

11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

Ferroelectric thin film nano-generators

Ingo Münch^{1*}, Matthias Krauß² and Werner Wagner³

¹ Karlsruhe Institute of Technology, Institute for Structural Analysis, Kaiserstr. 12, D-76131 Karlsruhe, ingo.muench@kit.edu, <http://www.kit.edu>

² Karlsruhe Institute of Technology, Kaiserstr. 12, D-76131 Karlsruhe, matthias.krauss@kit.edu

³ Karlsruhe Institute of Technology, Kaiserstr. 12, D-76131 Karlsruhe, w.wagner@kit.edu

Key Words: *Multiphysics Problems, Phase Field Modelling, Energy Harvesting.*

We investigate the behaviour of epitaxial sputtered ferroelectric thin films with uniform lattice orientation for the design of nano-generators to convert mechanical into electrical energy. Therefore, we use a phase field model to simulate the domain topology. For the efficiency of the generator, it is important to consider an appropriate substrate layer to pre-stress the ferroelectric material. Further, the BaTiO₃ film needs a structured field of top electrodes. Both, pre-stress and structured electrodes enforce a domain topology which allows for energy conversion.

Alternating interfacial strain between the substrate and the ferroelectric, e.g. by bending the substrate, leads to alternating domain configurations. Thus, opposite surface charges between the electrodes generate an electric flux. Due to the mechanical cycle load there is need for an electrical circuit to transform single-phase alternating current into co-current flow. It is essential to store the generated electric energy within an accumulator or capacitor. However, the contact and charge status of the electric storage medium strongly influences the performance of the generator.

We numerically couple the phase field model to a standard full-wave rectifier and a capacitor. Non-linear diode characteristics as well as energy losses are under consideration. The amount and the type of connections within the harvesting field are discussed to bridge from the nano-scale to electrical quantities for microelectronics. Naturally, the generators exhibit a favourable working point. The numerical simulation considers an electro-mechanical phase-field model with polarization as state variable. The complex boundary conditions can be considered within a finite element formulation. An enhanced numerical algorithm is required to handle the coupling.

REFERENCES

- [1] I. Münch, M. Krauß, W. Wagner and M. Kamlah, “Ferroelectric nanogenerators coupled to an electric circuit for energy harvesting”, *Smart Mat. Struct.*, Vol. **21**, 115026, (2012).
- [2] I. Münch, M. Krauß, C. M. Landis, J. E. Huber, “Domain engineered ferroelectric energy harvesters on a substrate”, *Journal of Applied Physics*, Vol. **109**(10), 104106, (2011).