Two-Scale Modeling of Ferroelectric Materials

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The continuum mechanical description of ferroelectric material behaviour in gereral follows a phenomenological approach that represents the main characteristics of the polycrystalline material. However, when it is desired to capture a wider range of microscopic effects, the phenomenological ansatz on the macroscale is often no longer applicable or at least not sufficient. To offer the opportunity of incorporating the microscopic effects directly into the model, numerical approaches will be presented that are able to connect the microscopic structure to the macroscopic model. To this end two homogenization approaches are formulated, which are both reflecting the heterogeneous crystal setup of the ferroelectric material. Both models represent the crystallographic lattice structure up to a certain accuracy. For the individual domains on the mesoscale we use a transversely isotropic model [1],[2].
The first approach uses orientation distribution functions for the domain orientations, that are installed in every material point of the macroscopic model [3]. In this context a thermodynamically consistent formulation for the description of the polycrystalline behaviour of the ferroelectric material will be derived and several applications will show the efficiency of the proposed formulation.
The second approach is based on an FE^2-formulation and accounts for a discrete representation of the mesoscopic scale [4]. The mesoscopic scale is represented by representative volume elements and is connected to the macroscopic scale by use of boundary integrals. The thermodynamically consistent formulation is able to integrate arbitrary mesoscopic setups into the macroscopic model and therewith to generate the individual macroscopic material response without using a macroscopic material law.

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