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Simulation of Domain Reorientation and Phase Transformation in Unpoled PZT95/5 under Triaxial Stress with a Micromechanical Model

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Motivation

PZT95/5 can transform at room temperature from a ferroelectric rhombohedral (FER) to an antiferroelectric orthorhombic (AFO) state under pressure because it has a smaller unit volume. Poled PZT is depolarized by the ferroelectric to antiferroelectric phase transformation triggering a release of bound charge, which makes this material interesting for pulse power applications. The ferroelectric-antiferroelectric phase transformation is highly nonlinear, hysteretic, and operates in a stress and electric field domains that also experiences other nonlinear phenomena such as domain-reorientation. This poses a substantial challenge for macroscale continuum models because these inherently microstructural changes are not resolved. A ferroelectric material model has been developed to simulate phase transition and domain reorientation for PZT95/5. A micromechanical approach approximates the domain microstructure with volume fractions representing all possible domain orientations. Energy-based switching criteria are used to capture the phase transformation and domain reorientation. The validated model successfully explains the combined domain reorientation and ferroelectric-antiferroelectric phase transformation observed in PZT95/5 under triaxial compressive loading.

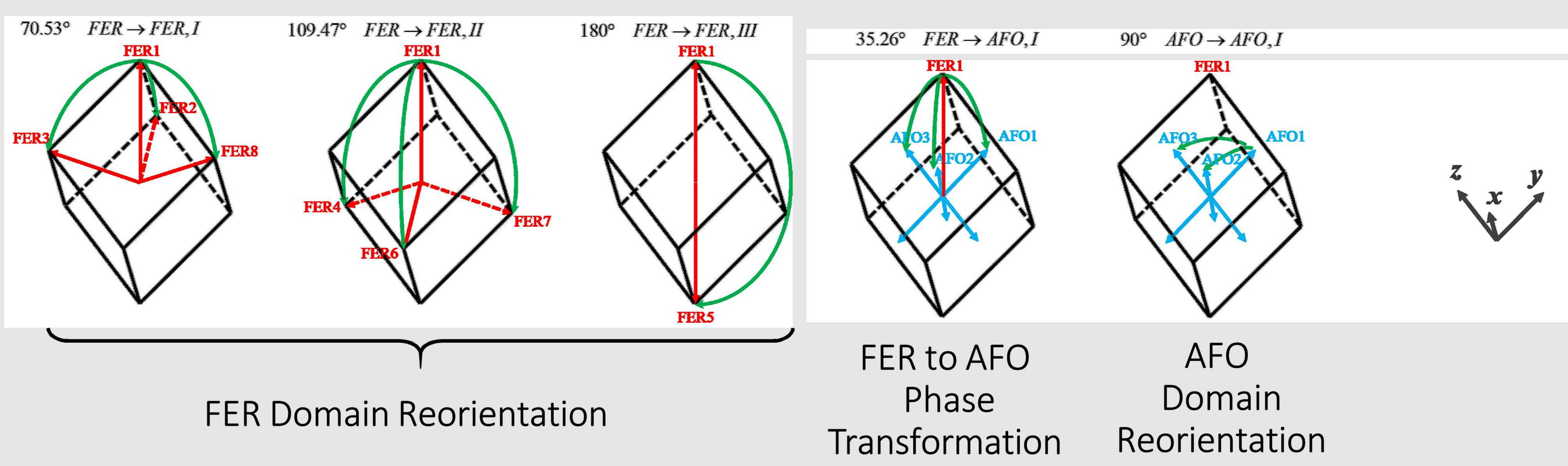
Material and Model Behavior

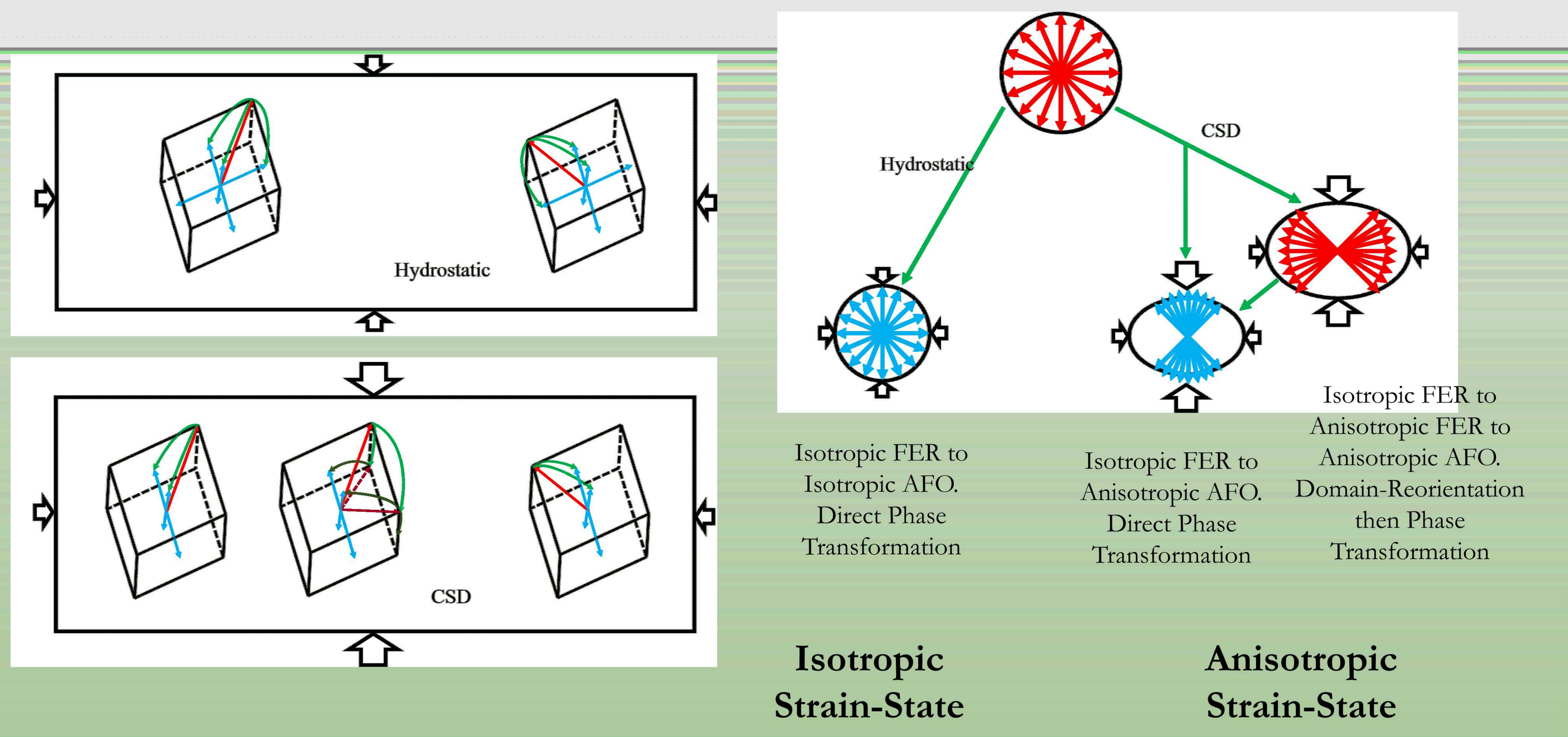
Within each single crystallite grain, the material model defines each of the 8 unique FER domain states and 3 unique AFO domain states as individual variants each defined by a spontaneous strain. Energy-based switching criterion governing transformation between two variants is satisfied when the availability of the system to do positive work from the spontaneous strain change of the transformation exceeds the transformation energy barrier.

$$\sigma_i \Delta\varepsilon_i^{0,\alpha\rightarrow\beta} - b^{\alpha\rightarrow\beta} \geq 0$$

Under hydrostatic compression, FER variants are equally likely to transform to all three AFO variants leading to isotropic remnant strain in the AFO phase. When deviatoric stresses are present, FER variants will only transform to the most energetically favorable AFO variant (mechanically compatible with the stress state). This causes anisotropy in the AFO remnant strain. Sufficiently large deviatoric stresses could also trigger a ferroelastic domain-reorientation in the FER phase prior to phase transformation.

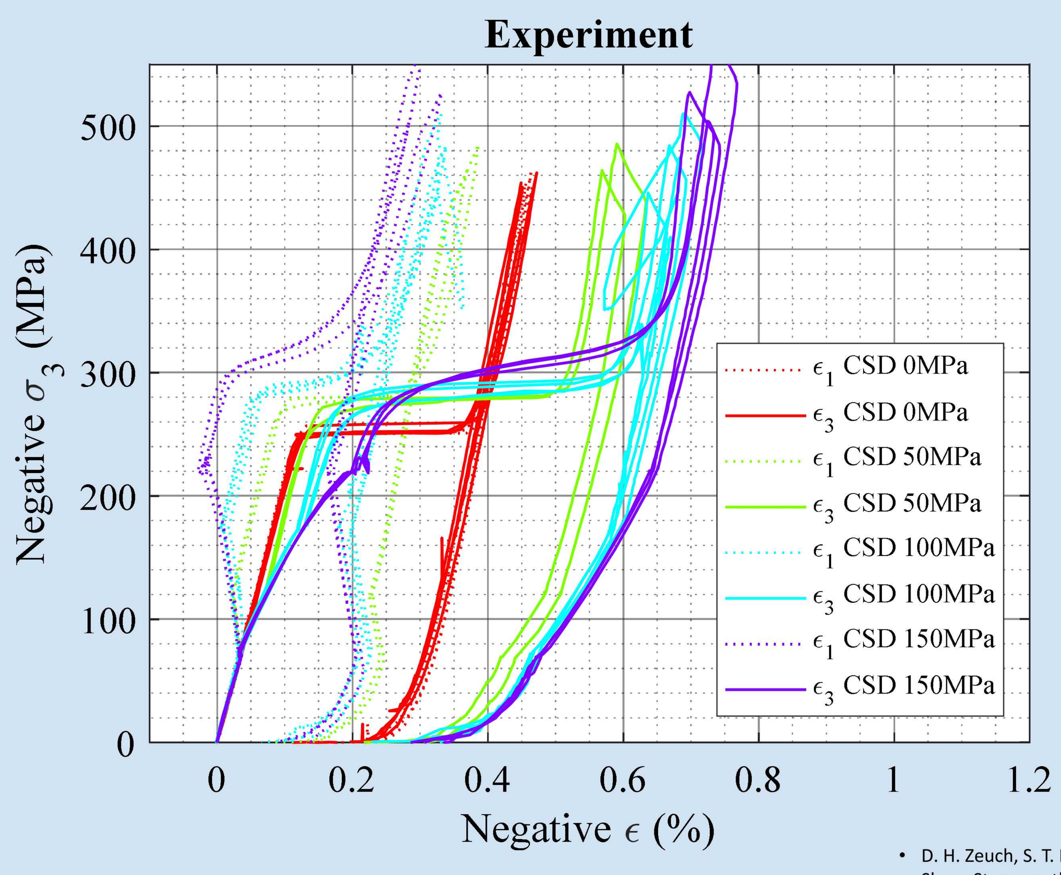
Variant Transformation Types

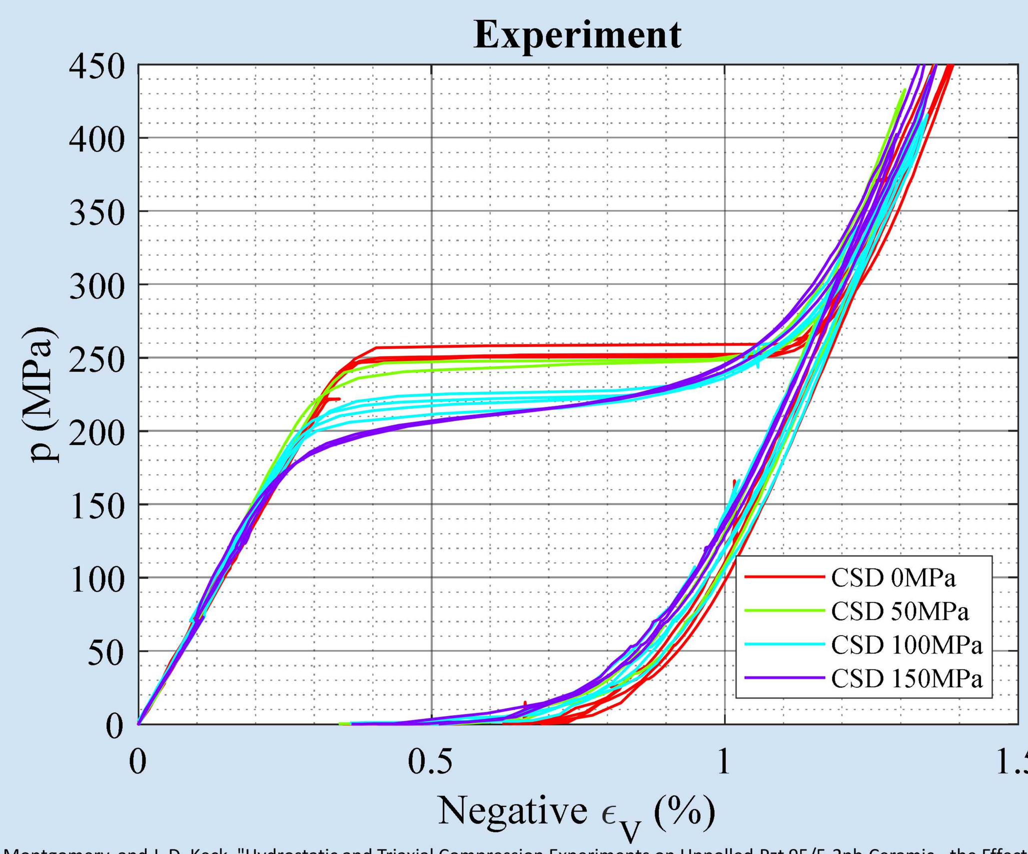




Experimental Material Response

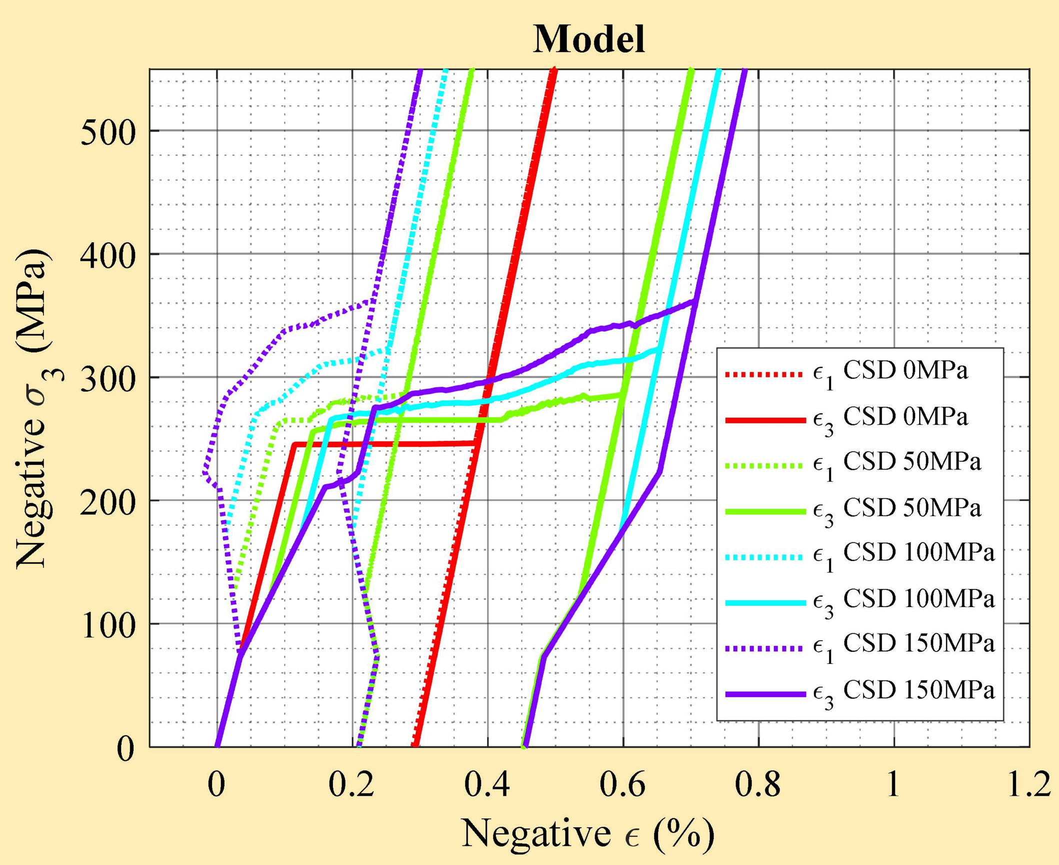
The modeling effort aims to reproduce and validate the experimental characterization work conducted by Zeuch *et al.**, which triaxially loaded unpoled PZT95/5 specimens under a combination of constant uniaxial and ramped hydrostatic compressive stress. This creates a constant stress difference (CSD) between the axial and transverse stresses. Zeuch's study found remnant axial and transverse strains of phase transformation to be isotropic under hydrostatic loads and severely anisotropic under CSD conditions while remnant volumetric strains of transformations were unchanged. Increasing CSD was also shown to decrease the phase transformation initialization pressure and increase the completion pressure.

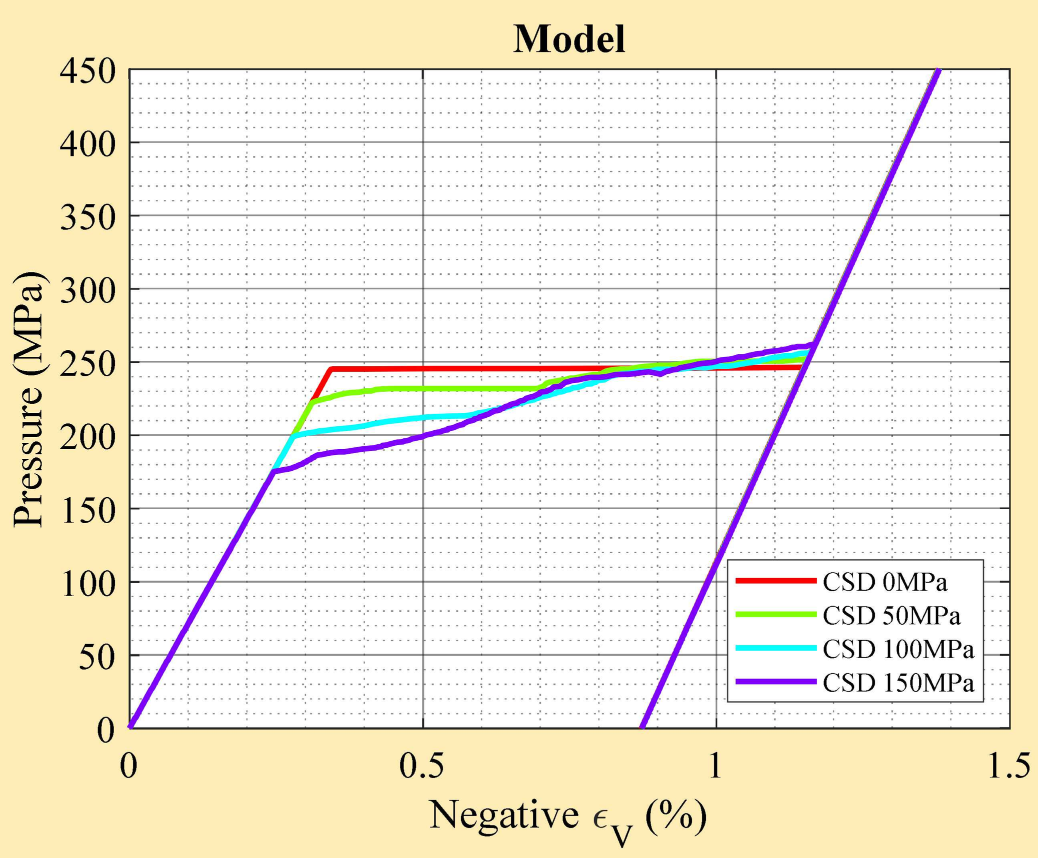




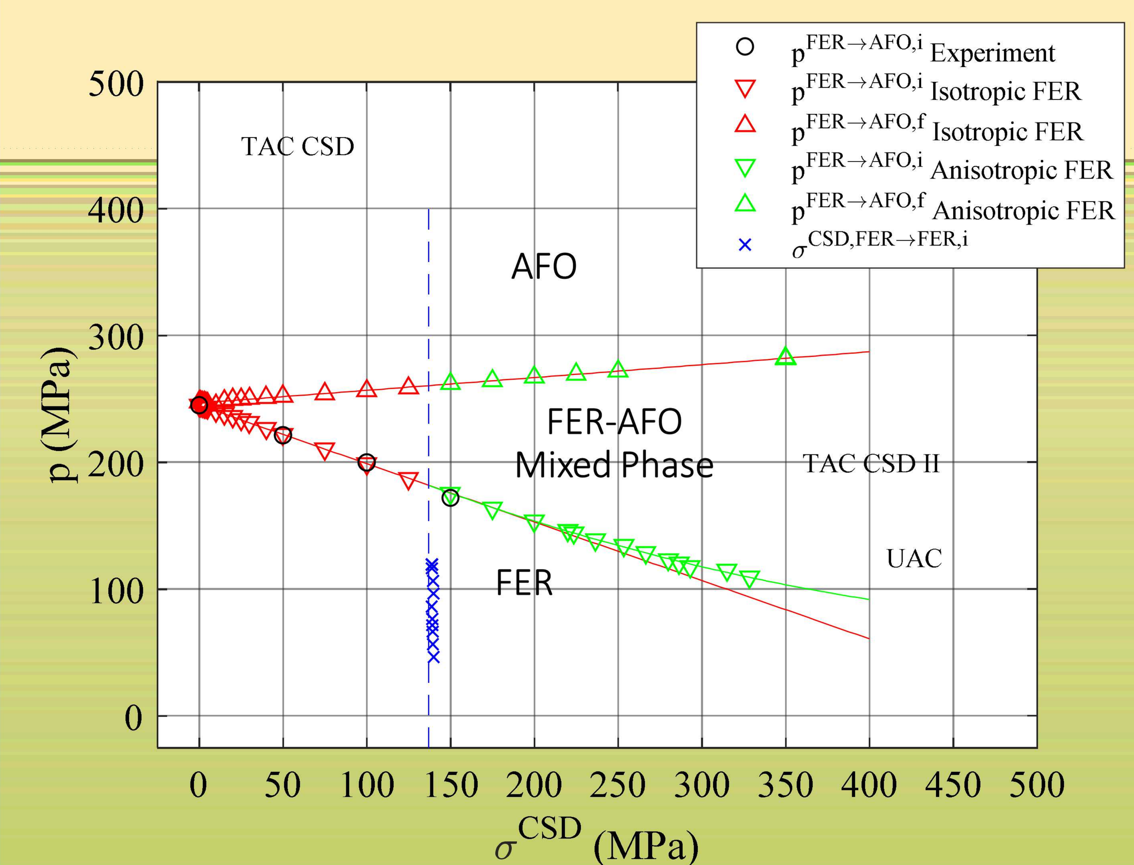
• D. H. Zeuch, S. T. Montgomery, and J. D. Keck, "Hydrostatic and Triaxial Compression Experiments on Unpoled Pzt 95/5-2nb Ceramic - the Effects of Shear-Stress on the Fr1-Ao Polymorphic Phase-Transformation," (in English), Journal of Materials Research, vol. 7, no. 12, pp. 3314-3332, Dec 1992.

Modeling Response





Predicted Phase Map of FER-AFO Phase Transformation in Hydrostatic-Uniaxial Stress Space



The modeling approach is capable of closely capturing the triaxial loading response of PZT95/5 including the FER and AFO elastic response, the transformation strain under both hydrostatic and triaxial loading, the initiation and termination stress states for phase transformation, and the initiation stress for domain reorientation.

For pulse power applications loaded under a mixture of hydrostatic and deviatoric stress, the model is capable of predicting a phase diagram in hydrostatic-deviatoric stress space outlining conditions for full, partial, and no phase transformation.

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