DFG FOR 1509 **Ferroische Funktionsmaterialien**
Mehrskalige Modellierung und experimentelle Charakterisierung

TP1 "Design und Analyse funktioneller Komposit-Materialien mit verzerrungsinduzierter magneto-elektrischer Kopplung"

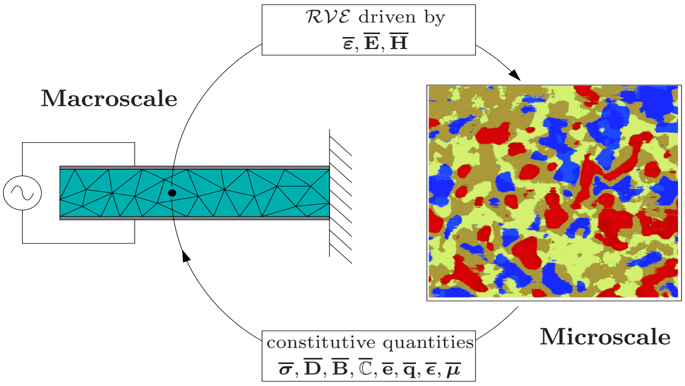
Multiferroic composites with strain-induced magneto-electric coupling

Introduction

Materials that exhibit strong magneto-electric (ME) coupling find application in sensor technology and data storage. Since natural materials have a very low ME coupling at room temperature, synthetic (composite) materials consisting of electro- and magneto-active phases become relevant. In such composites the ME coupling arises as a strain-induced product property.

Computational homogenization of ME composites

For the simulation of the effective ME coupling behavior we make use of the FE^2-method. This homogenization procedure allows for the determination of effective properties in consideration of attached representative volume elements ($\mathcal{RVE}$s), see [1].



The $\mathcal{RVE}$ is driven by boundary conditions, which have to ensure energetic consistency of both scales. This is fulfilled by postulating the following macrohomogeneity condition of the form

$$\overline{\boldsymbol{\sigma}} : \dot{\overline{\boldsymbol{\varepsilon}}} - \overline{\mathbf{D}} \cdot \dot{\overline{\mathbf{E}}} - \overline{\mathbf{B}} \cdot \dot{\overline{\mathbf{H}}} = \int_{\mathcal{RVE}} \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \mathbf{D} \cdot \dot{\mathbf{E}} - \mathbf{B} \cdot \dot{\mathbf{H}} \, dv,$$

In order to connect the macro- and microscopic quantities, we define the macroscopic variables in terms of volume integrals

$$\overline{\boldsymbol{\xi}} = \frac{1}{V_{\mathcal{RVE}}} \int_{\mathcal{RVE}} \boldsymbol{\xi} \, dv \quad \text{with} \quad \boldsymbol{\xi} := \{\boldsymbol{\varepsilon}, \boldsymbol{\sigma}, \mathbf{E}, \mathbf{D}, \mathbf{H}, \mathbf{B}\}$$

The incremental macroscopic constitutive equations result in

$$\begin{bmatrix} \Delta\overline{\boldsymbol{\sigma}} \\ -\Delta\overline{\mathbf{D}} \\ -\Delta\overline{\mathbf{B}} \end{bmatrix} = \begin{bmatrix} \overline{\mathbb{C}} & -\overline{\mathbf{e}}^T & -\overline{\mathbf{q}}^T \\ -\overline{\mathbf{e}} & -\overline{\boldsymbol{\epsilon}} & -\overline{\boldsymbol{\alpha}}^T \\ -\overline{\mathbf{q}} & -\overline{\boldsymbol{\alpha}} & -\overline{\boldsymbol{\mu}} \end{bmatrix} \begin{bmatrix} \Delta\overline{\boldsymbol{\varepsilon}} \\ \Delta\overline{\mathbf{E}} \\ \Delta\overline{\mathbf{H}} \end{bmatrix},$$

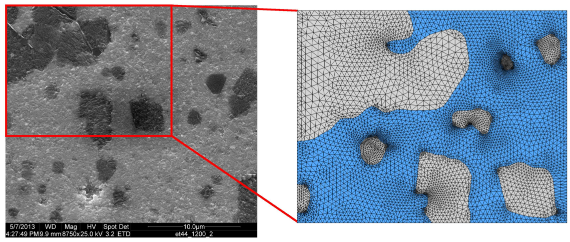
where the ME coupling modulus of the two phases is zero ($\boldsymbol{\alpha} \equiv \mathbf{0}$). However, the overall macroscopic ME modulus $\overline{\boldsymbol{\alpha}}$ of the composite material is in general non-zero and defined as follows

$$\overline{\boldsymbol{\alpha}} = \frac{\partial \overline{\mathbf{B}}}{\partial \overline{\mathbf{E}}} = \left[\frac{\partial \overline{\mathbf{D}}}{\partial \overline{\mathbf{H}}}\right]^T .$$

This ME coefficient significantly depends on the microstructure.

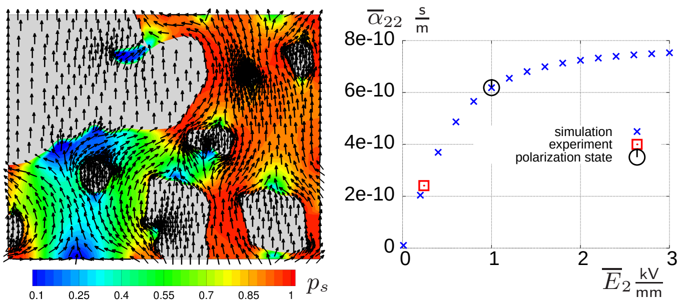
ME coefficient of experimental microstructures

We analyze the magneto-electric response of a real composite microstructure. The composite consists of a piezoelectric matrix ($BaTiO_3$) with particulate piezomagnetic inclusions ($CoFe_2O_4$).



The ME coupling in a real composite is zero without creating a pre-polarization and pre-magnetization of the phases. In order to arrive at different polarization states of the piezoelectric matrix, we determine the piezoelectric coupling properties on the microscale as follows, see also [2].

1. Apply macroscopic field $\overline{\mathbf{E}}$; compute local distribution $\mathbf{E}$
2. Preferred directions (for each Gauss point): $\mathbf{a} = \mathbf{E}/||\mathbf{E}||$
3. Relative amplitude of rem. polarization $p_s = \tanh(c \cdot ||\mathbf{E}||)$
4. Piezoelectric moduli $\mathbf{e} = p_s(-\beta_1 \mathbf{a} \otimes \underline{1} - \beta_2 \mathbf{a} \otimes \mathbf{a} \otimes \mathbf{a} - \beta_3 \overline{\mathbf{e}})$



$$\overline{\alpha}_{22}^{sim} = \frac{\overline{B}_2}{\overline{E}_2} = 7.78 \cdot 10^{-10} \ \frac{s}{m}$$

$$\overline{\alpha}_{22}^{exp} = 2.368 \cdot 10^{-10} \ \frac{s}{m}$$
(Etier et al.)

The deviation can be explained by the simplified modeling assumptions and the experimentally not yet obtained optimal pre-polarization and -magnetization state. However, due to the scaling factor p_s the model is capable to simulate different polarization states and to coincide with measured values, also for [3].

Future work: challenge for modeling and experiment

The model will be improved by accounting for highly resolved 3D microstructures and fundamental non-linearities (polarization/magnetization process). Most efficiently this can be realized by fully coupled FE^2 simulations in a powerful HPC framework.

References

[1] J. Schröder and M.-A. Keip, *Comput. Mech.* 50:229–244, 2012.
[2] Labusch et al., *Computational Mechanics* 2014.
[3] M. Etier et al., *Proc. Eur. Conf. Applic. Polar Dielec.* 1–4, 2012.

J. Schröder, M. Labusch
University of Duisburg-Essen
Department of Civil Engineering
Institute of Mechanics

M.-A. Keip
University of Stuttgart
Institute of Appled Mechanics (CE)
Chair I

D. C. Lupascu, M. Etier
University of Duisburg-Essen
Department of Civil Engineering
Institute for Materials Science