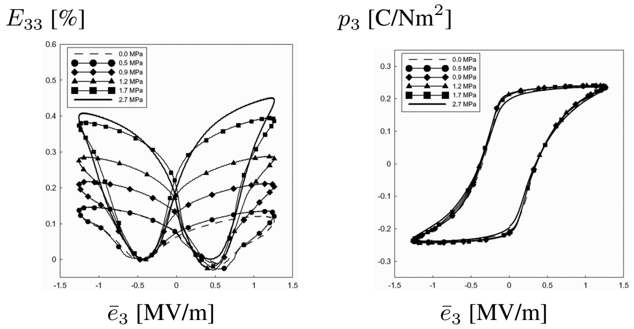
Laminate-based modelling of switching in ferroelectrics

Polarization switching

Loading-rate dependent, dissipative (e.g., $BaTiO_3$ [1]).



Continuum thermodynamic / electrostatic approach

- Pairwise compatibility
- Energetics & kinetics
- Variational formulation boundary-value problem

Pairwise compatibility

Strain-polarization variants $\alpha = 1, \ldots$ [2]

$$\boldsymbol{E}_\alpha = \boldsymbol{E}_\beta + \mathrm{sym}(\boldsymbol{a}_{\alpha\beta} \otimes \boldsymbol{n}_{\alpha\beta}) \ , \ \boldsymbol{p}_\alpha \cdot \boldsymbol{n}_{\alpha\beta} = \boldsymbol{p}_\beta \cdot \boldsymbol{n}_{\alpha\beta} \ .$$

Variant & laminate volume fractions $\boldsymbol{\mu} = (\mu_1, \ldots)$ [2]

$$\lambda_\alpha(\boldsymbol{\mu}) = \begin{cases} \mu_\alpha \prod_{i=1}^{\alpha-1} (1-\mu_i) \ , & \alpha = 1, \ldots, v-1 \ , \\ \prod_{i=1}^{\alpha-1} (1-\mu_i) \ , & \alpha = v \ . \end{cases}$$

Energetics (free energy)

Model 1 (average properties $p_\mathrm{R}(\boldsymbol{\mu}) = \sum_\alpha \lambda_\alpha(\boldsymbol{\mu}) \, p_\alpha$) [2, 4]

$$\begin{aligned} \psi(\boldsymbol{E}, \boldsymbol{p}, \boldsymbol{\mu}) &= \tfrac{1}{2} \{\boldsymbol{E} - \boldsymbol{E}_\mathrm{R}(\boldsymbol{\mu})\} \cdot \boldsymbol{C} \{\boldsymbol{E} - \boldsymbol{E}_\mathrm{R}(\boldsymbol{\mu})\} \\ &- \{\boldsymbol{p} - \boldsymbol{p}_\mathrm{R}(\boldsymbol{\mu})\} \cdot \boldsymbol{J} \{\boldsymbol{E} - \boldsymbol{E}_\mathrm{R}(\boldsymbol{\mu})\} \\ &+ \tfrac{1}{2} \{\boldsymbol{p} - \boldsymbol{p}_\mathrm{R}(\boldsymbol{\mu})\} \cdot \boldsymbol{X}^{-1} \{\boldsymbol{p} - \boldsymbol{p}_\mathrm{R}(\boldsymbol{\mu})\} \ . \end{aligned}$$

Model 2 (energy additivity) [3]

$$\psi(\boldsymbol{E}, \boldsymbol{p}, \boldsymbol{\mu}) = \sum\nolimits_\alpha \lambda_\alpha(\boldsymbol{\mu}) \, \psi_\alpha(\boldsymbol{E}, \boldsymbol{p}) \ .$$

Kinetics (resistance to domain wall motion)

Volume fraction evolution $\dot{\mu}_i = \partial_{f_i} \varphi$.
Driving force f_i (see example).
Dissipation potential $\varphi(f_1, \ldots)$.

Example: Switching during uniform loading ($BaTiO_3$) [4]

- Flat plate $\overline{\boldsymbol{e}} = \overline{e}_3 \, \boldsymbol{i}_3$, $\overline{\boldsymbol{T}} = \overline{T}_{33} \, \boldsymbol{i}_3 \otimes \boldsymbol{i}_3$.
- Switching system $\{(\boldsymbol{E}_i, \boldsymbol{p}_i), \ i = 1, \ldots, 4\}$.
- Spotaneous polarization $p_s = 0.26$ C/m^2.
- Coercivities $e_{90^\circ} = 0.26$ MV/m, $e_{180^\circ} = 0.23$ MV/m.

Simplified potential energy (constrained to $\langle \psi \rangle \approx 0$)

$$\langle I \rangle = \frac{K}{2\epsilon_0} \langle p_3 \rangle^2 - \overline{e}_3 \langle p_3 \rangle - \overline{T}_{33} \langle E_{33} \rangle \ .$$

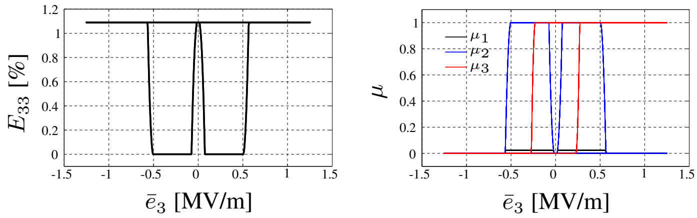
Driving force $f_i = -\partial_{\mu_i} \langle I \rangle$.
Volume fraction evolution ($\{x\}$ ramp function)

$$\dot{\mu}_i = \partial_{f_i} \varphi = \frac{1}{\eta} \{|f_i| - g_i\} \, \mathrm{sign}(f_i) \ .$$

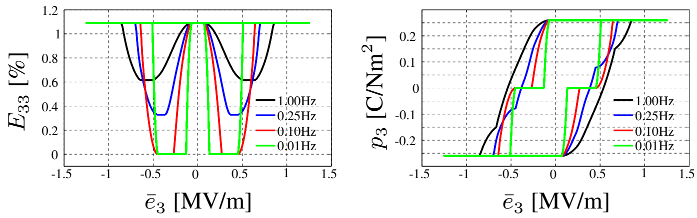
Switching threshhold $g_i(\boldsymbol{\mu}; p_s, e_{90^\circ}, e_{180^\circ})$.

Simulation results ($K = 0$, $\eta = 0.01$ s)

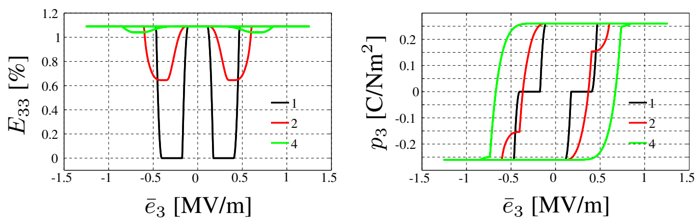
Volume fraction ($m = 1$, $\bar{T}_{33} = -5.84$ MPa, rate 0.01 Hz)



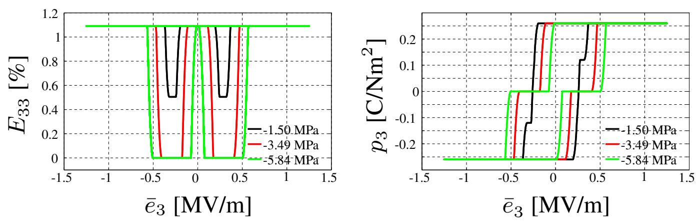
Variable loading rate ($m = 1$, $\bar{T}_{33} = -4.5$ MPa)



Variable rate sensitivity m ($\bar{T}_{33} = -3.49$ MPa, rate 0.01 Hz)



Variable stress $\bar{T}_{33}$ ($m = 1$, rate 0.01 Hz)



References

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[2] Y. C. Shu, K. Bhattacharya, *Phil. Mag. B* 81:2021, 2001.
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