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MECHANIK

Direct and Inverse Problems in Piezoelectricity

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Continuum mechanical modeling of non-linear ferroelectric material behavior

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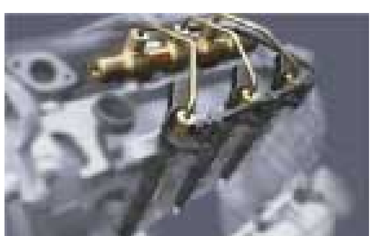

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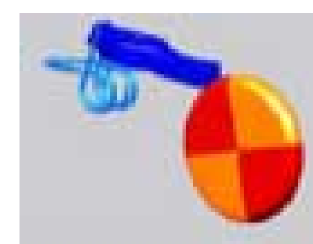
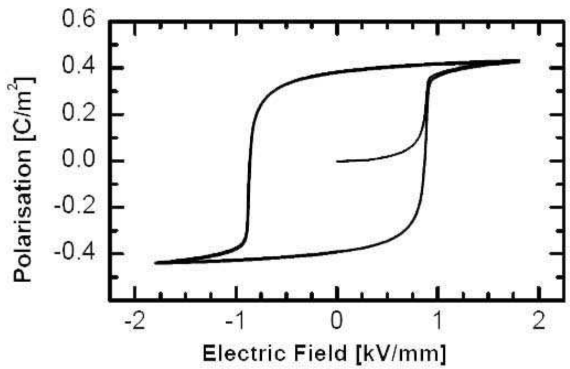


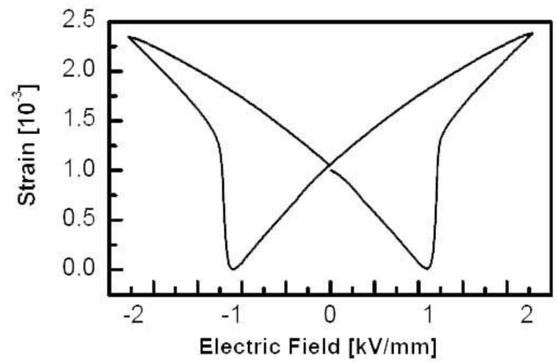
Outline

- Introduction: Phenomenology and Structure of Ferroelectrics
- Modeling of ferroelectric material behavior
  - Modeling through the lengthscales
  - Micromechanical Models
  - **Thermodynamically consistent modeling**
- Numerical Examples

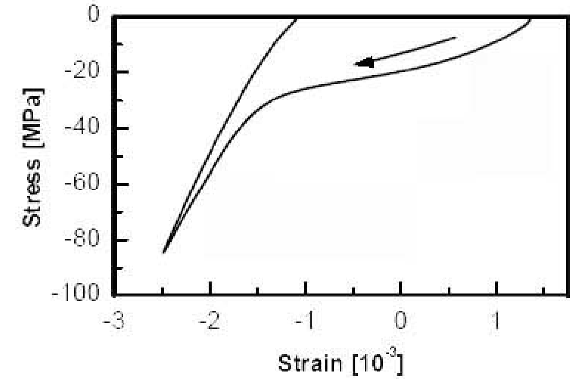
Motivation

Phenomenology of polycrystalline ferroelectrics (large field)

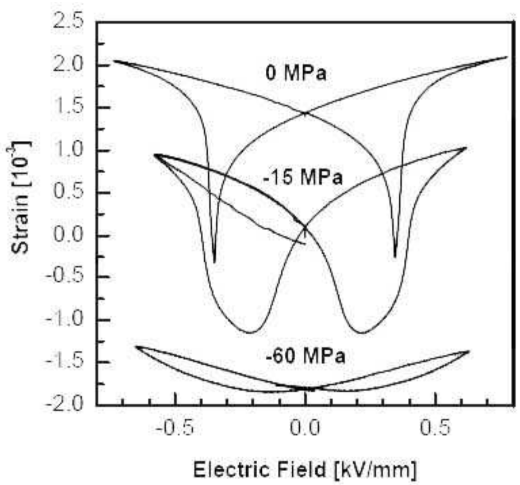




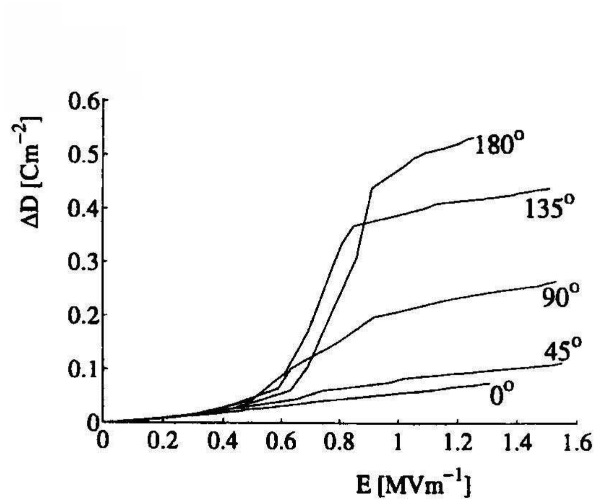
electric cyclic loading



mechanical depolarization



el.cycling + compression



repolarization

Experimental data:

LYNCH, 1996

FETT,MÜLLER,MUNZ&THUN, 1998

HUBER&FLECK, MPS, 2001

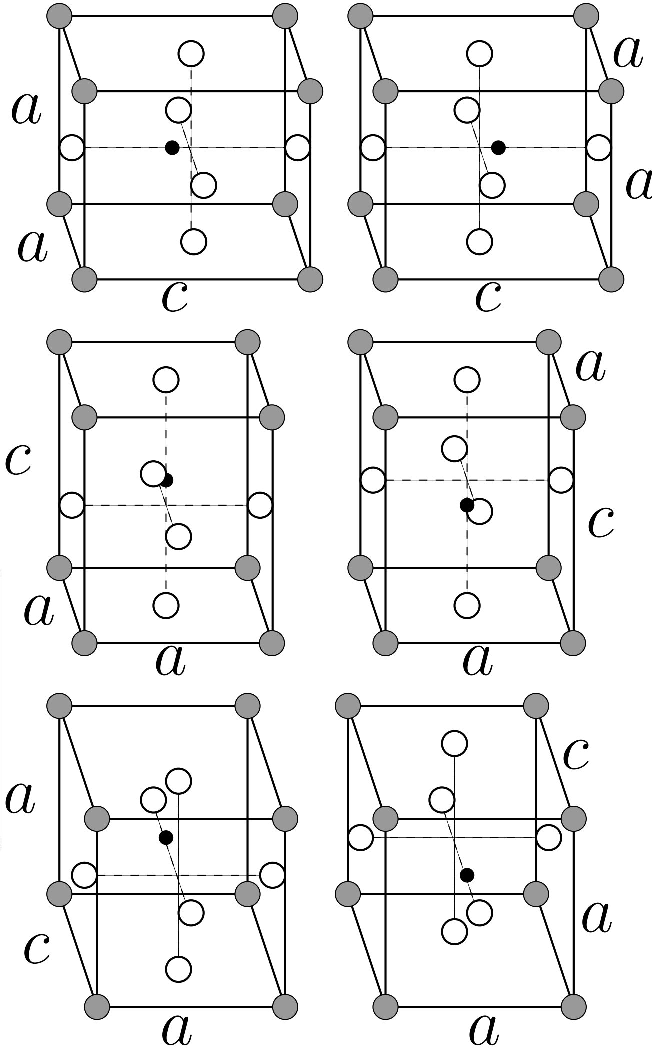
ZHOU, 2003

LUPASCU&RÖDEL, AEM, 2005

and others.

Examples:

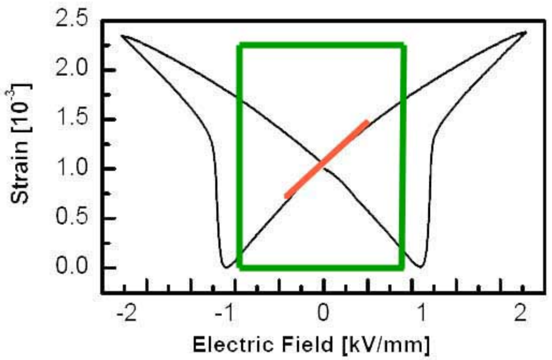
tetragonal PZT, $BaTiO_3$



$T < T_c$

Piezoelectric behavior

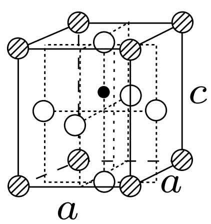
- coupling of electric/mechanic quantities
- direct/inverse piezoelectric effect
- 'small' fields – no switching
- often considered as linear
- reversible, i.e. non-dissipative



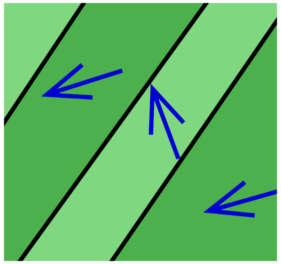
Ferroelectric behavior

- 'large' fields
- switching of unit-cells
- non-linear
- irreversible, i.e. dissipative

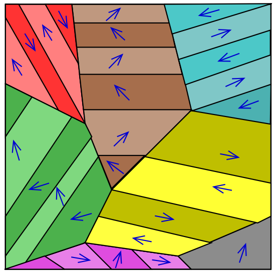
Polycrystalline Structure



Unit cell

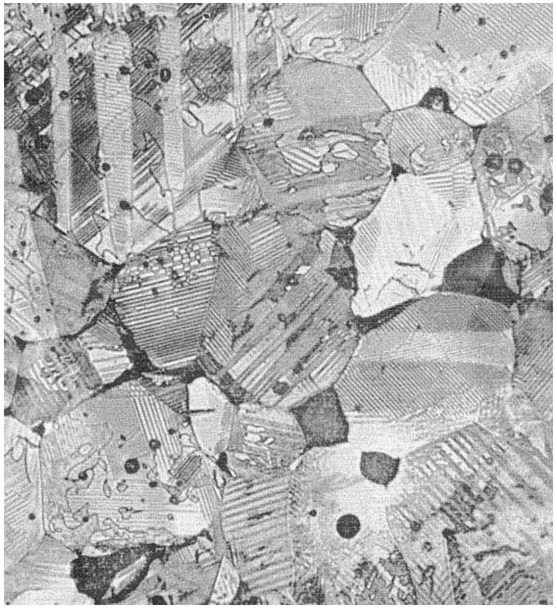


Domain Structure



Polycrystal

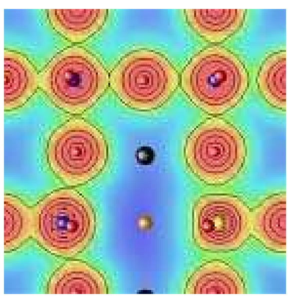
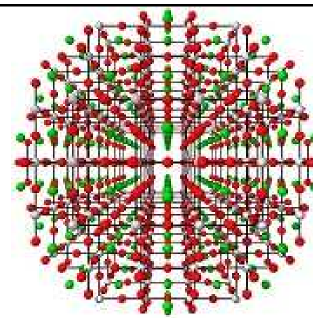
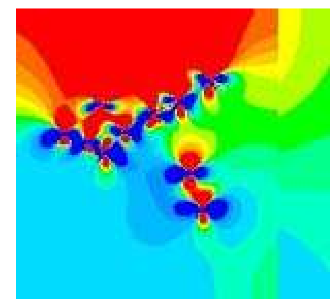
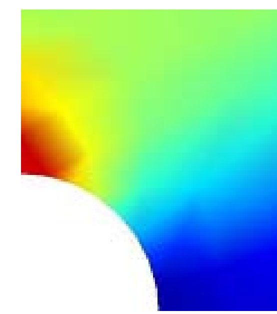
Picture: JAFFE ET AL. 1964



Micrograph ($BaTi0_3$)

- Single crystal grains consist of domains of uniform polarization
- Polycrystals constist of multiple grains
- The virgin state of the polycrystal
  (after cooling below the Curie-Temperature is random and unpolarized)

Modeling through the scales

Electron	Atom	Single / Polycrystal	Device
Quantum Mechanics	Statistical Mechanics	Micromechanics, Homogenization, Cont.Mechanics	Cont. Mechanics
			
$<<$nm	nm$-\mu$m	$<$mm	$>$mm
DFT	MD, Mol. Statics Monte-Carlo-Sim.	Finite Diff., FEM Phase-Field-Sim.	FEM

HERE: Micromechanics + Continuum Mechanics Models

Modeling Approaches Literature

- Micro-electromechanical approaches:

  HWANG,LYNCH&MCMEEKING,1995, CHEN,FANG&HWANG,1997,

  HWANG,HUBER,MCMEEKING&FLECK,1998, MICHELITSCH&KREHER,1998,

  HWANG&MCMEEKING,1998, LU,FANG,LI,HWANG,1999, KESSLER&BALKE,2001,

  HUBER,FLECK,LANDIS,MCMEEKING,1999, WANG,SHI,CHEN,LI, ZHANG, 2005 and others.

- Phenomenological modeling approaches:

  CHEN 1980, BASSIOUNY,GHALEB&MAUGIN 1988, GHANDI&HAGOOD 1996,

  FAN,STOLL&LYNCH 1999, COCKS&MCMEEKING 1999, KAMLAH&JIANG 1999,

  KAMLAH&TSAKMAKIS 1999, LANDIS&MCMEEKING 1999, MCMEEKING&LANDIS 1999,

  KAMLAH&BOEHLE 2001, LANDIS, JMPS, 2002, KAMLAH&WANG, FZKA, 2003,

  LANDIS,WANG,SHENG, JIMSS, 2004, LANDIS, ASME, 2003B and others.

- **Reviews:** KAMLAH 2001, LANDIS 2004.

Micromechanical Modeling

Single crystal models

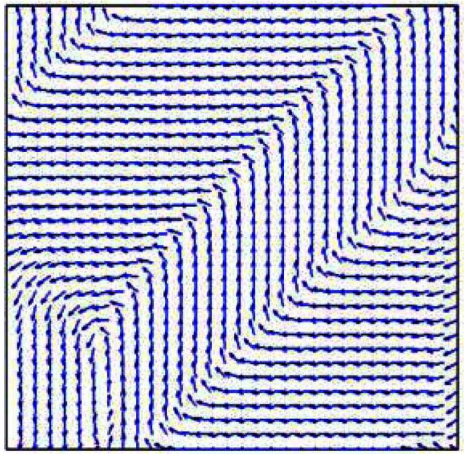
- Single-crystal – Single-domain: Complete switch

  (e.g. HWANG, LYNCH& MCMEEKING 1995, LU, FANG, LI& HWANG 1999)

- Single-crystal – Multi-domain: Incremental switching

  (e.g. HUBER, FLECK, LANDIS& MCMEEKING 1999)

- Phase-field simulations (e.g. WANG,LI,CHEN&ZHANG, 2005)



Phase-field simulation

Homogenization

- REUSS-assumption: Volume-averaging

  (e.g. LU, FANG, LI & HWANG 1999)

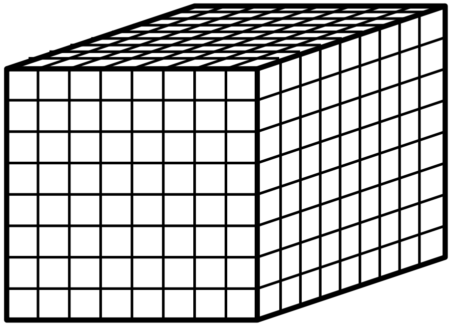
- Self-consistent scheme

  (e.g. HUBER, FLECK, LANDIS & MCMEEKING 1999)

- Finite Element Simulations

  (e.g. HWANG&MCMEEKING 1998, 1999)

- Other homogenization techniques ...



FEM-mesh

Phenomenological modeling

Thermodynamically consistent modeling

- Thermodynamic and Electrostatic Balances
- Assumptions and Simplifications
- Modeling Reversible Processes: Piezoelectricity, Electrostriction
- Modeling Irreversible Processes: Internal Variables
- Three Examples of Models for Ferroelectricity

Other approaches

There are models, wich are not based on the 2nd law of thermodynamics

e.g. models based on loading and saturation conditions (*see Presentation by Marc Kamlah)*

e.g. KAMLAH&TSAKMAKIS 1999, KAMLAH&BÖHLE 2001

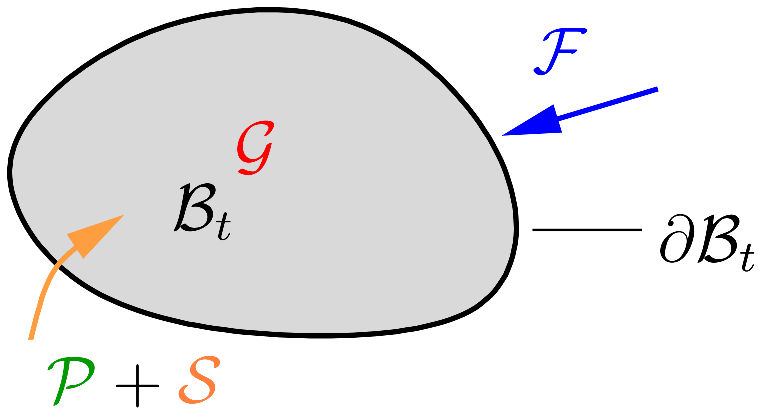
Thermodynamical balance statements see e.g. Hutter&Jöhnk 04

General balance statement for material body $\mathcal{B}$ (global form):

$$\frac{d}{dt}\mathcal{G} = \mathcal{P} + \mathcal{S} + \mathcal{F}$$

$\mathcal{G}$: balanced quantity | $\mathcal{P}$: production inside $\mathcal{B}$

$\mathcal{S}$: supply inside $\mathcal{B}$ | $\mathcal{F}$: flux through the surface $\partial\mathcal{B}$



Thermodynamical balance statements see e.g. Hutter&Jöhnk 04

General balance statement (global form):

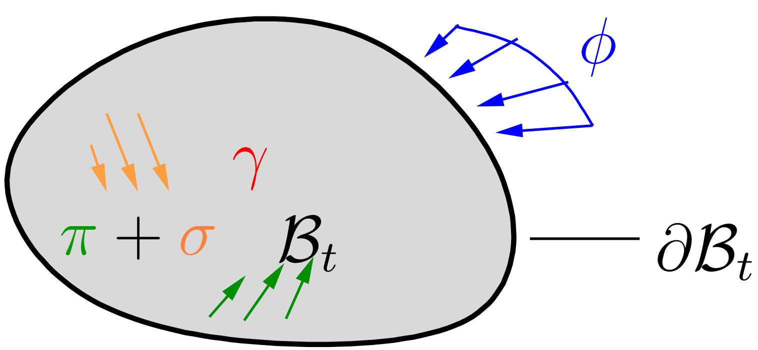
$$\frac{d}{dt}\int_{\mathcal{B}} \gamma(\vec{x},t)dv = \int_{\mathcal{B}} (\pi(\vec{x},t) + \varsigma(\vec{x},t))dv + \int_{\partial\mathcal{B}} \tilde{\phi}(\vec{x},t,\vec{n})da$$

γ: density of balanced quantity $\mathcal{G}$

π : production-density inside $\mathcal{B}$

ς: supply-density inside $\mathcal{B}$

$\tilde{\phi}$: flux-density through the surface $\partial\mathcal{B}$



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γ: density of balanced quantity $\mathcal{G}$

π : production-density inside $\mathcal{B}$

ς: supply-density inside $\mathcal{B}$

$\tilde{\phi}$: flux-density through the surface $\partial\mathcal{B}$

CAUCHY LEMMA: $\tilde{\phi}(\vec{x},t,\vec{n}) = -\phi(\vec{x},t)\vec{n}$

Divergence theorem: $\int_{\partial\mathcal{B}} \phi\vec{n}da = \int_{\mathcal{B}} \text{div}\,\phi dv$

REYNOLDS' transport theorem: $\frac{d}{dt}\int_{\mathcal{B}} \gamma(\vec{x},t)dv = \int_{\mathcal{B}} \left(\frac{d}{dt}\gamma + \gamma\ \text{div}\,\vec{v}\right)dv$

$$\int_{\mathcal{B}} \frac{d}{dt}\gamma(\vec{x},t) + \gamma\ \text{div}\,\vec{v}(\vec{x},t) - \pi(\vec{x},t) - \varsigma(\vec{x},t) + \ \text{div}\,\phi(\vec{x},t)dv = 0$$

Thermodynamical balance statements see e.g. Hutter&Jöhnk 04

General balance statement (global form):

$$\frac{d}{dt}\int\limits_{\mathcal{B}} \gamma(\vec{x},t)dv = \int\limits_{\mathcal{B}} (\pi(\vec{x},t) + \varsigma(\vec{x},t))dv + \int\limits_{\partial\mathcal{B}} \tilde{\phi}(\vec{x},t,\vec{n})da$$

γ: density of balanced quantity $\mathcal{G}$

π : production-density inside $\mathcal{B}$

ς: supply-density inside $\mathcal{B}$

$\tilde{\phi}$: flux-density through the surface $\partial\mathcal{B}$

CAUCHY Lemma: $\tilde{\phi}(\vec{x},t,\vec{n}) = -\phi(\vec{x},t)\vec{n}$

Divergence theorem: $\int\limits_{\partial\mathcal{B}} \phi\vec{n}da = \int\limits_{\mathcal{B}} \text{div}\,\phi dv$

REYNOLDS' transport theorem: $\frac{d}{dt}\int\limits_{\mathcal{B}} \gamma(\vec{x},t)dv = \int\limits_{\mathcal{B}} \left(\frac{d}{dt}\gamma + \gamma\ \text{div}\,\vec{v}\right)dv$

General balance statement for point inside material body $\mathcal{B}$ (local form):

$$\frac{d}{dt}\gamma(\vec{x},t) + \gamma\ \text{div}\,\vec{v}(\vec{x},t) - \pi(\vec{x},t) - \varsigma(\vec{x},t) + \text{div}\,\phi(\vec{x},t) = 0$$

Specific thermodynamical balances

General balance: $\frac{d}{dt}\gamma + \gamma \,\mathrm{div}\, \vec{v} - \pi(\vec{x},t) - \varsigma(\vec{x},t) + \,\mathrm{div}\, \phi(\vec{x},t) = 0$

quantity	density γ	production π	supply ς	flux $\tilde{\phi}$
mass	ϱ	0	0	0
momentum	$\varrho\vec{v}$	0	$\vec{f} + \vec{f}^e$	$-\vec{t}$
ang. mom.	$\vec{x} \times \varrho\vec{v}$	0	$\vec{x} \times (\vec{f} + \vec{f}^e) + \vec{m}^e$	$-\vec{x} \times \vec{t}$
energy	$\varrho u + \frac{1}{2}\varrho\vec{v} \cdot \vec{v}$	0	$(\vec{f} + \vec{f}^e) \cdot \vec{v} + \varrho r + \varrho p^e$	$-\vec{t} \cdot \vec{v} + \vec{q} \cdot \vec{n}$
entropy	ϱs	$\varrho\pi_s \geq 0$	$\varrho\varsigma_s = \varrho\frac{r}{\theta}$	$\vec{\phi}_s \cdot \vec{n} = \varrho\frac{\vec{q}}{\theta} \cdot \vec{n}$

$\vec{f}$: body forces (e.g. gravitational force $\varrho\vec{g}$), $\vec{f}^e$: electric body force, $\vec{t} = \boldsymbol{\sigma}\vec{n}$: Surface tractions, $\boldsymbol{\sigma}$: CAUCHY stress tensor, $\vec{x} \times (\vec{f} + \vec{f}^e)$: moment of body forces, $\vec{m}^e$: electric body couple, $-\vec{x} \times \vec{t}$: moment of surface tractions, $\varrho u + \frac{1}{2}\varrho\vec{v} \cdot \vec{v}$: internal plus kinetic energy density, $\varrho\vec{f} \cdot \vec{v} + \varrho r + \varrho p^e$: power of volume forces, radiation and electric power, θ: abs. temperature, $-\vec{t} \cdot \vec{v} + \vec{q} \cdot \vec{n}$: power of surface tractions and heat flux through the surface

$\pi_s \geq 0$: Second Law of Thermodynamics

Local thermodynamical balance equations

balance of mass $$\frac{d}{dt}\varrho + \varrho \,\mathrm{div}\,\vec{\mathrm{v}} = 0$$

balance of momentum $$\varrho \frac{d}{dt}\vec{\mathrm{v}} = \mathrm{div}\,\boldsymbol{\sigma} + \vec{\mathrm{f}} + \vec{\mathrm{f}}^{\mathrm{e}}$$

'Equations of motion'

balance of ang.mom. $$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{T}} + \bar{\boldsymbol{\sigma}}(\vec{\mathrm{m}}^{\mathrm{e}})$$

balance of tot.energy $$\varrho \tfrac{d}{dt} u = -\,\mathrm{div}\,\vec{\mathrm{q}} + \mathrm{tr}\,(\mathbf{L}\boldsymbol{\sigma}) + \varrho r + \varrho p^{\mathrm{e}} \qquad (1)$$

balance of entropy $$\varrho \tfrac{d}{dt} s = -\,\mathrm{div}\left(\frac{\vec{\mathrm{q}}}{\theta}\right) + \varrho \frac{r}{\theta} + \varrho \pi_s \qquad (2)$$

2nd law $$\pi_s \geq 0 \qquad (3)$$

CLAUSIUS-DUHEM inequality: (1)-$\theta\cdot$(2), (3) HELMHOLTZ free energy ψ

$$\rightarrow \boxed{\varrho\dot{\psi} + \varrho\dot{\theta}s - \mathbf{L}\cdot\boldsymbol{\sigma} - \varrho p^{\mathrm{e}} + \tfrac{1}{\theta}\vec{\mathrm{q}}\cdot\ \mathrm{grad}\,\theta = -\varrho\pi_s \leq 0}\ ,\ \dot{u} - \theta\dot{s} - \dot{\theta}s =: \dot{\psi}$$

Electric contributions to the mechanical balance equations

- Force exerted on an electric monopole: $\vec{\mathrm{f}} = q\vec{\mathrm{E}}$
- Force exerted on an electric dipole: $\vec{\mathrm{f}} = \vec{\mathrm{p}} \cdot \text{grad}\,\vec{\mathrm{E}}$
- Angular momentum exerted on a dipole: $\vec{\mathrm{m}} = \vec{\mathrm{p}} \times \vec{\mathrm{E}}$

⇝ Contributions to **balance of momentum / ang. momentum**

electric body force: $\vec{\mathrm{f}}^{\mathrm{e}} = q^{\mathrm{f}}\vec{\mathrm{E}} + \text{grad}\,\vec{\mathrm{E}}\vec{\mathrm{P}}$

electric body couple: $\vec{\mathrm{m}}^{\mathrm{e}} = \vec{\mathrm{P}} \times \vec{\mathrm{E}}$

- Work done by change of a dipole: $dW = d\vec{\mathrm{p}} \cdot \vec{\mathrm{E}}$
- Work done by moving free charges: $dW = \vec{\mathrm{I}} \cdot \vec{\mathrm{E}}dt$

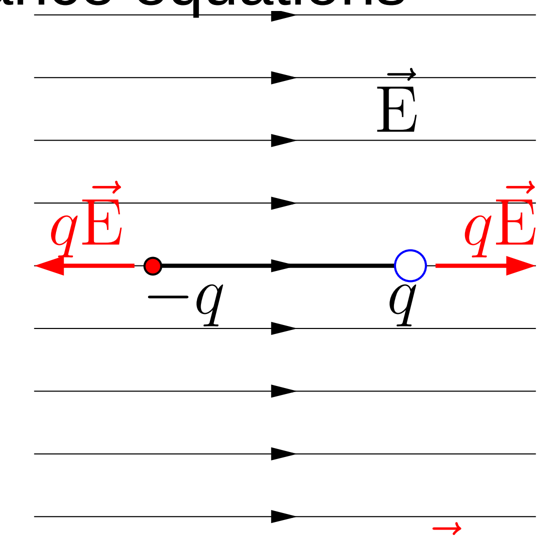
⇝ Contribution to **energy balance**

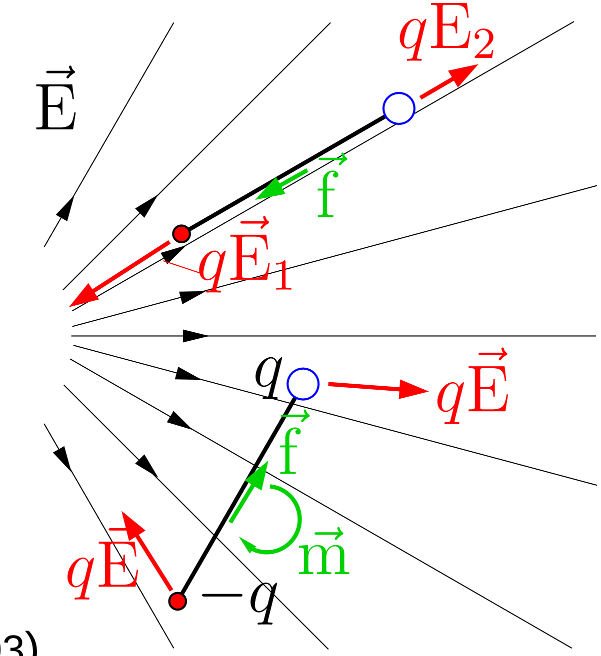
electric power: $\varrho p^{\mathrm{e}} = \vec{\mathrm{E}} \cdot (\dot{\vec{\mathrm{D}}} + \vec{\mathrm{I}})$

- Maxwell-stresses: $\boldsymbol{\sigma}^{\mathrm{e}} = \vec{\mathrm{E}} \otimes \vec{\mathrm{D}} - \epsilon_0 \frac{1}{2}(\vec{\mathrm{E}} \cdot \vec{\mathrm{E}})\mathbf{1}$

$\vec{\mathrm{f}}^{\mathrm{e}} = \text{div}\,\boldsymbol{\sigma}^{\mathrm{e}}$ and $\vec{\mathrm{m}}^{\mathrm{e}}$ is axial vector of $\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^{\mathrm{e}} - \boldsymbol{\sigma}^{\mathrm{eT}}$

BUT: $||\boldsymbol{\sigma}^{\mathrm{e}}|| < 1$MPa $\ll \sigma_{\mathrm{c}} \sim 30..40$MPa (KAMLAH&WANG '03)





MAXWELL Equations (1)(e.g. HUTTER&VAN DE VEN 1978)

Balance of electric charge

GAUSS law: $\epsilon_0 \int_{\partial\mathcal{B}} \vec{\mathrm{E}} \cdot \vec{\mathrm{n}} da = \int_{\mathcal{B}} q dv,$ local form: $\boxed{\epsilon_0 \operatorname{div} \vec{\mathrm{E}} = q^{\mathrm{f}} + q^{\mathrm{b}}}$

Introduce $\vec{\mathrm{D}}, \vec{\mathrm{P}}$ such that:
$$\begin{cases} \vec{\mathrm{D}}/\epsilon_0 & : \text{ el. field of the free charges } q^{\mathrm{f}} \\ -\vec{\mathrm{P}}/\epsilon_0 & : \text{ el. field of the bound charges } q^{\mathrm{b}} \end{cases}$$

then: $\boxed{\vec{\mathrm{D}} = \epsilon_0 \vec{\mathrm{E}} + \vec{\mathrm{P}}}$ and $\boxed{\operatorname{div} \vec{\mathrm{D}} = q^{\mathrm{f}}}$

Conservation of free charge

$$\frac{d}{dt} \int_{\mathcal{B}} \underbrace{\operatorname{div} \vec{\mathrm{D}}}_{q^{\mathrm{f}}} dv + \int_{\partial\mathcal{B}} \vec{\mathrm{I}} \cdot d\vec{\mathrm{a}} = 0$$

local form:

$$\boxed{\dot{q}^{\mathrm{f}} + q^{\mathrm{f}} \operatorname{div} \vec{\mathrm{v}} + \operatorname{div} \vec{\mathrm{I}} = 0}$$

$\vec{\mathrm{I}}$: conductive electric current, $\vec{\mathrm{D}}$: electric displacement, $\vec{\mathrm{P}}$: Polarization

MAXWELL Equations (2)

Balance of magnetic flux

$$\frac{d}{dt}\int_{\mathcal{A}} \vec{\mathrm{B}} \cdot \vec{\mathrm{n}}\,da = -\oint_{\partial\mathcal{A}} \vec{\mathrm{E}} \cdot d\vec{\mathrm{s}} \quad \text{(FARADAY law)}$$

in case of quasi-electrostatics:

$$\boxed{\mathrm{curl}\,\vec{\mathrm{E}} = \vec{0}}$$

There exists a scalar field φ, such that

$$\boxed{\vec{\mathrm{E}} = -\,\mathrm{grad}\,\varphi}$$

$\vec{\mathrm{B}}$: magnetic flux, $\vec{\mathrm{E}}$: electric field strength, φ: electric potential $\overset{*}{(\ )}$: convective time derivative

Summary: Local balance equations

$$\dot{\varrho} + \varrho\,\text{div}\,\vec{\mathrm{v}} = 0$$

$$\varrho\dot{\vec{\mathrm{v}}} - \vec{\mathrm{f}} - \text{div}\,\boldsymbol{\sigma} = \vec{0}$$

$$\boldsymbol{\sigma} - \boldsymbol{\sigma}^{\mathrm{T}} = \mathbf{0}$$

$$-s\dot{\theta} - \frac{1}{\theta}\vec{\mathrm{q}}\cdot\,\text{grad}\,\theta + \text{tr}\,(\mathbf{L}\boldsymbol{\sigma}) + \vec{\mathrm{E}}\cdot(\dot{\vec{\mathrm{D}}} + \vec{\mathrm{I}}) \geq \varrho\dot{\psi}$$

$$\text{div}\,\vec{\mathrm{D}} = q^{\mathrm{f}}$$

$$\dot{q}^{\mathrm{f}} + q^{\mathrm{f}}\,\text{div}\,\vec{\mathrm{v}} = -\,\text{div}\,\vec{\mathrm{I}}$$

$$\text{curl}\,\vec{\mathrm{E}} = \vec{0}, \qquad -\,\text{grad}\,\varphi = \vec{\mathrm{E}}$$

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$$

small deformations:

$\mathbf{F} \approx \mathbf{1}$, $\dot{(\ )} \approx \frac{\partial}{\partial t}(\ )$, $\text{sym}(\mathbf{L}) \approx \dot{\boldsymbol{\varepsilon}}$

$\dot{\rho} \approx 0$, $\text{div}\,\vec{\mathrm{v}} \approx 0$

no external charges in bulk

$q^{\mathrm{f}} \approx 0, \vec{\mathrm{I}} \approx \vec{0}$

(Resistance$\approx 10^{10}..10^{12}\Omega/$cm)

isothermal processes:

$\theta \approx$const., $\vec{\mathrm{q}} \approx \vec{0}$

quasi-static processes: $\dot{\vec{\mathrm{v}}} \approx 0$

Reduced set of basic equations

$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T\,, \quad \text{div}\,\boldsymbol{\sigma}$	$=$	$-\vec{\mathrm{f}}$	momentum balances
$\text{div}\,\vec{\mathrm{D}}$	$=$	0	GAUSS' law
$-\nabla\varphi$	$=$	$\vec{\mathrm{E}}$	electric potential φ
$\frac{1}{2}(\nabla\vec{\mathrm{u}} + (\nabla\vec{\mathrm{u}})^{\mathrm{T}})$	$=$	$\boldsymbol{\varepsilon}$	linearized strains
$\boldsymbol{\sigma}\cdot\dot{\boldsymbol{\varepsilon}} + \vec{\mathrm{E}}\cdot\dot{\vec{\mathrm{D}}}$	$\geq$	$\rho\dot{\psi}$	CLAUSIUS–DUHEM inequality
		ψ	HELMHOLTZ free energy

Boundary conditions:

$\vec{\mathrm{u}}$	$=$	$\bar{\vec{\mathrm{u}}}$	on boundary with prescribed displacement
φ	$=$	$\bar{\varphi}$	on boundary with prescribed el. potential
$\boldsymbol{\sigma}\vec{\mathrm{n}}$	$=$	$\bar{\vec{\mathrm{t}}}$	on boundary with prescribed traction
$\vec{\mathrm{D}}\cdot\vec{\mathrm{n}}$	$=$	$\bar{q}^{\mathrm{f}}$	on boundary with prescribed free charge

Reduced set of basic equations

$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T\,,\quad \text{div}\,\boldsymbol{\sigma}$	$=$	$-\vec{\mathrm{f}}$	momentum balances	6 var.	3 equ.
$\text{div}\,\vec{\mathrm{D}}$	$=$	0	GAUSS' law	3 var.	1 equ.
$-\nabla\varphi$	$=$	$\vec{\mathrm{E}}$	electric potential φ	4 var.	3 equ.
$\frac{1}{2}(\nabla\vec{\mathrm{u}} + (\nabla\vec{\mathrm{u}})^{\mathrm{T}})$	$=$	$\boldsymbol{\varepsilon}$	linearized strains	9 var.	6 equ.
$\boldsymbol{\sigma}\cdot\dot{\boldsymbol{\varepsilon}} + \vec{\mathrm{E}}\cdot\dot{\vec{\mathrm{D}}}$	$\geq$	$\rho\dot{\psi}$	CLAUSIUS–DUHEM inequality	22 var.	13 equ.
		ψ	HELMHOLTZ free energy		

Reduced set of basic equations

$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T\,,\quad \mathrm{div}\,\boldsymbol{\sigma}$	$=$	$-\vec{\mathrm{f}}$	momentum balances	6 var.	3 equ.
$\mathrm{div}\,\vec{\mathrm{D}}$	$=$	0	GAUSS' law	3 var.	1 equ.
$-\nabla\varphi$	$=$	$\vec{\mathrm{E}}$	electric potential φ	4 var.	3 equ.
$\frac{1}{2}(\nabla\vec{\mathrm{u}} + (\nabla\vec{\mathrm{u}})^{\mathrm{T}})$	$=$	$\boldsymbol{\varepsilon}$	linearized strains	9 var.	6 equ.
$\boldsymbol{\sigma}\cdot\dot{\boldsymbol{\varepsilon}} + \vec{\mathrm{E}}\cdot\dot{\vec{\mathrm{D}}}$	$\geq$	$\rho\dot{\psi}$	CLAUSIUS–DUHEM inequality	22 var.	13 equ.
		ψ	HELMHOLTZ free energy		

Modeling Task (simplified):

Construct a thermodynamic potential function which best **fits the physical material behavior** and derive constitutive equations, which **comply with the 2nd law of thermodynamics**!

Examples:

Potentials, LEGENDRE-Transforms, Internal state variables $\mathbf{q}$

HELMHOLTZ free energy: $\psi = \hat{\psi}(\boldsymbol{\varepsilon}, \vec{\mathrm{D}}, \mathbf{q})$

GIBBS free energy: $\varrho G = \varrho\psi - \boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon} - \vec{\mathrm{E}}\cdot\vec{\mathrm{D}} = \hat{G}(\boldsymbol{\sigma}, \vec{\mathrm{E}}, \mathbf{q})$

Electric enthalpy: $\varrho H = \varrho\psi - \vec{\mathrm{E}}\cdot\vec{\mathrm{D}} = \varrho\hat{H}(\boldsymbol{\varepsilon}, \vec{\mathrm{E}}, \mathbf{q})$

Modeling of reversible processes

- state is defined by $(\boldsymbol{\varepsilon}, \vec{\mathrm{E}})$ or $(\boldsymbol{\sigma}, \vec{\mathrm{D}})$ or $(\boldsymbol{\varepsilon}, \vec{\mathrm{D}})$ or $(\boldsymbol{\sigma}, \vec{\mathrm{E}})$

$\rightsquigarrow$ the HELMHOLTZ free energy is a function of $(\boldsymbol{\varepsilon}, \vec{\mathrm{D}})$: $\boxed{\psi = \hat{\psi}(\vec{\mathrm{D}}, \boldsymbol{\varepsilon})}$

Conservation of energy (no dissipation):

$$\begin{aligned} \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} + \vec{\mathrm{E}} \cdot \dot{\vec{\mathrm{D}}} - \varrho \dot{\psi} &= 0 \\ \left(\boldsymbol{\sigma} - \varrho \frac{\partial \hat{\psi}}{\partial \boldsymbol{\varepsilon}} \right) \cdot \dot{\boldsymbol{\varepsilon}} + \left(\vec{\mathrm{E}} - \varrho \frac{\partial \hat{\psi}}{\partial \vec{\mathrm{D}}} \right) \cdot \dot{\vec{\mathrm{D}}} &= 0 \end{aligned}$$

must hold for any $\dot{\boldsymbol{\varepsilon}}$ and $\dot{\vec{\mathrm{D}}}$ imposed by boundary conditions

$$\text{therefore} \begin{cases} \boldsymbol{\sigma} = \varrho \dfrac{\partial \hat{\psi}}{\partial \boldsymbol{\varepsilon}} \\ \vec{\mathrm{E}} = \varrho \dfrac{\partial \hat{\psi}}{\partial \vec{\mathrm{D}}} \end{cases}$$

Linear piezoelectric law

Quadratic form for ψ^{pe}:

$$\hat{\psi}^{\mathrm{pe}}(\bar{\boldsymbol{\varepsilon}}, \bar{\vec{\mathrm{D}}}) = \frac{1}{2}\bar{\boldsymbol{\varepsilon}} \cdot \mathbb{C}\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}} \cdot \mathbb{h}\bar{\vec{\mathrm{D}}} + \frac{1}{2}\bar{\vec{\mathrm{D}}} \cdot \boldsymbol{\beta}\bar{\vec{\mathrm{D}}}$$

$$\boldsymbol{\sigma} = \frac{\partial \hat{\psi}^{\mathrm{pe}}}{\partial \boldsymbol{\varepsilon}} = \mathbb{C}\bar{\boldsymbol{\varepsilon}} - \mathbb{h}\bar{\vec{\mathrm{D}}}$$

$$\vec{\mathrm{E}} = \frac{\partial \hat{\psi}^{\mathrm{pe}}}{\partial \vec{\mathrm{D}}} = -\mathbb{h}^{\mathrm{T}}\bar{\boldsymbol{\varepsilon}} + \boldsymbol{\beta}\bar{\vec{\mathrm{D}}}$$

$\mathbb{C}$	Elastic stiffness at const. $\vec{\mathrm{D}}$
$\mathbb{h}$	Tensor of piezoelectric coupling
$\boldsymbol{\beta}$	Dielectric compliance at const. $\boldsymbol{\varepsilon}$

$\bar{\boldsymbol{\varepsilon}}$ and $\bar{\vec{\mathrm{D}}}$ are given relative to the unloaded state.

- Moduli $\mathbb{C}$, $\boldsymbol{\beta}$, $\mathbb{h}$ are in general anisotropic
- Moduli $\mathbb{C}$, $\boldsymbol{\beta}$ considered isotropic in most models
- $\mathbb{h}$ is considerd transversely isotropic with respect to polarization direction

Quadratic electrostrictive law

Cubic form for ψ^{es}:

$$\hat{\psi}^{\mathrm{es}}(\bar{\boldsymbol{\varepsilon}}, \bar{\vec{\mathrm{D}}}) = \frac{1}{2}\bar{\boldsymbol{\varepsilon}} \cdot \mathbb{C}\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}} \cdot \mathbb{h}\bar{\vec{\mathrm{D}}} + \frac{1}{2}\bar{\vec{\mathrm{D}}} \cdot \boldsymbol{\beta}\bar{\vec{\mathrm{D}}} + \boldsymbol{\varepsilon} \cdot \mathbb{A}(\bar{\vec{\mathrm{D}}} \otimes \bar{\vec{\mathrm{D}}})$$

Modeling irreversible processes (1)

Additional (internal) variables are necessary to describe the state of the material.

Decomposition of strains and electric displacements:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\mathrm{r}} + \boldsymbol{\varepsilon}^{\mathrm{i}} \quad , \qquad \vec{\mathrm{D}} = \vec{\mathrm{D}}^{\mathrm{r}} + \vec{\mathrm{P}}^{\mathrm{i}}$$

$\boldsymbol{\varepsilon}^{\mathrm{r}}, \vec{\mathrm{D}}^{\mathrm{r}}$: reversible, piezoelectric $\qquad$ $\boldsymbol{\varepsilon}^{\mathrm{i}}, \vec{\mathrm{P}}^{\mathrm{i}}$: irreversible, ferroelectric

The irreversible quantities are described by the set of internal state variables $\mathbf{q}$

Free Energy:

$$\psi = \hat{\psi}(\boldsymbol{\varepsilon}, \vec{\mathrm{D}}, \mathbf{q})$$

Clausius–Duhem inequality:

$$\boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} + \vec{\mathrm{E}} \cdot \dot{\vec{\mathrm{D}}} - \varrho \dot{\psi} \quad \geq \quad 0$$

$$\left(\boldsymbol{\sigma} - \varrho \frac{\partial \hat{\psi}}{\partial \boldsymbol{\varepsilon}}\right) \cdot \dot{\boldsymbol{\varepsilon}} + \left(\vec{\mathrm{E}} - \varrho \frac{\partial \hat{\psi}}{\partial \vec{\mathrm{D}}}\right) \cdot \dot{\vec{\mathrm{D}}} - \sum_j \varrho \frac{\partial \hat{\psi}}{\partial q_j} \dot{q}_j \quad \geq \quad 0$$

Remaining inequality: Driving forces for the internal variables

$$\sum_j -\varrho \frac{\partial \hat{\psi}}{\partial q_j} \dot{q}_j = \sum_j f_j \dot{q}_j \geq 0 \quad \Rightarrow \quad \dot{q}_j = \lambda f_j, \quad \lambda \geq 0$$

f_j: Driving forces

Modeling irreversible processes (2)

Techniques:

- Simple visco-plasticity model (continous switching)

$$\dot{q}_j = \lambda f_j$$

- Visco-plasticity model with (loading function F)

$$\dot{q}_i = \langle F(f_k) \rangle \lambda f_i \ , \quad \langle \ \rangle = 0 \text{ if}(\ ) < 0$$

- Rate-independent plasticity model with loading function (cf. yield function)

$$F(f_j) \begin{cases} < 0 \ : \ \text{piezoelectric process, then} & \dot{q}_j = 0 \\ = 0, \dot{F}|_{q=\text{fixed}} > 0 \ : \ \text{ferroelectric process, then} & \dot{q}_j = \lambda \frac{\partial F}{\partial f_j} \end{cases}$$

λ: consistency parameter, determined from consistency condition $\dot{F} = 0$

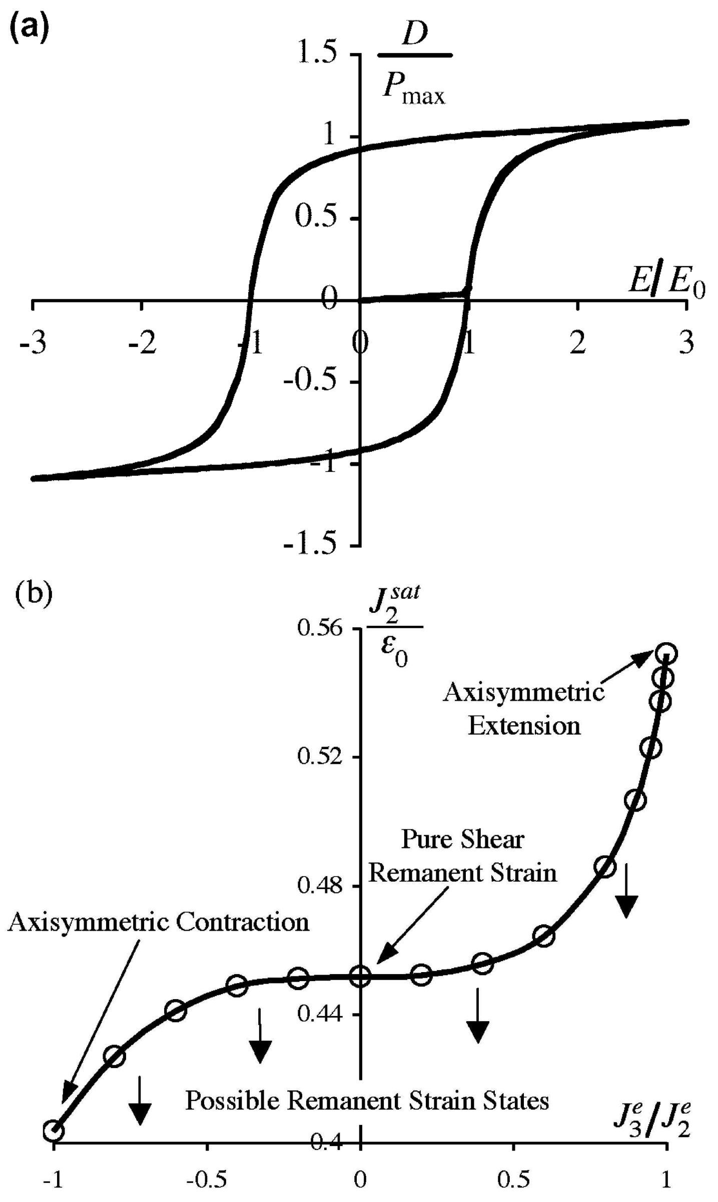
Saturation of switching

Saturation is handled by confining the internal variables to admissible ranges

- by energy barriers (hardening potentials)
- by additional saturation criteria, lock-up

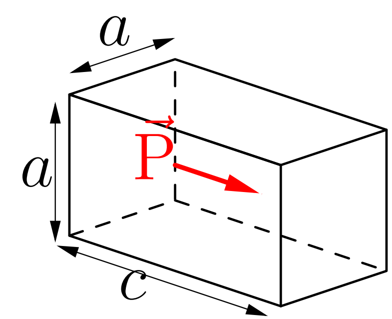
Model by C.M.LANDIS 2002

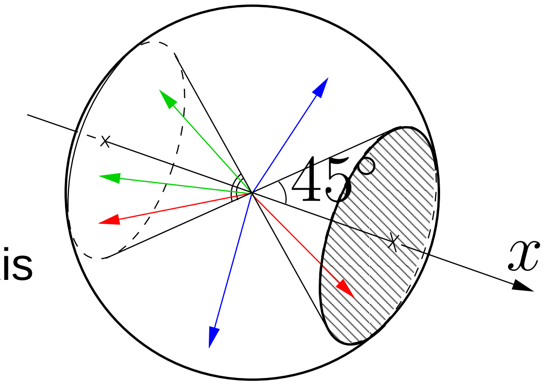
- In tradition of plasticity theory
- Thermodynamical potential:
  HELMHOLTZ free energy ψ
- Internal variables: $\boldsymbol{\varepsilon}^{\mathrm{i}}, \vec{\mathrm{P}}^{\mathrm{i}}$
- Driving forces: $\boldsymbol{\sigma}, \vec{\mathrm{E}}$
- No assumptions about micro-structure
- Strain saturation: $J_2^{\boldsymbol{\varepsilon}} < J_2^{\max}(J_2^{\boldsymbol{\varepsilon}} / J_3^{\boldsymbol{\varepsilon}})$
  (fitted to micro-mech. simulations LANDIS 2003)
- Polarization saturation: $|\vec{\mathrm{P}}^{\mathrm{i}}| < P_{\mathrm{m}}^{\mathrm{i}}(\boldsymbol{\varepsilon}^{\mathrm{i}})$
  (fitted to micro-mech. simulations LANDIS, WANG&SHENG 2004)
- Kinematic hardening with energy-barrier



Model by M.Kamlah&Jiang 1999

see presentation by Marc Kamlah!





- Thermodyn. potential: Gibbs energy
- Internal variables

β : Fraction of c-axis, within 45° -cone

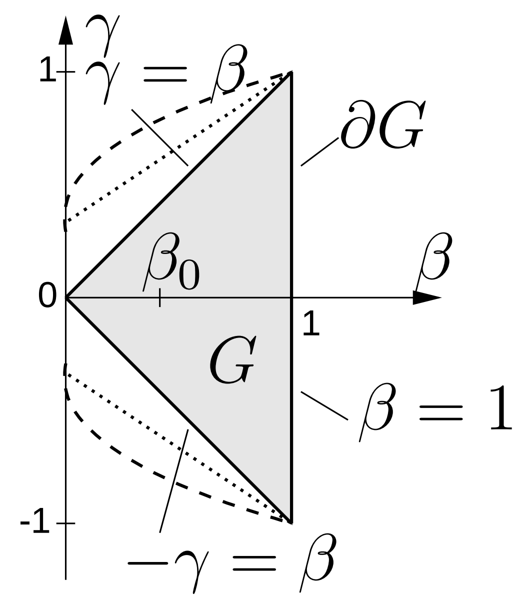
γ : Measure for polarisation resulting from these c-axis

$\vec{e}^{\gamma/\beta}$: later versions: Additional internal variables

for rotation of cone and polarization

- Admissible states: $0 \leq \beta \leq 1$ and $|\gamma| \leq \beta$
- Irreversible quantities:

$$\boldsymbol{\varepsilon}^{\mathrm{i}}(\beta) = \varepsilon_0 \frac{3}{2} \frac{\beta - \beta_0}{1 - \beta_0} \left(\vec{n} \otimes \vec{n} - \frac{1}{3} \mathbf{1} \right), \quad \vec{P}^{\mathrm{i}}(\gamma) = P_0 \gamma \vec{n}$$



- Later versions:

Kamlah&Jiang 2002, Kamlah&Wang 2003

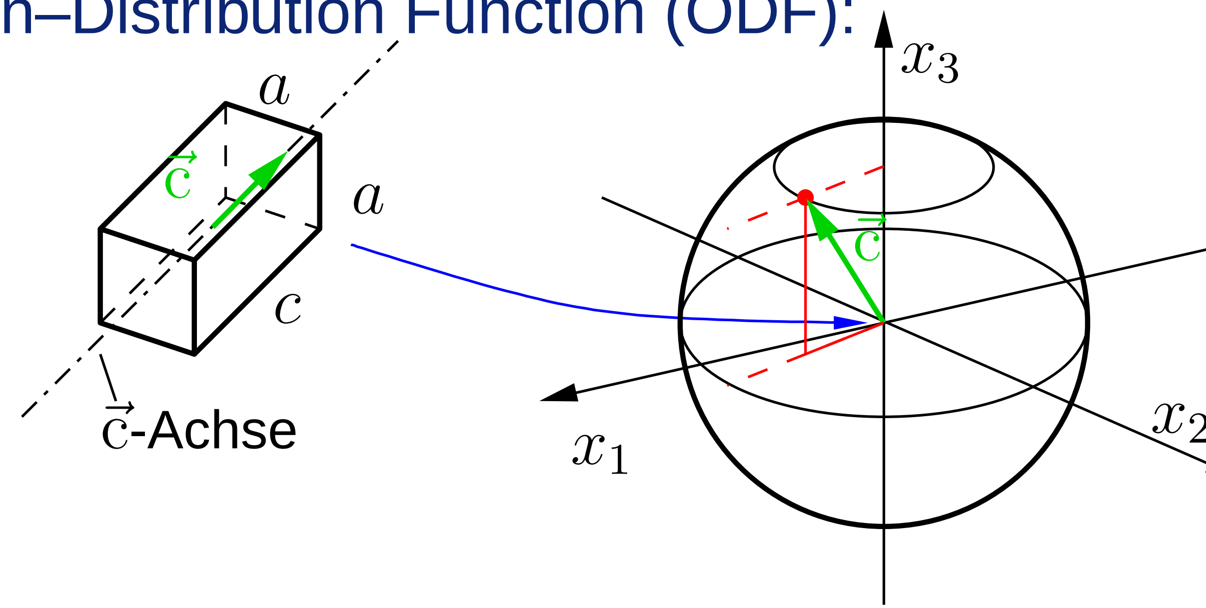
Model by V.Mehling & al. 2005

Continuous Orientation–Distribution Function (ODF):

- c-Axes

  (Tetragonal unit cell)

  with strain state $\varepsilon^{\mathrm{i}}_{\mathrm{uc}}$



Model by V. Mehling & al. 2005

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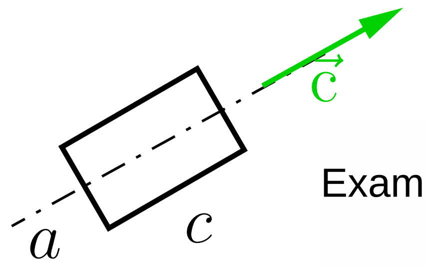
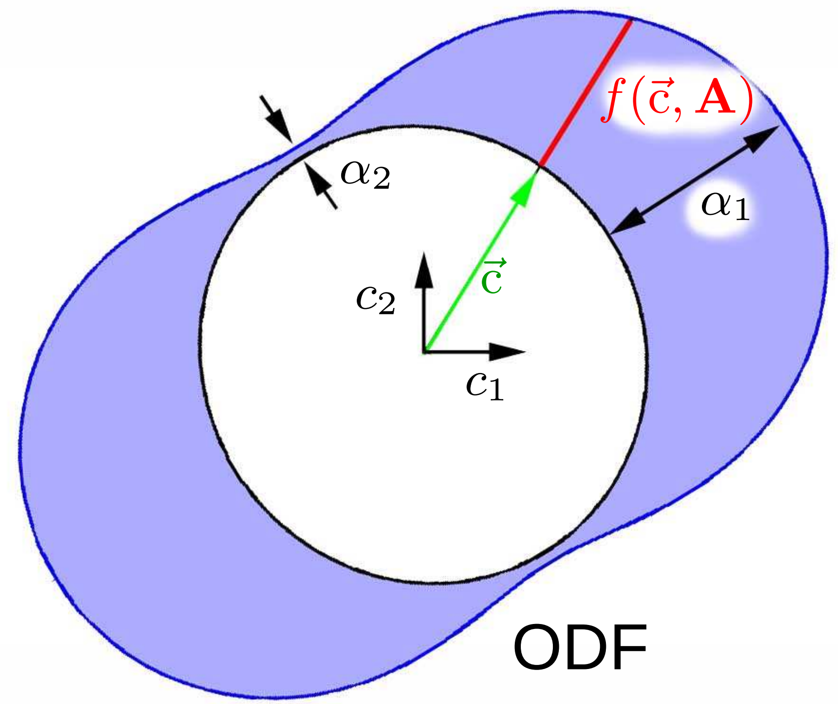


Example: $\alpha_1 = 0.95, \alpha_2 = 0.05, \alpha_3 = 0.0$

- ODF: $f(\vec{\mathrm{c}}; \mathbf{A})$

$$\boxed{f = \vec{\mathrm{c}} \cdot \mathbf{A}\vec{\mathrm{c}}}, \ \mathrm{tr}\ \mathbf{A} = 1$$

α_j: Eigenvalues of $\mathbf{A}$ (Texture-tensor)



Model by V.Mehling & al. 2005

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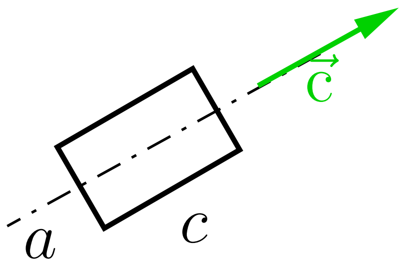

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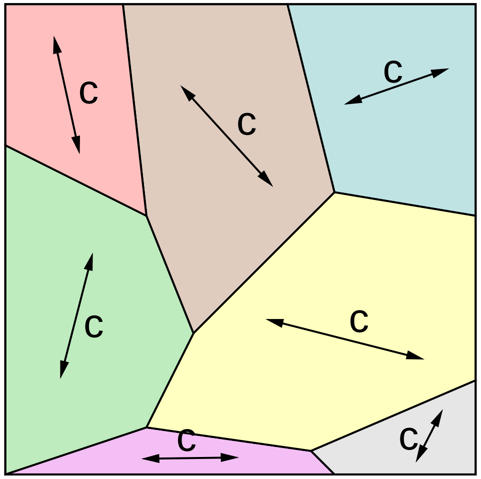
- Volume-averaging results in macroscopic strain

$$\boldsymbol{\varepsilon}^{\mathrm{i}} = \langle \boldsymbol{\varepsilon}^{\mathrm{i}}_{\mathrm{uc}} \rangle = \hat{\boldsymbol{\varepsilon}}^{\mathrm{i}}(\mathbf{A}) = \tfrac{3}{2}\varepsilon_0(\mathbf{A} - \mathbf{1}/3)$$



Model by V.Mehling & al. 2005

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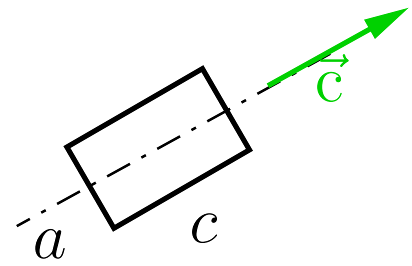

- ODF: $f(\vec{c}; \mathbf{A})$

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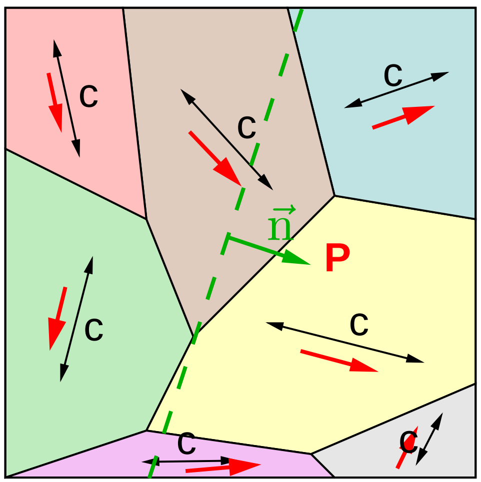

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- Polarizability: Sum of possible contributions from all cells to macroscopic polarization in direction $\vec{n}$ at a fixed strain state

  $$\vec{P}^{\mathrm{i}}_{\mathrm{m}} = \hat{\vec{P}}^{\mathrm{i}}_{\mathrm{m}}(\vec{n}; \mathbf{A}) = P_0(\mathbf{A} + \tfrac{1}{2}\mathbf{1}(1 - \vec{n} \cdot \mathbf{A}\vec{n}))\vec{n}$$

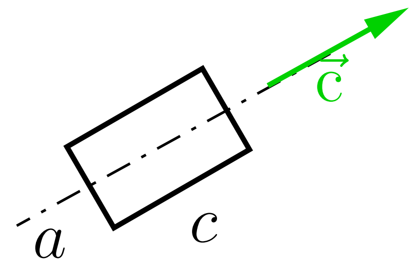
Model by V.Mehling & al. 2005

Continuous Orientation–Distribution Function (ODF):

- c-Axes

  (Tetragonal unit cell)

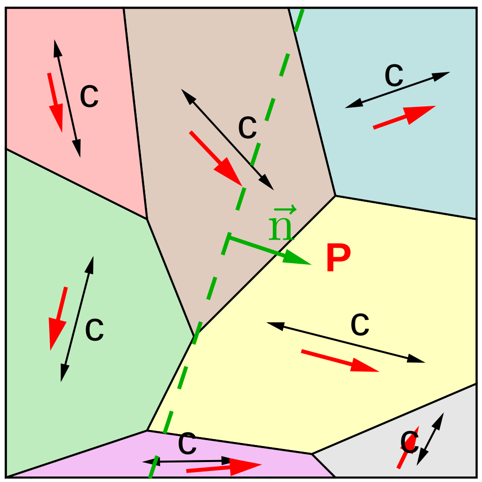
  with strain state $\boldsymbol{\varepsilon}^{\mathrm{i}}_{\mathrm{uc}}$



- ODF: $f(\vec{c}; \mathbf{A})$

  $\boxed{f = \vec{c} \cdot \mathbf{A} \vec{c}}$, tr $\mathbf{A} = 1$

  α_j: Eigenvalues of $\mathbf{A}$ (Texture-tensor)



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- Polarization generated by additional internal variables: relative remanent polarization $\vec{p}$

$$\vec{P}^{\mathrm{i}} = \hat{\vec{P}}^{\mathrm{i}}(\vec{p}) = P_0 \vec{p};$$

Set of Internal Variables: $\mathbf{q} = \{\mathbf{A}, \vec{p}\}$

Admissible Range: $|\vec{p}| \leq P^{\mathrm{i}}_{\mathrm{m}}/P_0;\ \alpha_j \geq 0$

Model Summary (MEHLING, TSAKMAKIS, GROSS, 2005)

Internal variables, irrev. quantities $\mathbf{q} = \{\mathbf{A}, \vec{\mathrm{p}}\}$, $\left(\boldsymbol{\varepsilon}^{\mathrm{i}} = \hat{\boldsymbol{\varepsilon}}^{\mathrm{i}}(\mathbf{A}), \vec{\mathrm{P}}^{\mathrm{i}} = \hat{\vec{\mathrm{P}}}^{\mathrm{i}}(\vec{\mathrm{p}})\right)$

Additive decomposition $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\mathrm{r}} + \boldsymbol{\varepsilon}^{\mathrm{i}}; \quad \vec{\mathrm{D}} = \vec{\mathrm{D}}^{\mathrm{r}} + \vec{\mathrm{P}}^{\mathrm{i}}$

Electric enthalpy $H = \hat{H}^{\mathrm{r}}(\vec{\mathrm{E}}, \boldsymbol{\varepsilon}, \vec{\mathrm{p}}) + \hat{H}^{\mathrm{i}}(\mathbf{A}, \vec{\mathrm{p}})$

Piezoelectric constitutive law $H^{\mathrm{r}} = \bar{H}^{\mathrm{r}}(L_k(\vec{\mathrm{E}}, \boldsymbol{\varepsilon}, \vec{\mathrm{p}}))$ (cf. SCHRÖDER&GROSS 2004)

(invariant formulation) $= \frac{1}{2}\boldsymbol{\varepsilon}^{\mathrm{r}} \cdot \mathbb{C}^{\mathrm{E}}(\vec{\mathrm{p}})\boldsymbol{\varepsilon}^{\mathrm{r}} - \boldsymbol{\varepsilon}^{\mathrm{r}} \cdot \mathfrak{e}(\vec{\mathrm{p}})\vec{\mathrm{E}} - \frac{1}{2}\vec{\mathrm{E}} \cdot \boldsymbol{\epsilon}^{\varepsilon}(\vec{\mathrm{p}})\vec{\mathrm{E}}$

$$\vec{\mathrm{D}} = -\partial H^{\mathrm{r}}/\partial \vec{\mathrm{E}}, \qquad \boldsymbol{\sigma} = \partial H^{\mathrm{r}}/\partial \boldsymbol{\varepsilon}$$

Hardening potential $H^{\mathrm{i}} = \hat{H}^{\mathrm{i}}(\mathbf{A}, \vec{\mathrm{p}})$

Dissipation inequality, driving forces $-\varrho\frac{\partial \hat{H}}{\partial \mathbf{A}} \cdot \dot{\mathbf{A}} - \varrho\frac{\partial \hat{H}}{\partial \vec{\mathrm{p}}} \cdot \dot{\vec{\mathrm{p}}} = \mathbf{f}^{\mathrm{A}} \cdot \dot{\mathbf{A}} + \vec{\mathrm{f}}^{\mathrm{p}} \cdot \dot{\vec{\mathrm{p}}} \geq 0$

Coupled switching criterion
(HUBER&FLECK 2001, LANDIS 1999)

$$F = \left(\frac{\|\mathrm{dev}\,(\mathbf{f}^{\mathrm{A}})\|}{f_{\mathrm{c}}^{\mathrm{A}}}\right)^2 + \left(\frac{|\vec{\mathrm{f}}^{\mathrm{p}}|}{f_{\mathrm{c}}^{\mathrm{p}}}\right)^2 + \phi\frac{\mathrm{dev}\,(\mathbf{f}^{\mathrm{A}})\cdot(\vec{\mathrm{p}} \otimes \vec{\mathrm{f}}^{\mathrm{p}})_{\mathrm{s}}}{f_{\mathrm{c}}^{\mathrm{A}} f_{\mathrm{c}}^{\mathrm{p}}} - 1 \leq 0$$

Evolution of internal variables $\dot{\mathbf{A}} = \lambda\partial F/\partial \mathbf{f}^{\mathrm{A}}, \dot{\vec{\mathrm{p}}} = \lambda\partial F/\partial \vec{\mathrm{f}}^{\mathrm{p}}$, iff $F = 0$ and loading

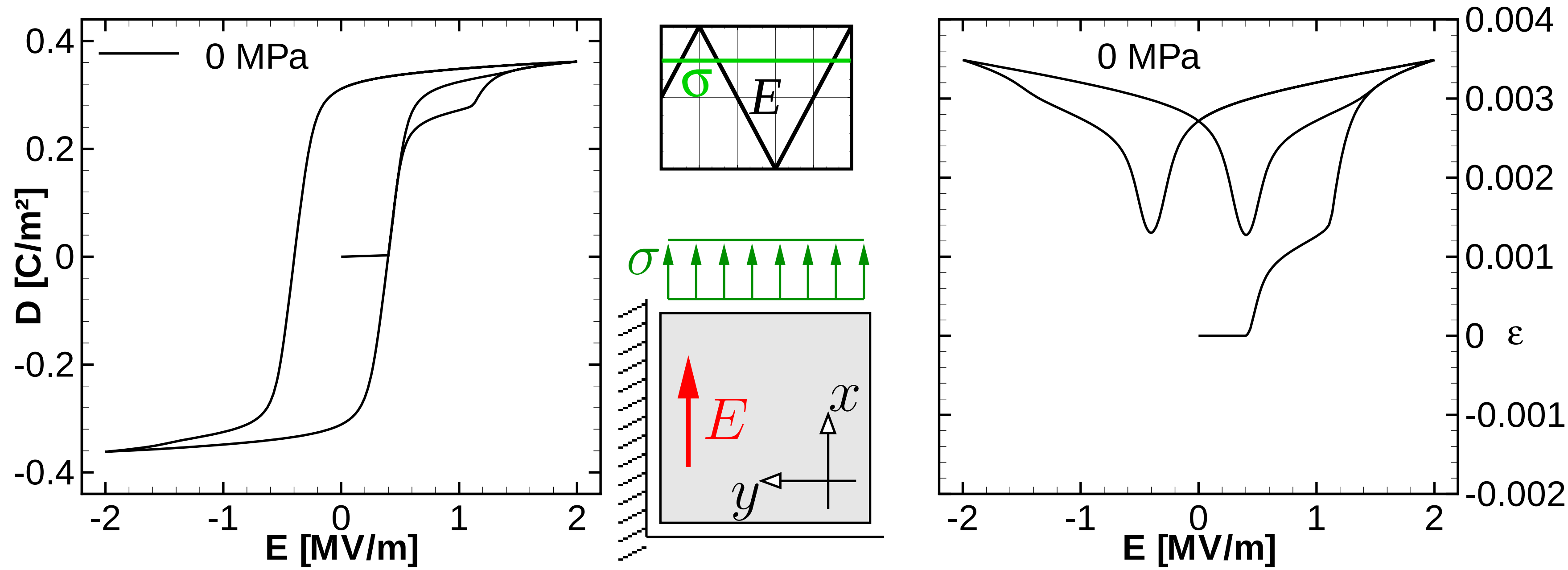
Numerical Implementation

- Implementation into standard-FEM
- Nodal degrees of freedom: u_x, u_y, u_z, φ (ALLIK&HUGHES, 1970)
- Implicit time integration method
- Predictor - corrector method
- Linear/quadratic volume-elements

Material Constants (poled PZT4) for Piezo-Constants see DUNN&TAYA '94

$$
\begin{aligned}
C_{11} &= 139000\mathrm{MPa} & C_{12} &= 77800\mathrm{MPa} & C_{44} &= 25600\mathrm{MPa} \\
C_{33} &= 115000\mathrm{MPa} & C_{13} &= 74300\mathrm{MPa} \\
e_{333} &= 15.1\mathrm{C/m^2} & e_{331} &= -5.2\mathrm{C/m^2} & e_{131} &= 12.7\mathrm{C/m^2} \\
\epsilon_{11} &= 646.4\mathrm{E\text{-}5C/MVm} & & & \epsilon_{33} &= 562.2\mathrm{E\text{-}5C/MVm} \\
\varepsilon_0 &= 0.32\% & P_0 &= 0.36\mathrm{C/m^2} & E_\mathrm{c} &= 0.4\mathrm{MV/m} & \sigma_\mathrm{c} &= 35\mathrm{MPa} \\
c_\mathrm{A} &= 0.02\mathrm{MPa} & m_\mathrm{A} &= 1 & a_\mathrm{A} &= 0.0001\mathrm{MPa} \\
c_\mathrm{p} &= 0.06\mathrm{MPa} & m_\mathrm{p} &= 1 & a_\mathrm{p} &= 0.0006\mathrm{MPa} & \phi &= 2.0
\end{aligned}
$$

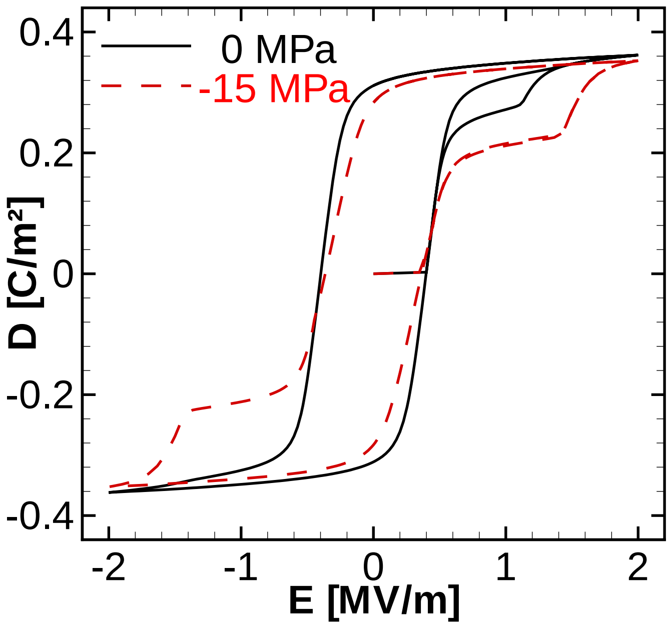
Example 1: Cyclic electric loading

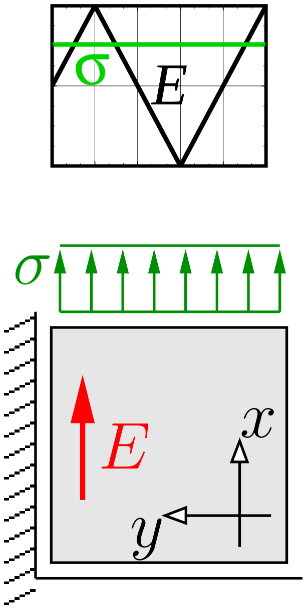


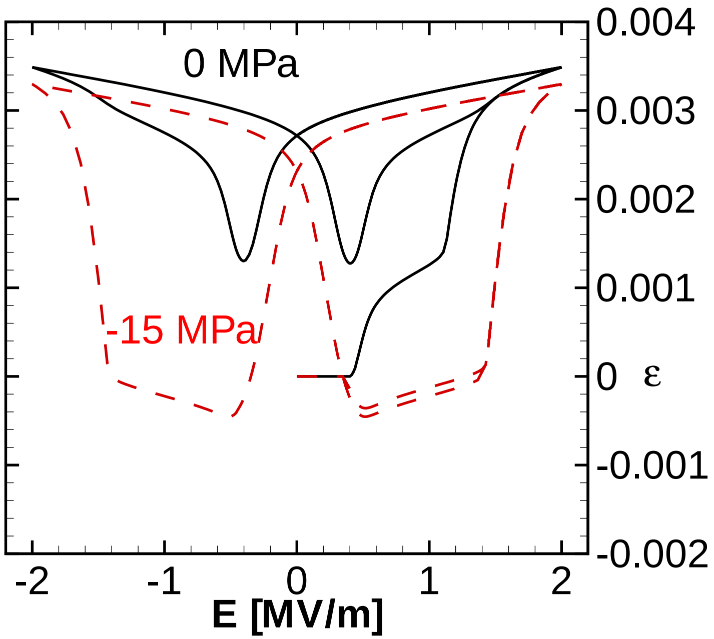
(cf. experiment, e.g. LYNCH 1996)

Example 1: Cyclic electric loading

...with constant mechanical compressive stress.







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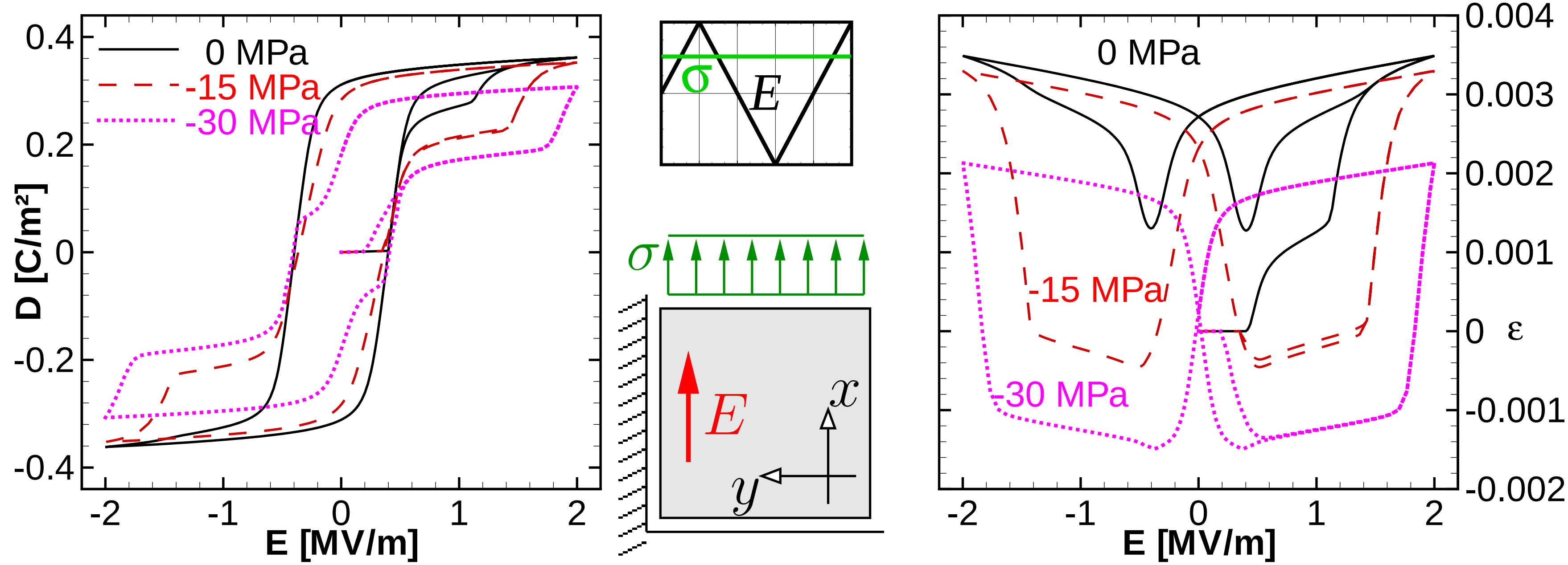

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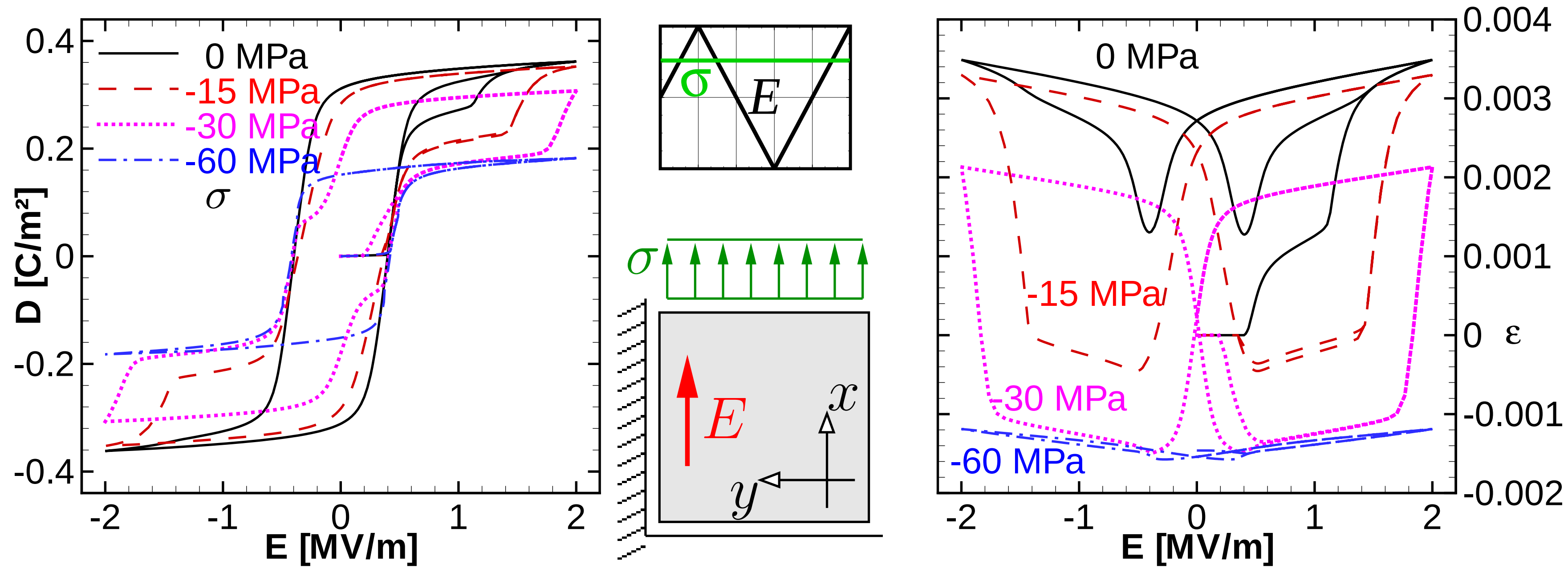
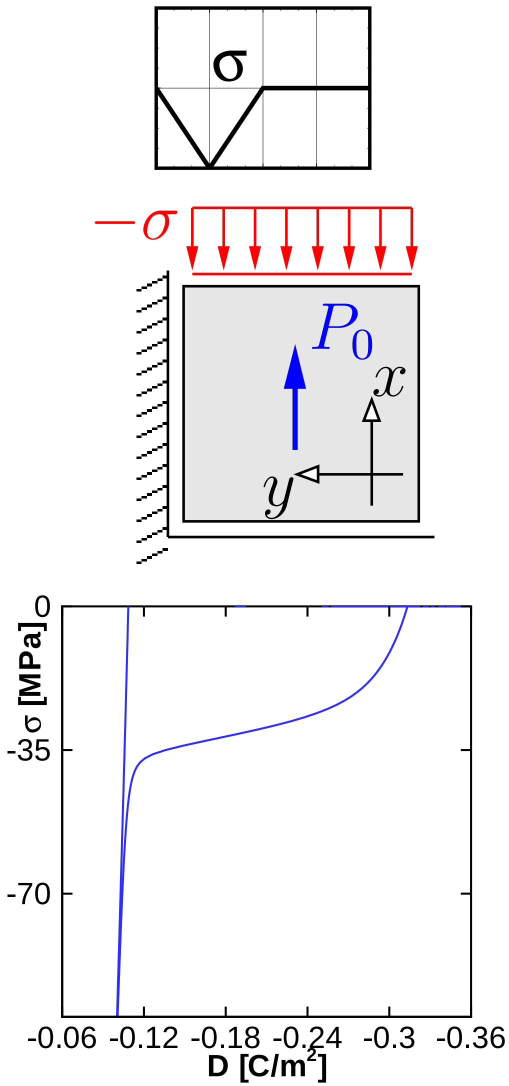


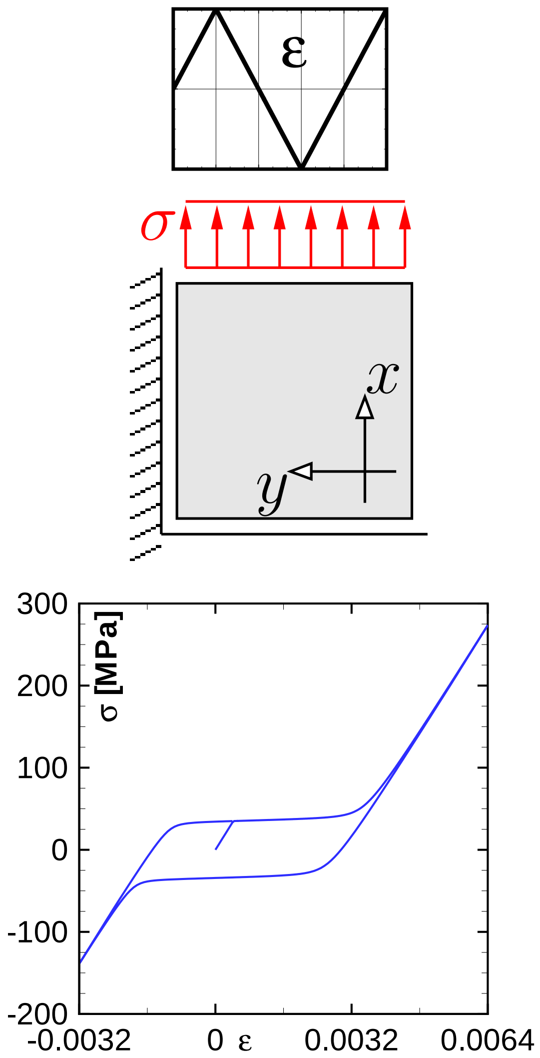
(cf. experiment, e.g. LYNCH 1996)

Example 2: Mechanical loading

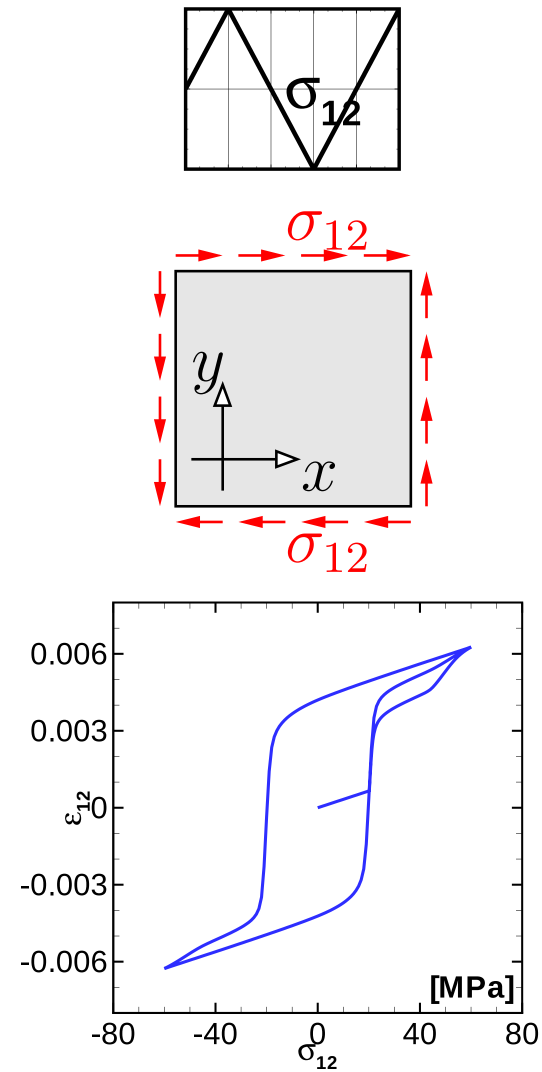
mech. depolarization



mech. cycling

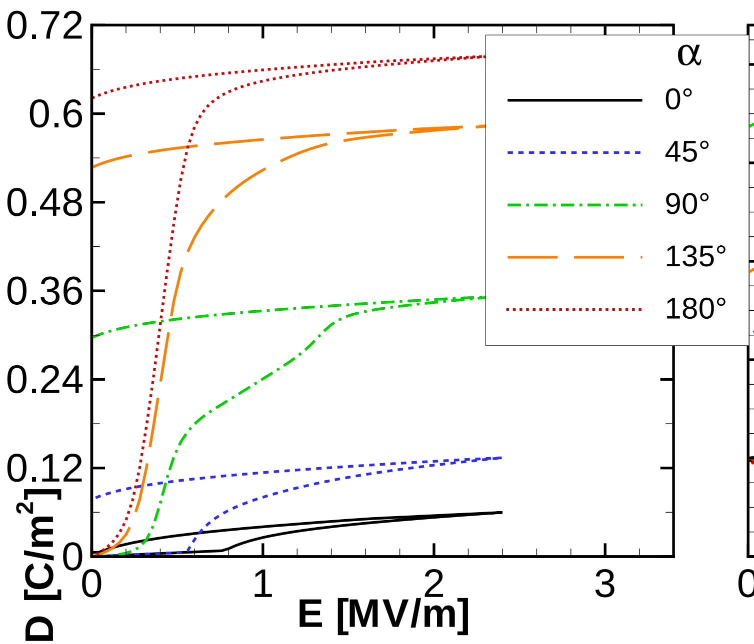


mech. shear cycling

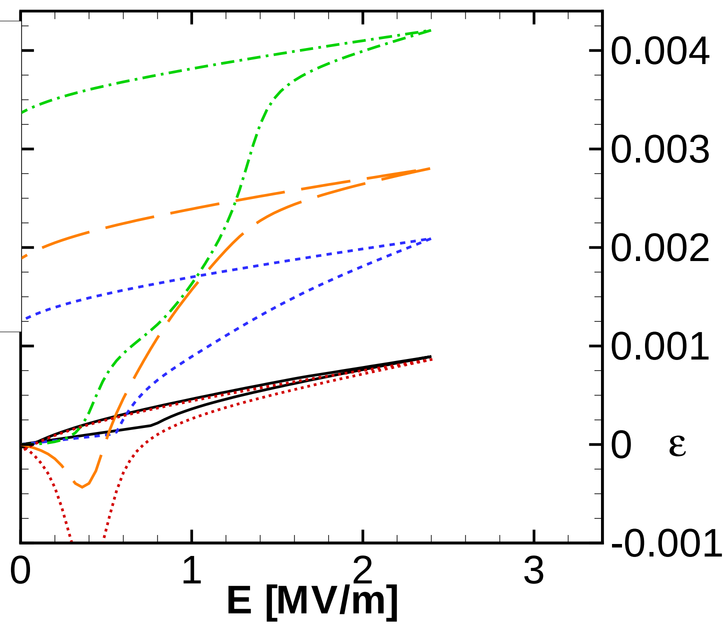


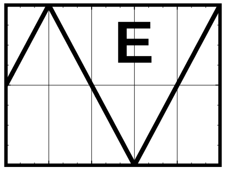
Example 3: Repolarization for $\vec{\mathrm{E}} \nparallel \vec{\mathrm{P}}^{\mathrm{i}}$

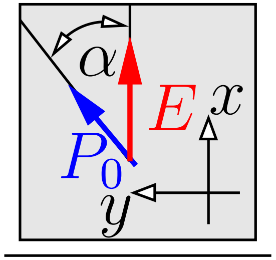
Polarization response



Strain response



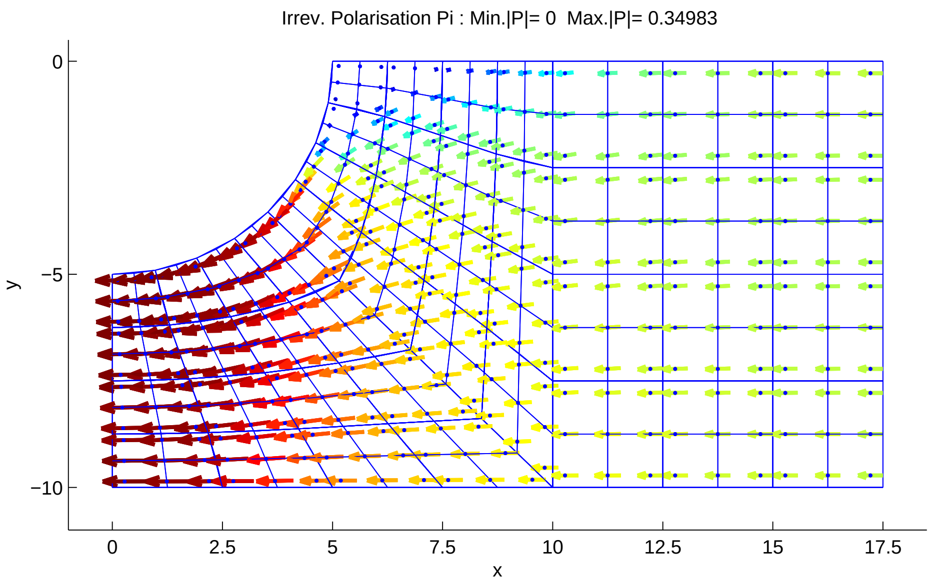




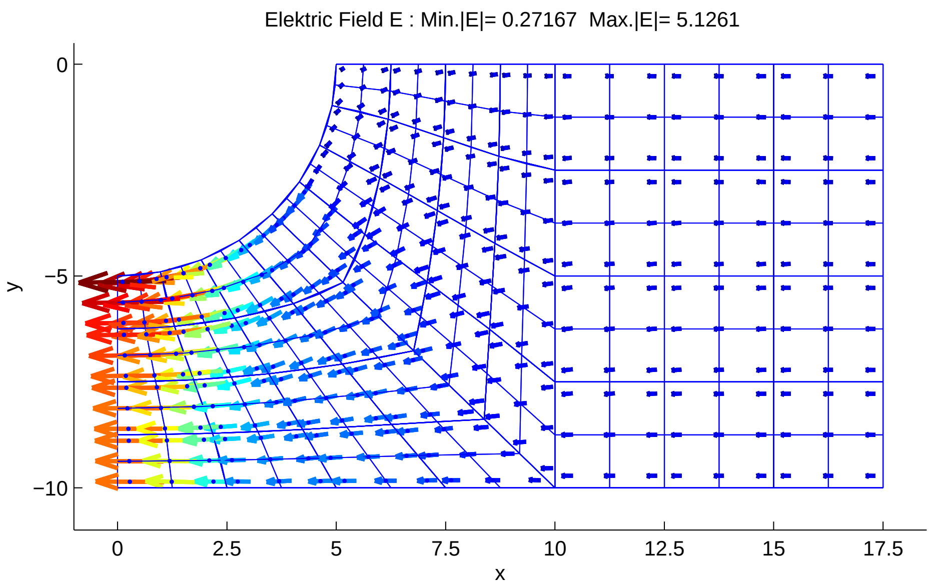
(cf. experiment, e.g. HUBER&FLECK 2001, ZHOU, 2003)

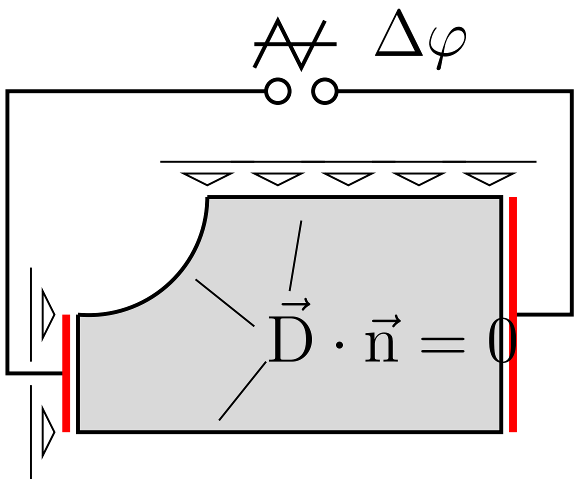
Example 4: Polarization of a strip with hole

Vector of irreversible Polarization $[\mathrm{C/m^2}]$



Vector of Electric Field Strength $[\mathrm{MV/m}]$





Conclusion

- Basic phenomenology and structure of ferroelectrics
- Modeling through the length-scales
- Overview over micromechanical modeling
- Fundamentals of continuum thermodynamics & electrostatics
- Thermodynamically consistent modeling

  Piezoelectricity – Electrostriction – Ferroelectricity
- Phenomenological models - three examples
- Numerical examples