Computational characterization of magneto-electric composites: the role of ferroelectric pre-polarization

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ABSTRACT

Coupling between electric and magnetic fields enable new smart devices and may find application in sensor technology and data storage [1]. Materials showing magneto-electric (ME) coupling properties combine two or more ferroic characteristics and are known as *multiferroics*. Since natural single-phase materials show a very low interaction between polarization and magnetization at room temperature, the manufacturing of composite materials becomes relevant. These ME composites consist of magnetically and electrically active phases and generate the ME coupling as a strain-induced *product property*. It has to be emphasized that for each of the two phases the ME coupling modulus is zero and the overall ME modulus is generated by the interaction between both phases. Here we distinguish between the direct and converse ME effect. The direct effect characterizes magnetically induced polarization, where an applied magnetic field yields a deformation of the magneto-active phase which is transferred to the electro-active phase. As a result, a *strain-induced* polarization in the electric phase is observed. On the other hand, the converse effect characterizes electrically activated magnetization. Several experiments on composite multiferroics showed remarkable ME coefficients that are orders of magnitudes higher than those of single-phase materials. Due to the significant influence of the microstructure on the ME effect, we derived a two-scale finite element (FE²) homogenization framework, which allows for the consideration of microscopic morphologies [2,3]. A further major influence on the overall ME properties is the polarization state of the ferroelectric phase. With this in mind, a material model is implemented that considers the switching behavior of the spontaneous polarization [4] and enables a more exact comparison to experimental measurements in [5].

REFERENCES

- [1] N.A. Spalding and M. Fiebig, "The renaissance of magnetoelectric multiferroics", *Materials Science*, **309**, 391-392 (2005).
- [2] J. Schröder and M.-A. Keip, "Two-scale homogenization of electro-mechanically coupled boundary value problems", *Computational Mechanics*, **50**, 229-244 (2012).
- [3] M. Labusch, M. Etier, D.C. Lupascu, J. Schröder and M.-A. Keip, "Product properties of a two-phase magneto-electric composite: Synthesis and numerical modeling", *Computational Mechanics*, **54**, 71-83 (2014).
- [4] S.C. Hwang, C.S. Lynch and R.M. McMeeking, "Ferroelectric/ferroelastic interactions and a polarization switching model", *Acta Metall. Mater.*, **43**, 2073-2084 (1995).
- [5] M. Etier, V.V. Shvartsman, Y. Gao, J. Landers, H. Wende and D.C. Lupascu, "Magnetoelectric effect in (0-3) CoFe₂O₄-BaTiO₃ (20/80) composite ceramics prepared by the organosol route", *Ferroelectrics*, 448, 77-85 (2013).