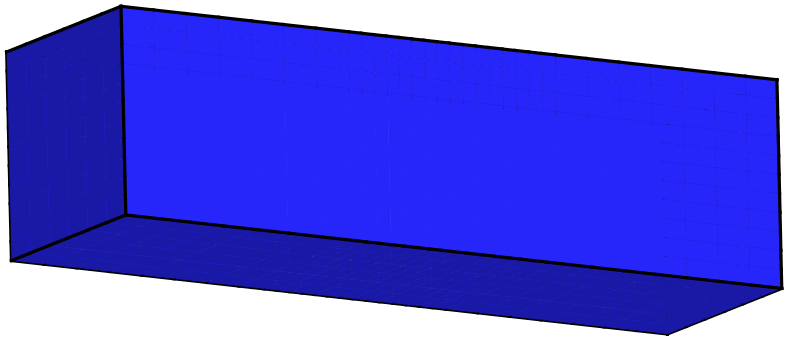

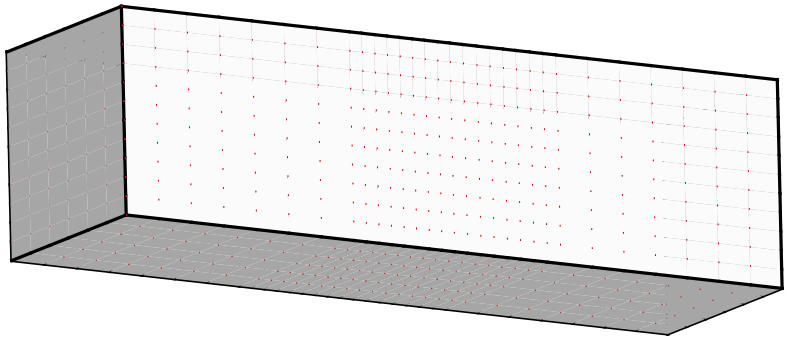

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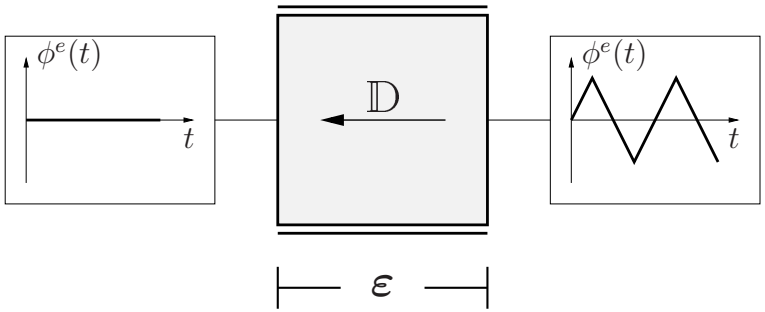
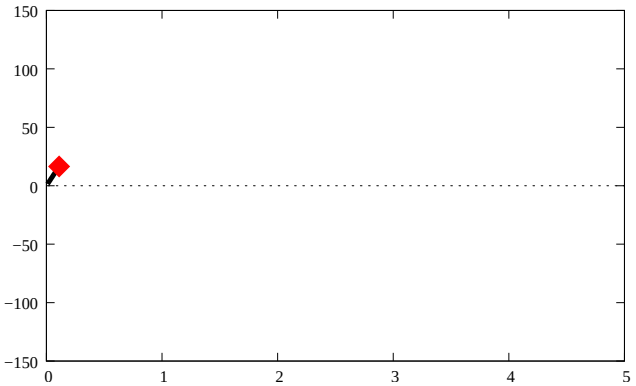
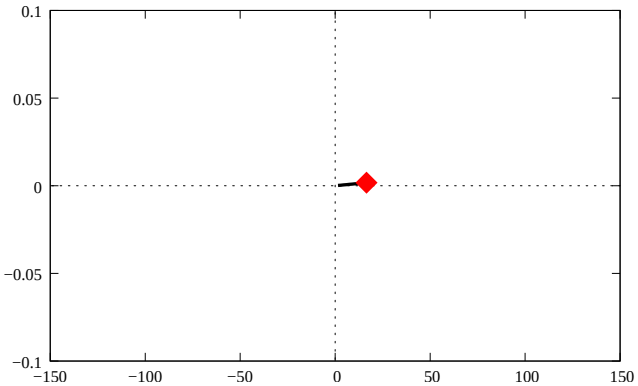
Dissipative Material Response of Ferroelectric Polymers

Time-Dependent Dielectric Hysteresis and Butterfly Curves

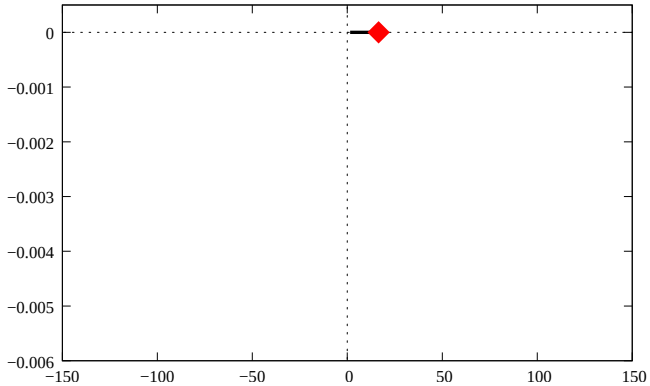




$\mathbb{E}$ vs t



$\mathbb{D}$ vs $\mathbb{E}$



ε vs $\mathbb{E}$

- Orientation of the microscopic unit cells produces an hysteretical behaviour
- The simulated response resemble the experimental one given by Zhang, Bharti & Zhao [1998] and Furukawa & Seo [1990]

Dissipative Material Response of Ferroelectric Polymers

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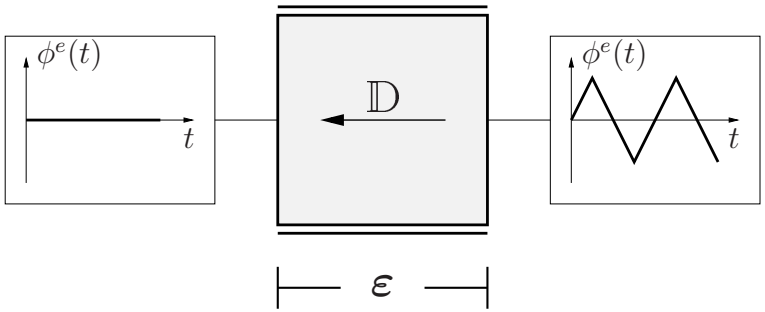

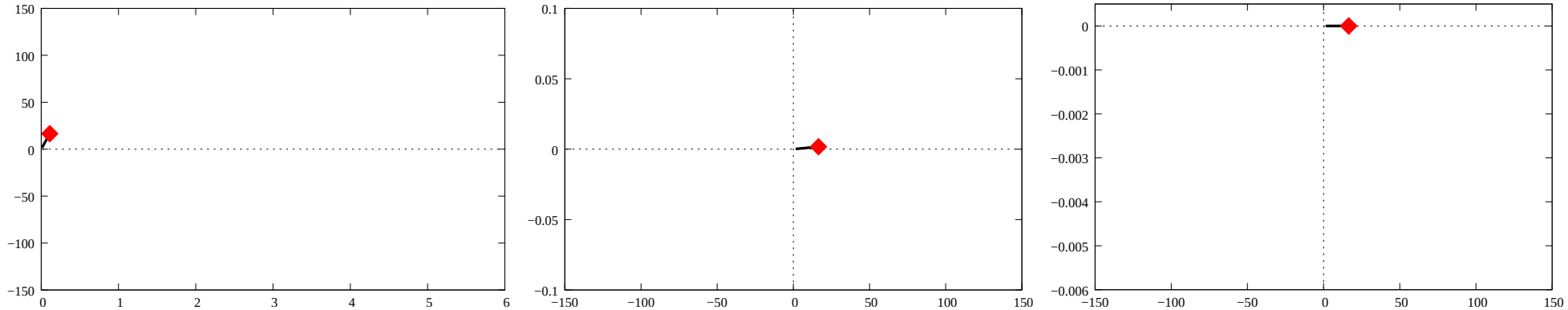

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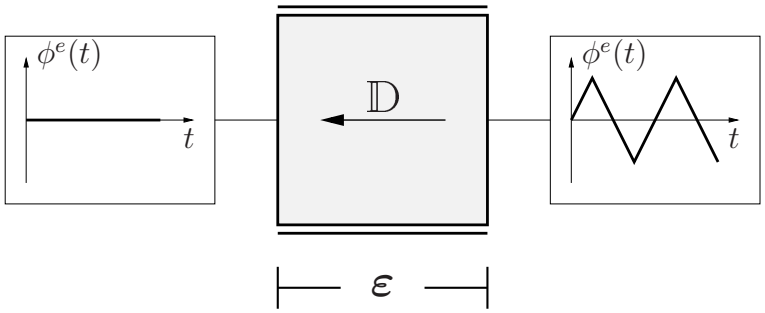
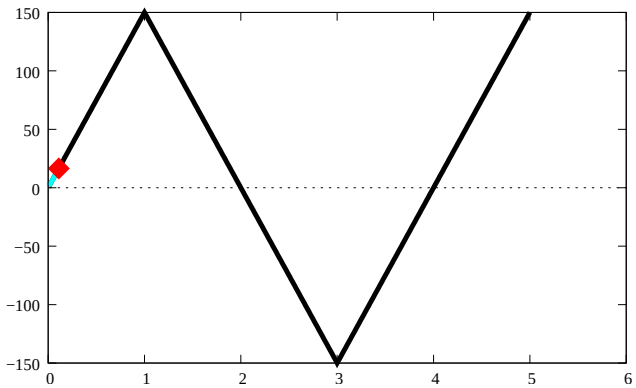
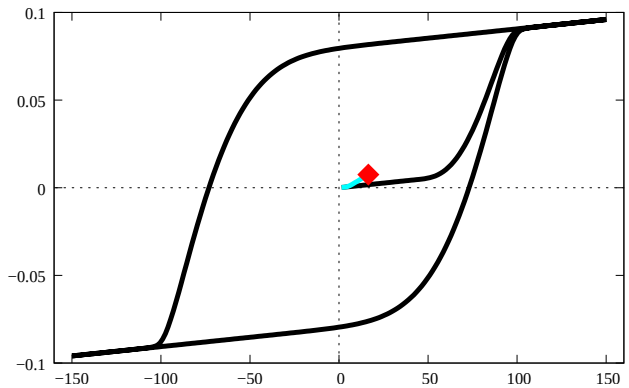
Dissipative Material Response of Ferroelectric Polymers

Time-dependent dielectric hysteresis and butterfly curves

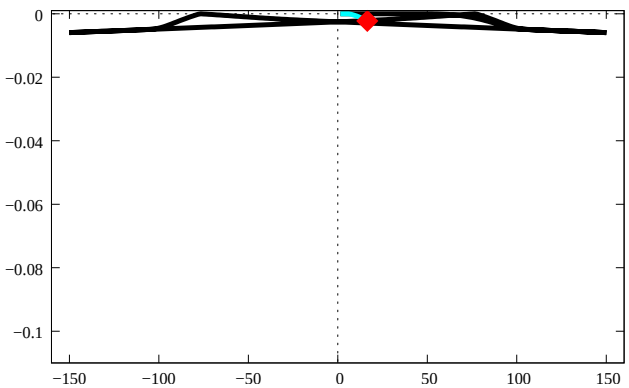




$\mathbb{E}$ vs t



$\mathbb{D}$ vs $\mathbb{E}$



ε vs $\mathbb{E}$

- Orientation of the microscopic unit cells produces an hysteretical behaviour
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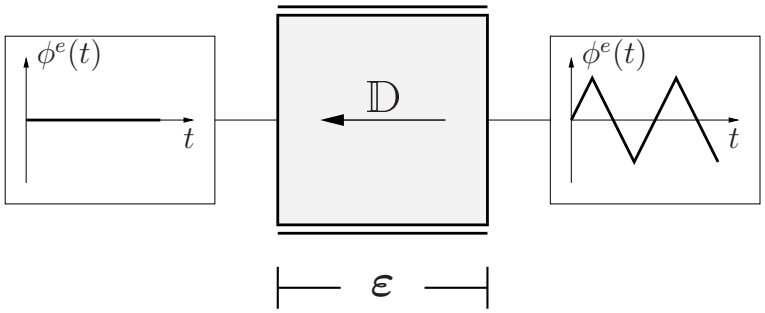
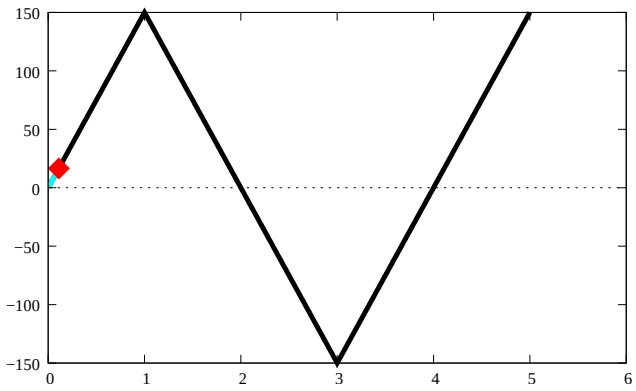
Dissipative Material Response of Ferroelectric Polymers

Time-dependent dielectric hysteresis and butterfly curves





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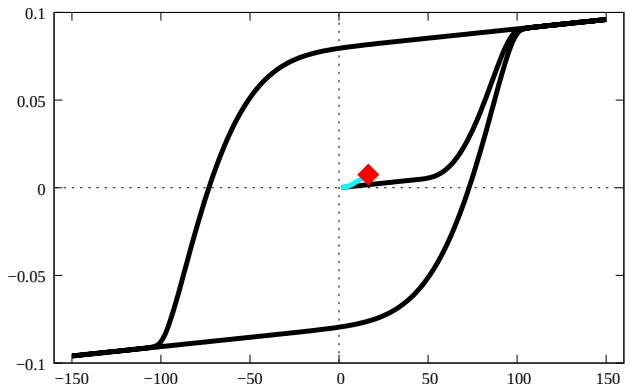

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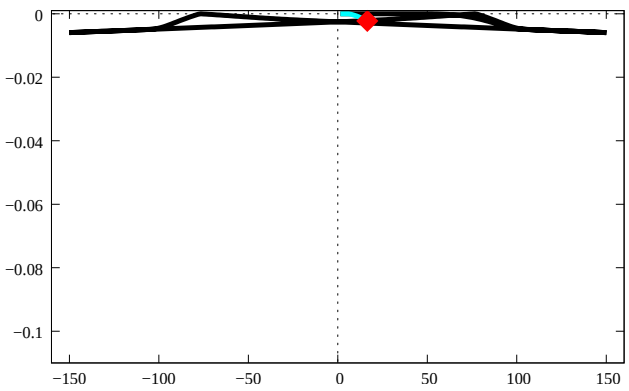

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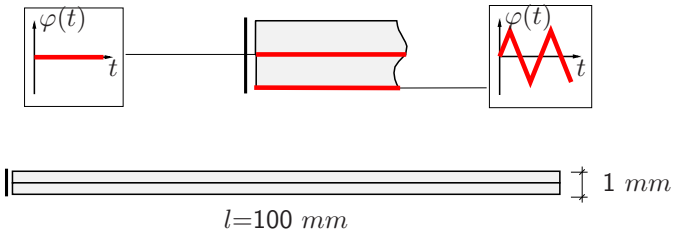
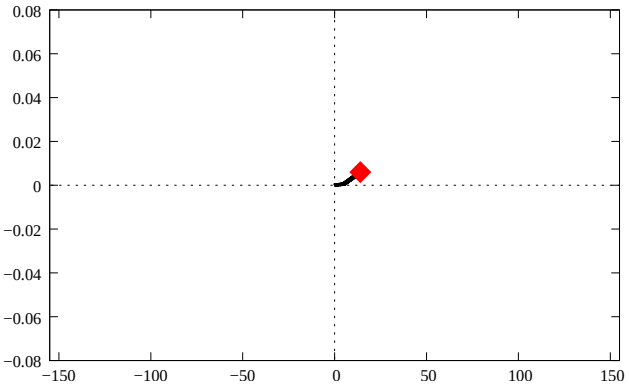
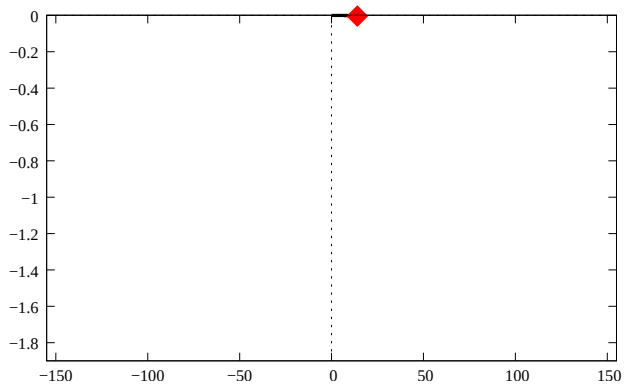
Application of Ferroelectric Polymers

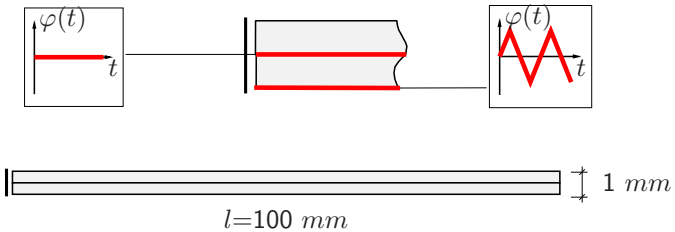


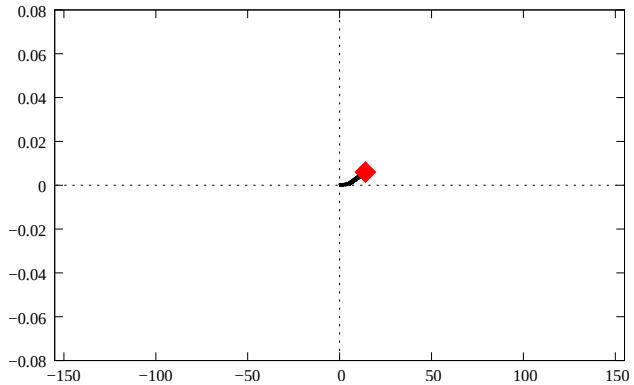


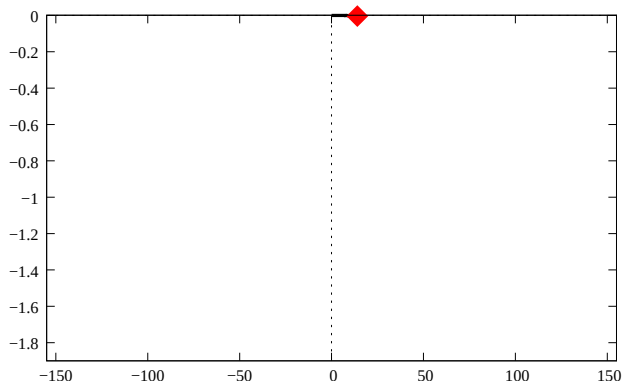


- Double finger actuator made up of two superimposed layers of ferroelectric polymers
- Only one of the two layers is activated with an electric potential difference between the upper and lower surface
- Dielectric hysteresis, butterfly curve and deformed configuration during a cyclic electric loading process
- Uniform polarization between the electrodes in the region not close to the electrode tip

Application of Ferroelectric Polymers







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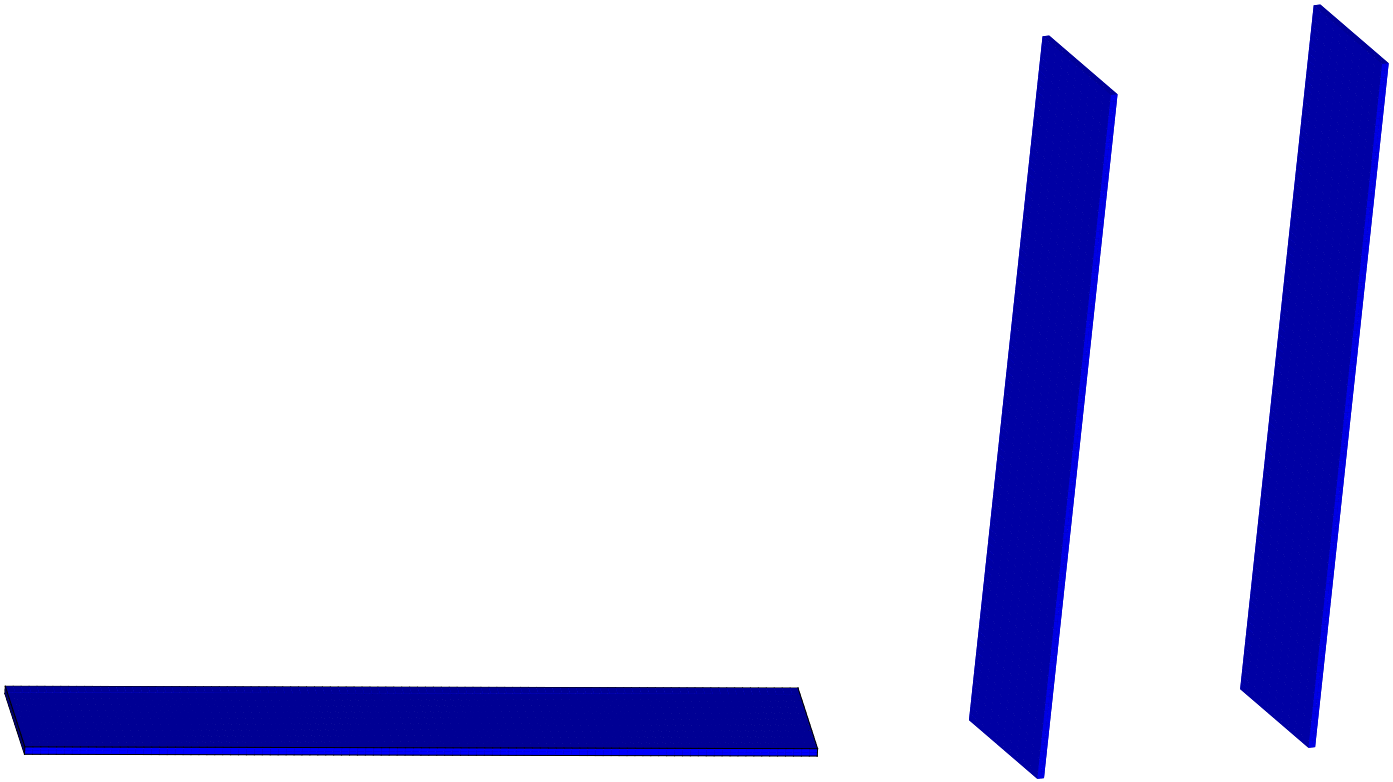

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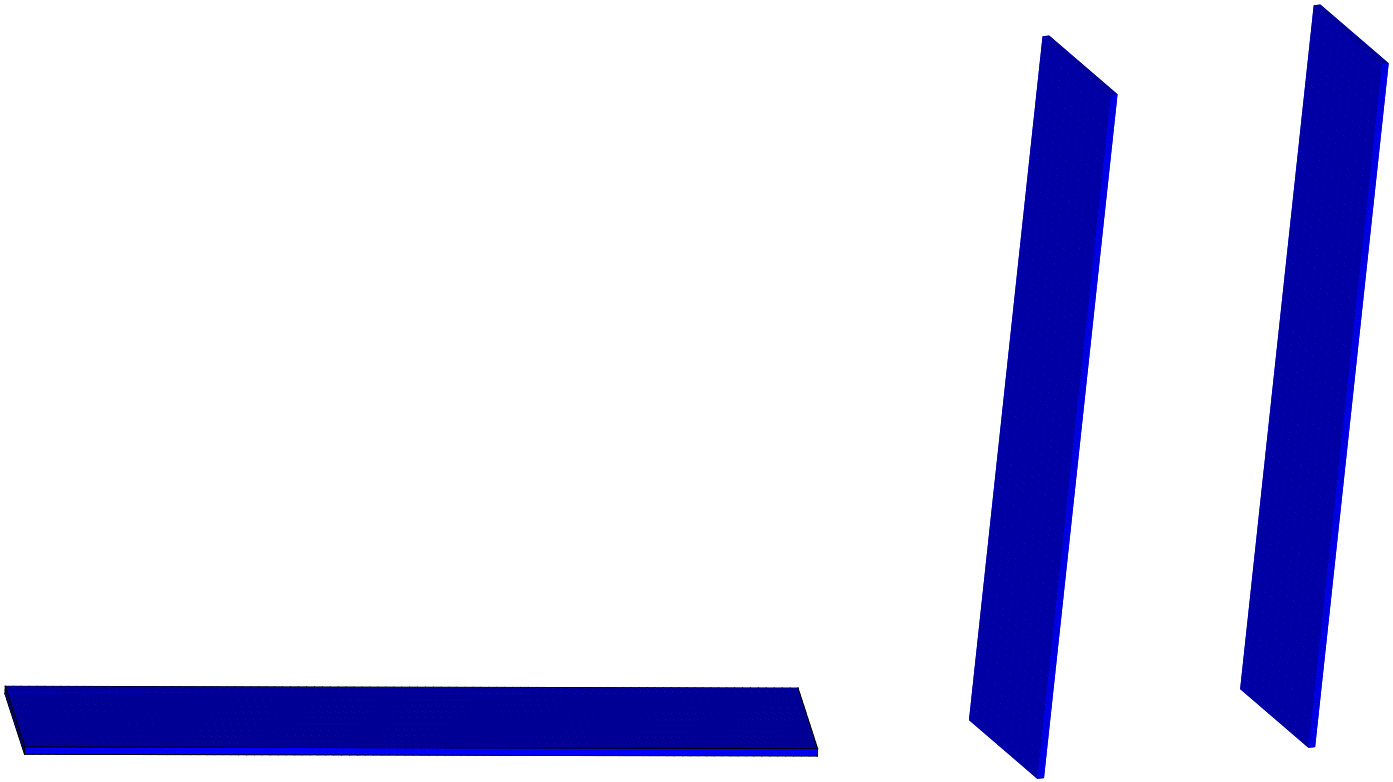

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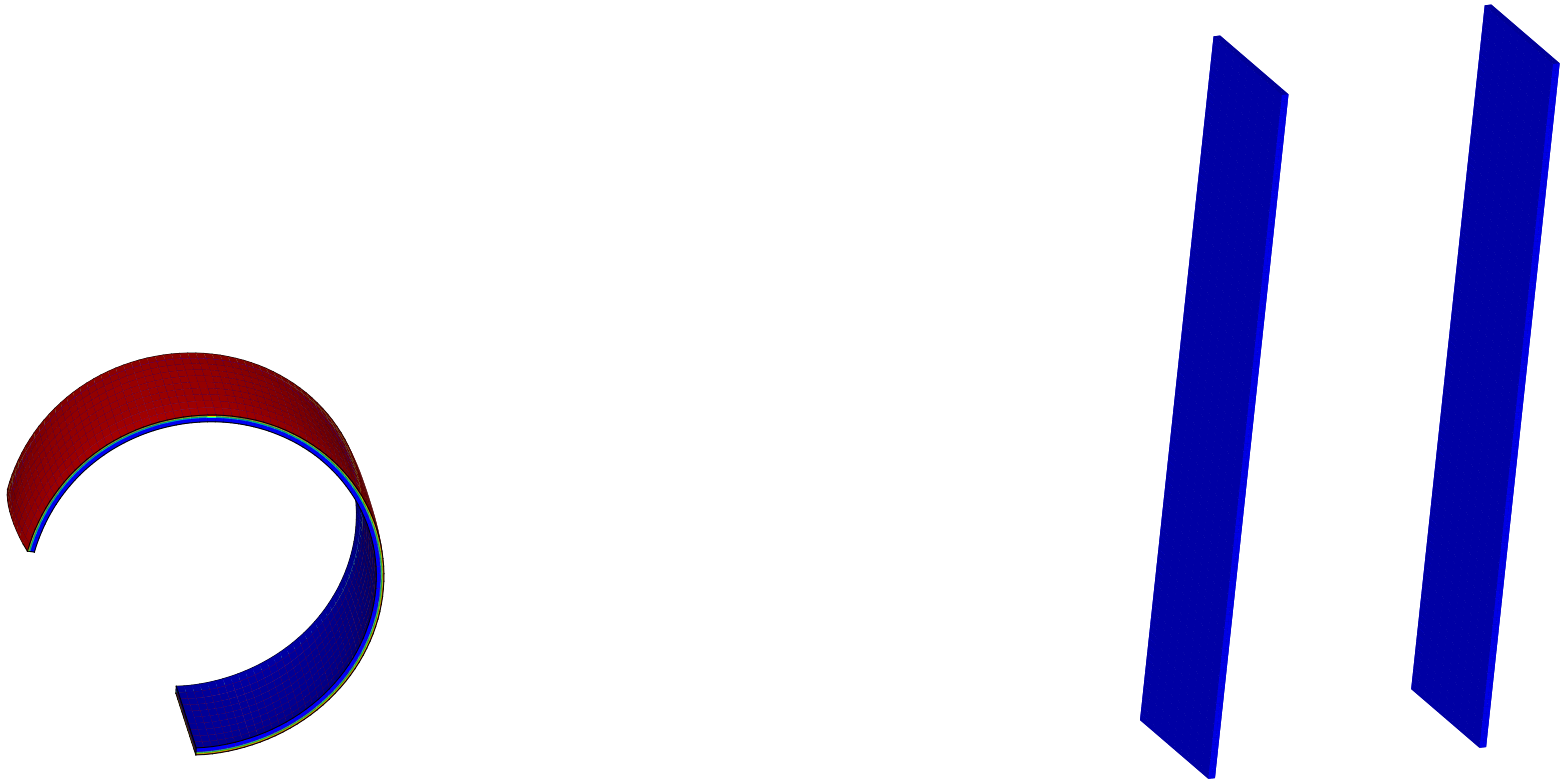

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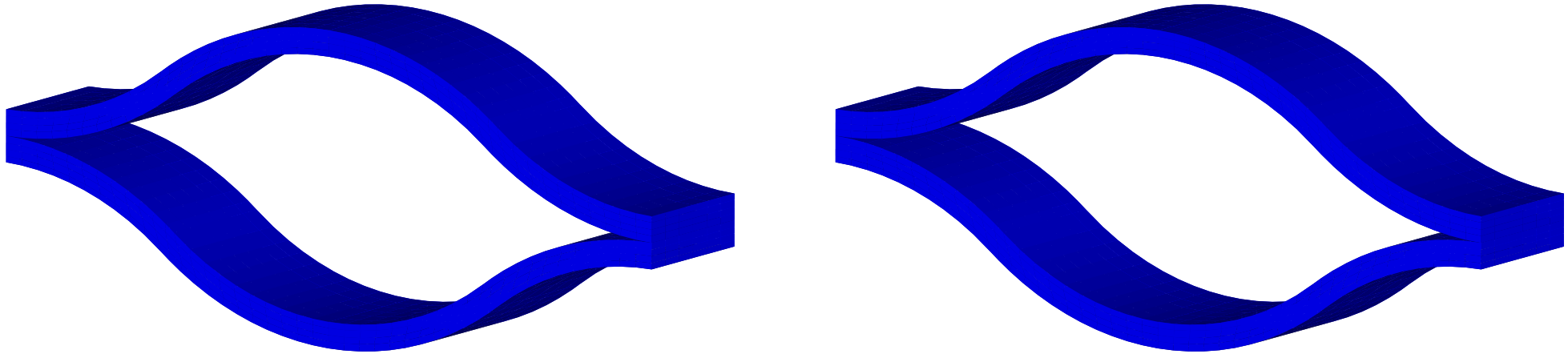
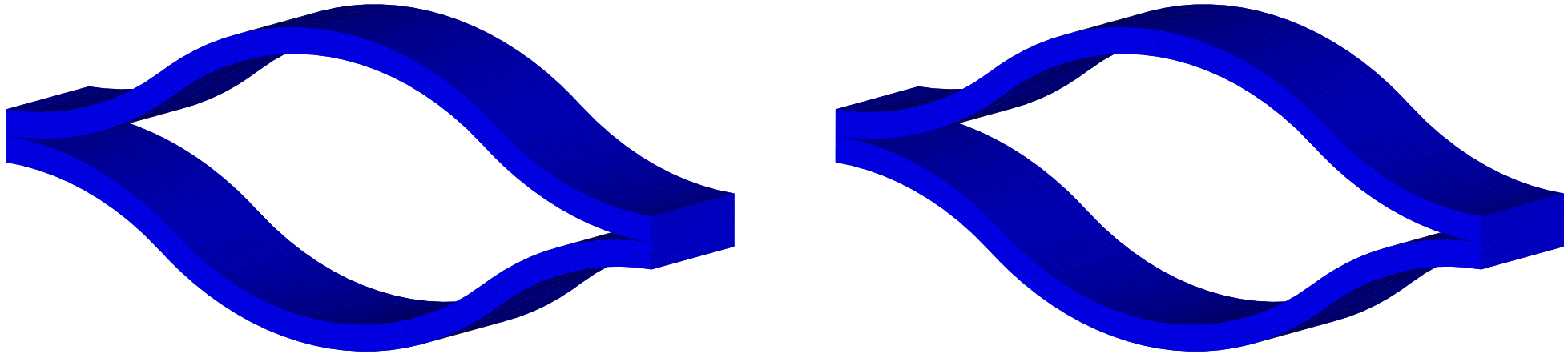


- Double-S-shaped actuator made up of two superimposed layers of ferroelectric polymers
- The inner or the outer layer is activeted with an electric potential difference
- A contact without friction between the two Double-S renders the system stiffer

Application of Ferroelectric Polymers



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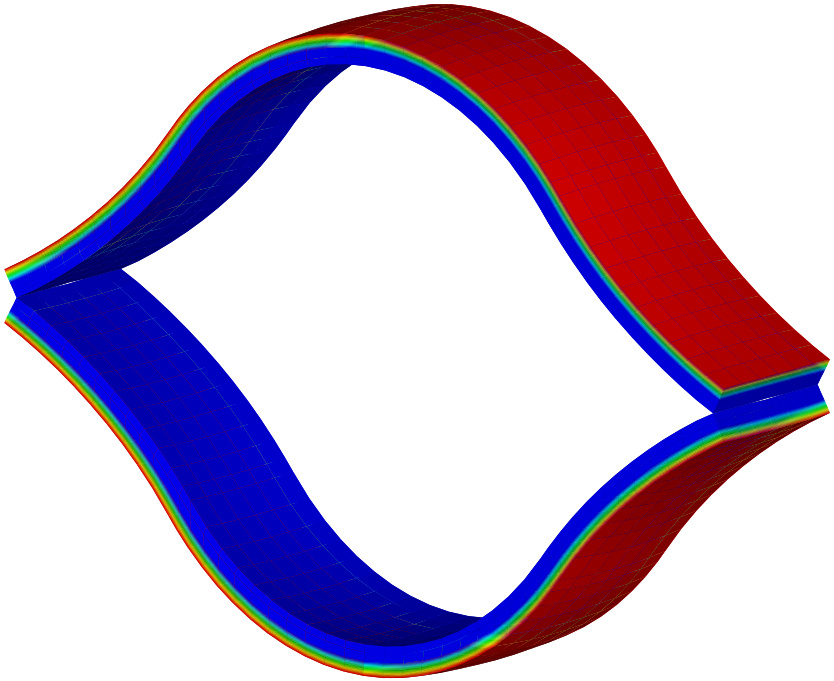

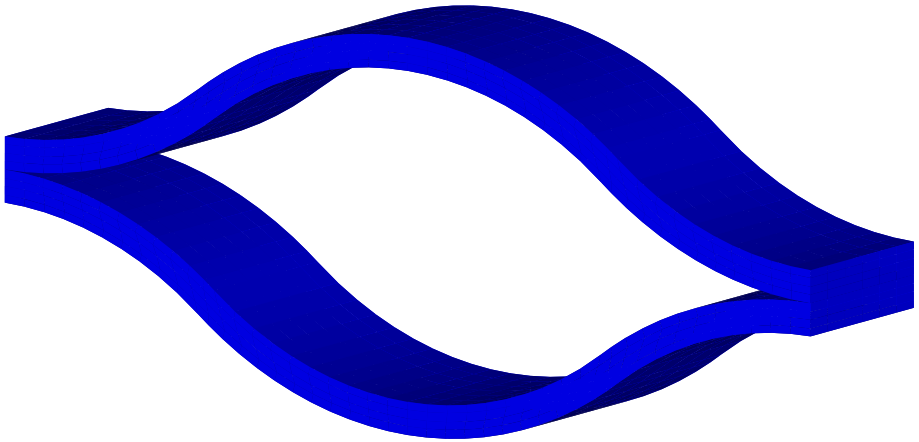

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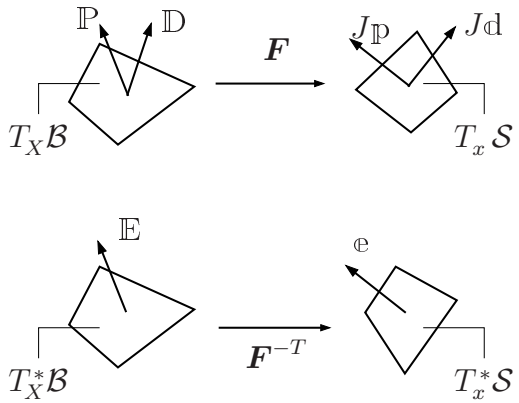
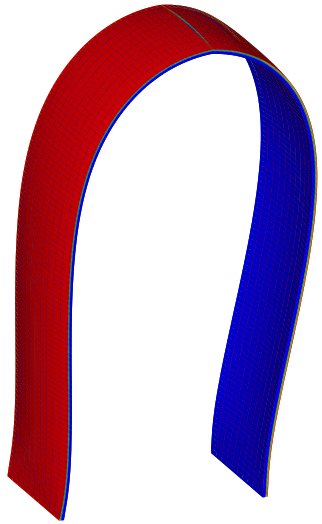
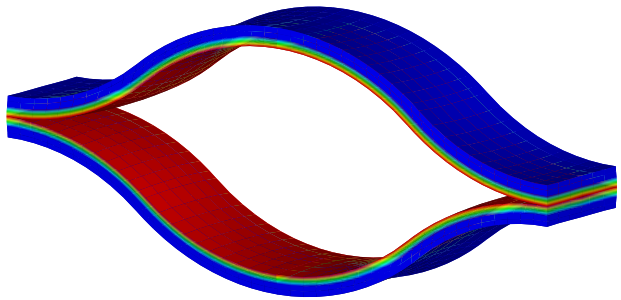
Summary

On the Formulation and Numerical Implementation of Dissipative Electro-Mechanics at Large Strains







Aspects Considered

- Formulation of electromechanics considering large deformations and using a differential geometry approach
- Incremental Variational Formulation for ferroelectrics at Large strains
- Model problem for a macroscopic response with a continuously rotating polarization vector
- Numerical examples reproducing the basic effects of ferroelectricity along with technical applications