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Multiferroic composites with strain-induced magneto-electric coupling

DFG-FOR 1509 "Ferroic Functional Materials"

The research group focusses on the continuum-mechanical modeling and experimental characterization of ferroic functional materials. The overall aim is to develop a new quality in reliable and robust modeling tools for the description of complex, non-linear, magneto-electro-mechanical interactions on multiple length scales. The coupled two-scale simulation of magneto-electric composites is of particular interest.

http://www.uni-due.de/ferroics

Introduction

Materials that exhibit strong magneto-electric (ME) coupling find application in sensor technology and data storage. Since all known natural materials have very low ME coupling at room temperature synthetic (composite) materials consisting of piezoelectric and -magnetic phases become relevant. In such composites ME coupling arises as a strain-induced product property [2].

Computational homogenization of ME composites

For the analysis of the coupled behavior of ME composites we take into account the kinematic quantities and balance equations

$$\begin{aligned} \boldsymbol{\varepsilon} &= \nabla^s \boldsymbol{u} & \mathbf{E} &= -\nabla\phi & \mathbf{H} &= -\nabla\varphi \\ \nabla\cdot\boldsymbol{\sigma} + \boldsymbol{f} &= \mathbf{0} & \nabla\cdot\mathbf{D} &= q & \nabla\cdot\mathbf{B} &= 0 \end{aligned}$$

The effective response of the ME composite is obtained from a representative volume element ($\mathcal{RVE}$). The micro-fields are decomposed into a macroscopic part $\overline{\bullet}$ and micro-fluctuations $\widetilde{\bullet}$

$$\boldsymbol{\xi} = \overline{\boldsymbol{\xi}} + \widetilde{\boldsymbol{\xi}} \quad \text{with} \quad \boldsymbol{\xi} := [\boldsymbol{\varepsilon}, \boldsymbol{\sigma}, \boldsymbol{E}, \boldsymbol{D}, \boldsymbol{H}, \boldsymbol{B}]\,.$$

Energetically consistent periodic boundary conditions are computed from a generalized Hill-Mandel condition [3] and are applied along the boundary of the $\mathcal{RVE}$. The homogenized response is computed by averaging over the microscopic fields on the $\mathcal{RVE}$

$$\overline{\boldsymbol{\xi}} := \frac{1}{V_{\mathcal{RVE}}} \int_{\mathcal{B}} \boldsymbol{\xi}\, dv\,.$$

We suppose linear, transversely isotropic material response of the piezoelectric and -magnetic phases on the microscale. The incremental constitutive equations of the individual phases are

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

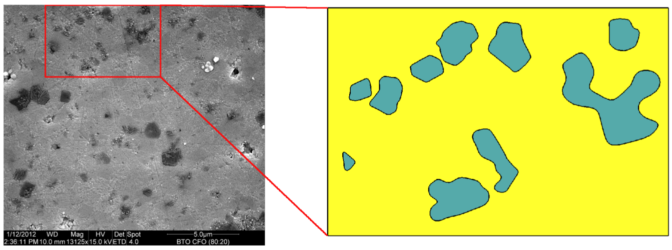
where the ME coupling modulus of the two phases is zero ($\boldsymbol{\alpha} \equiv \mathbf{0}$). However, the overall macroscopic ME modulus $\overline{\boldsymbol{\alpha}}$ of the composite material is in general non-zero and defined as follows

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

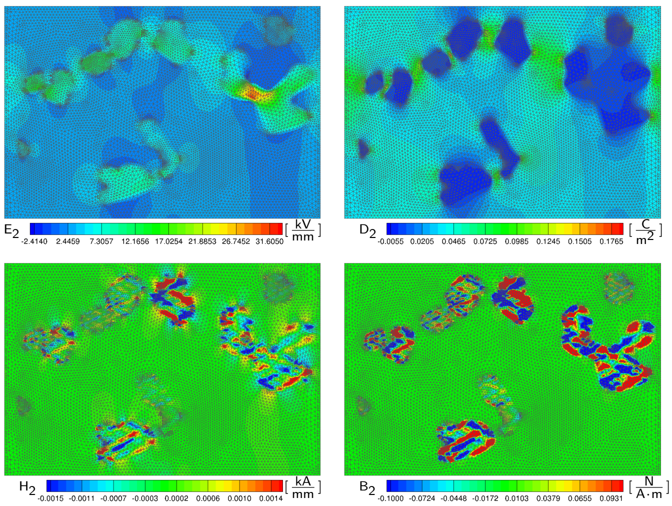
This effective ME coefficient is dependent on the properties of the individual phases and the morphology of the microstructure.

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 ($CoFe_2O_4$).



In order to analyze the ME coefficient we apply an external electric field $\overline{E}_2$ in vertical direction. The resulting deformation of the piezoelectric matrix is transferred to the piezomagnetic particles so that a (strain-induced) magnetic induction is generated.



The simulated effective ME coefficient $\overline{\alpha}_{22}^{\mathsf{sim}}$ is compared to the experimentally determined coefficient $\overline{\alpha}_{22}^{\mathsf{exp}}$ from [1] ($[\overline{\alpha}] = \frac{N\,s}{V\,C}$)

$$\overline{\alpha}_{22}^{\mathsf{sim}} = 3.893 \cdot 10^{-11} \quad \Leftrightarrow \quad \overline{\alpha}_{22}^{\mathsf{exp}} = 4.4 \cdot 10^{-12}\,.$$

The deviation can be explained by: i) the 2D simulation cannot render the 3D shape of the inclusions, ii) the assumed perfect polarity of the two phases cannot be obtained in experiment.

Future work: challenge for modeling and experiment

The challenge lies in both modeling and experiment. In *experiment*, the polarization/magnetization process will be improved so that optimal composites can be developed. 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] M. Etier et al., *Proc. Eur. Conf. Applic. Polar Dielec.* 1–4, 2012.
[2] J. Lee et al., *Int. J. Eng. Sci.* 43:790–825, 2005.
[3] J. Schröder and M.-A. Keip, *Comput. Mech.* 50:229–244, 2012.

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SCHR 570/12–1