



## Sonderforschungsbereich 595

### Elektrische Ermüdung in Funktionswerkstoffen



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## Compositional Design of Piezoelectric Transducer Materials: Lessons from Thermodynamics

Ceramics based on pseudo-binary ferroelectric solid solutions that exhibit morphotropic phase boundaries remain the most widely used materials for piezoelectric transducer applications. In this talk the generic case of a ferroelectric solid solution is considered wherein different symmetry phases located at opposing ends of the diffusionless composition-temperature phase diagram are separated by a morphotropic boundary (MB). It is shown that the classical Landau theory of weak first order phase transformations automatically predicts an extreme reduction in the anisotropy of polarization near the MB. In the lowest-order approximation the isothermal composition change producing the rhombohedral to tetragonal transition along the MB line is dictated by the condition that the polarization anisotropy energy vanishes. Under this condition there is a drastic decrease in domain wall energy that results in the formation of ferroelectric nanodomain states that produce the same diffraction pattern attributed to homogeneous monoclinic phases. The electric field or stress induced reconfiguration of these nanotwins necessarily produces extrinsic contributions to the dielectric and electromechanical properties. The spherical degeneration of the polarization direction also predicts the formation of a polar glass-like state wherein the nanodomains may assume irregular shapes and may exhibit high configurational sensitivity to external forces. A small lifting of the orientational degeneracy of the polarization leads to differing phase diagram topologies wherein an orthorhombic phase may interleave the rhombohedral and tetragonal phase fields. The curving of the MB line, the nearly continuous transitions between adjacent ferroelectric phases and the change in the order of the paraelectric to ferroelectric transitions with composition also arise naturally in the theory. If diffusional processes are operative, all equilibrium boundary lines of the diffusionless phase diagram must be replaced by two-phase fields. Possible topologies of the equilibrium MB phase diagram illustrating these two-phase equilibrium fields are computed. The theory provides insights into the influence of microstructure on the dielectric and piezoelectric properties of morphotropic ferroelectric solid solution systems and the implications for processing-property relations in these materials will be discussed. The theory of vanishing polarization anisotropy is also found to reproduce the phase diagram topologies of other technologically important perovskite-structured solid solution systems that do not display an MB. An extension of the theory to more complex systems provides a potential means to guide the compositional design of materials with phase diagram topologies tailored for use in specific transducer applications.

Die Vorträge finden, wenn nicht anders angegeben, jeweils um **16:15**  
im Gebäude der Materialwissenschaften, Lichtwiese, Petersenstr. 23, **Raum 77** statt