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Multifield-Driven Phase Transition and Domain Boundary Mechanisms in PZT95/5 Ceramics

Yujuan Peng[1], Yixuan Jiang[1,*], and Xingzhe Wang[1]

[1]Key Laboratory of Mechanics on Western Disaster and Environment, Ministry of Education, College of Civil Engineering and Mechanics, Key Laboratory of Special Function Materials and Structure Design of Ministry of Education, Lanzhou University, Lanzhou, 730000, China

[*]Corresponding Author: Yixuan Jiang. Email: jyix@lzu.edu.cn

ABSTRACT

PZT95/5 ceramics exhibit rich and field-tunable ferroelectric–antiferroelectric (FE–AFE) phase transitions under coupled mechanical, thermal, and electric fields, serving as promising candidates for high-power pulse power supplies, energy storage devices, and electromechanical conversion systems. However, existing models usually simplify phase transitions as pure polarization rearrangements, largely ignoring the strong coupling between polarization and oxygen octahedral tilting (OOT), as well as the critical role of antiferroelectric domain boundaries in multi-domain microstructures. These drawbacks severely restrict the quantitative understanding and precise regulation of transition pathways, intermediate phase structures, and domain switching dynamics.

This work establishes a unified Landau thermodynamic framework incorporating FE polarization, AFE polarization, and OOT as coupled order parameters, which accurately reproduces the temperature–pressure phase diagram and polar microstructure evolution of PZT95/5. The model reveals that OOT competes with polarization in the FE phase but synergizes with it in the AFE phase, thereby regulating the stability of incommensurate intermediate phases and pressure-induced transition pathways.

On this basis, a thermodynamically consistent multi-order-parameter phase-field model is further developed to simulate multi-domain evolution and phase boundary dynamics under coupled electromechanical loadings. Simulations show that by tuning the FE–AFE polarization coupling strength, pressure-induced FE–AFE transitions can be controlled to occur either directly or stepwise via a stable intermediate phase. Under electric fields, the antiferrodistortive–ferrodistortive (AFD–FD) structural transition of OOT determines the transition pathway, rendering AFE–FE conversion a two-stage AFE–FiE–FE behavior. Domain wall investigations demonstrate that in the FE rhombohedral phase, OOT-related antiphase boundaries coincide with non-180° FE domain walls and dominate domain wall thickness and mobility. The antiphase boundaries of the AFE phase exhibit a structure where a FE domain is sandwiched between two oppositely oriented AFE domains. With increasing pressure, the FE domain at the boundary gradually vanishes. The underlying mechanism is that pressure modifies the phase characteristics of the antiphase boundaries, eventually leading to a phase difference of π across the boundary; the two half-period AFE domains overlap reversely and cancel each other out, resulting in no net polarization component at the antiphase boundaries.

This work establishes a link between microscale domain dynamics and macroscale electromechanical responses. The revealed mechanical mechanisms of AFE domain boundaries and staged transition rules provide a theoretical foundation for the design and performance optimization of high-performance antiferroelectric ceramics for extreme environments.

KEYWORDS

PZT95/5; ferroelectric-antiferroelectric phase transition; oxygen octahedral tilting; domain boundary; phase-field



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model; Landau thermodynamics; electromechanical coupling

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