



Phase-field modeling for ferroelectrics

By Völker, Benjamin M.

Condition: New. Publisher/Verlag: Südwestdeutscher Verlag für Hochschulschriften | in a multi-scale approach | The primary objective of this work is to apply phase-field modeling in a knowledge based multi-scale simulation approach for the ferroelectric polycrystalline ceramics lead titanate and lead zirconate titanate (PZT) in order to bridge the gap between predictive atomistic and micromechanical modeling methods. Two interfaces in the multi-scale simulation chain are developed and established. Results of atomistic calculations are employed as input parameters for a phase-field model connecting the atomic level to the meso-scale. A novel and completely knowledge based adjustment method is developed for the core of the phase-field model-its thermodynamic free energy function. Furthermore, the elastic properties of the free energy function are improved by introducing higher order terms. In order to link the meso- to the micro-scale in the simulation chain, the phase-field model is implemented in a finite-element formulation. Typical ferroelectric domain configurations as well as defect mechanisms are investigated under electromechanical loading, identifying reversible domain wall motion and bending as governing mechanisms influencing small-signal parameters on the meso-scale. | Format: Paperback | Language/Sprache: english | 180 pp.



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