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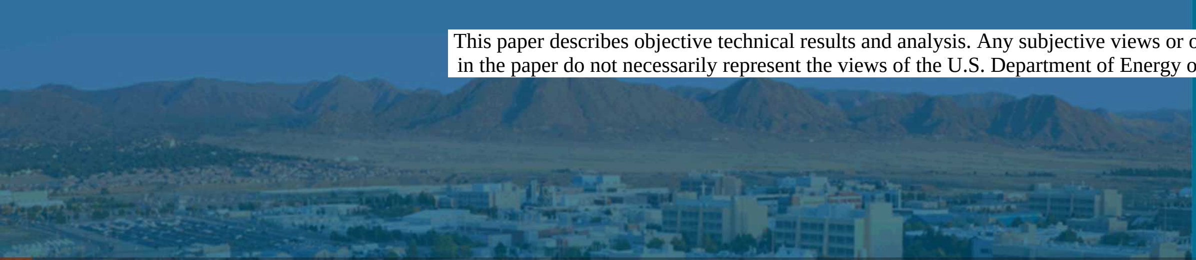

Simulation of Domain Reorientation and Phase Transformation in Unpoled PZT95/5 under Triaxial Stress with a Micromechanical Model

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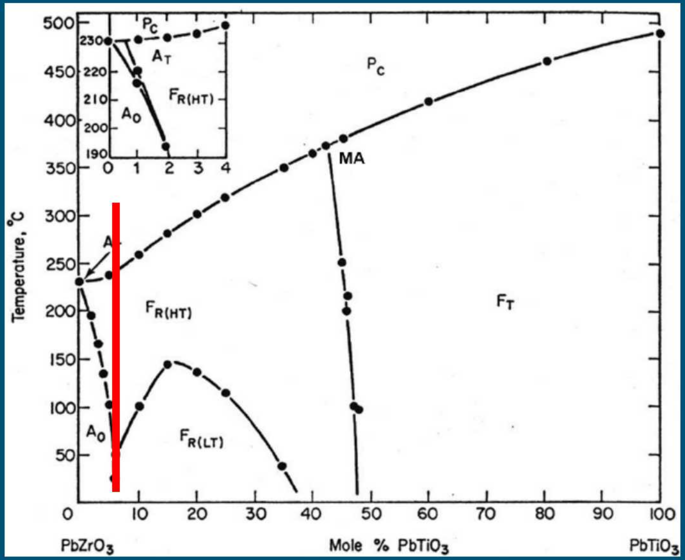
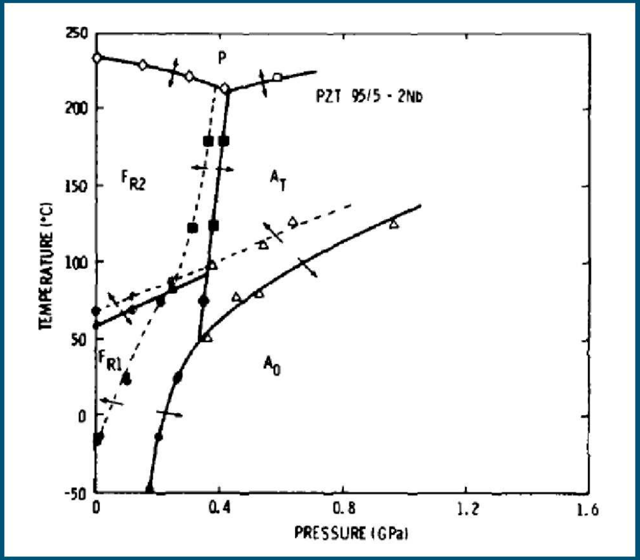
Introduction to PZT95/5



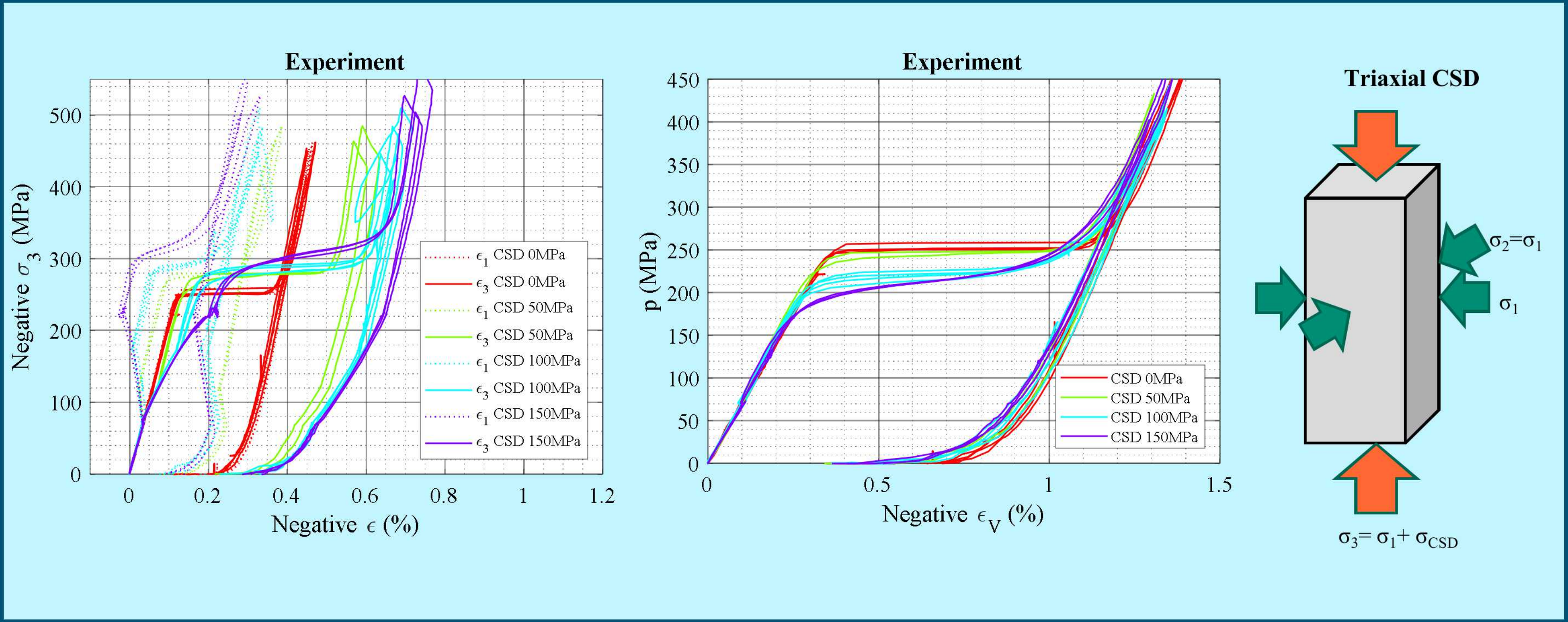
Jaffe Cook and Jaffe 1971.



Fritz and Keck 1978.

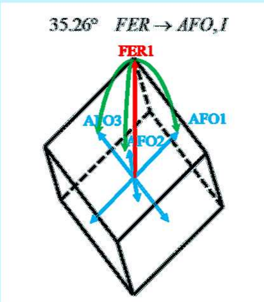
- PZT 95/5 lies on the FER side of the FER – AFO phase boundary.
- Pressure can induce FER to AFO phase transformation due to smaller unit volume of the AFO phase.
- Goal of this work is to model and understand previous work on anisotropic compressive stress induced FER to AFO transformation

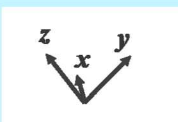
Triaxial Compression Loading in PZT95/5

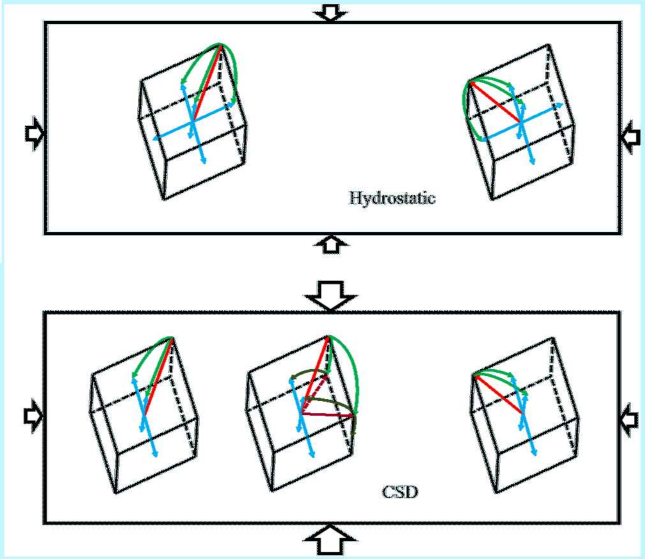


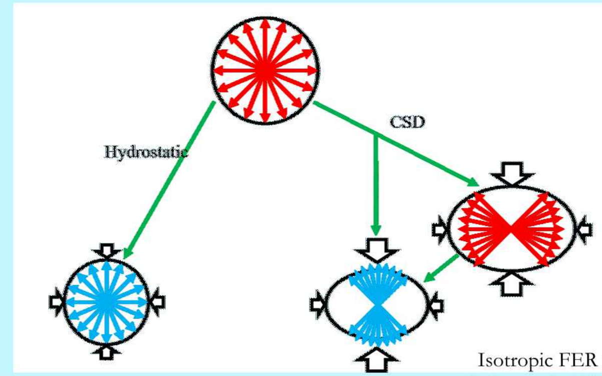
- Triaxial Constant Stress Difference (CSD) study conducted by Zeuch *et al*. 1992
- Large anisotropy in phase transformation strain remnant strain under CSD
- No difference in volumetric strain
- Lowering of phase transformation initiation pressure
- Increase of phase transformation termination pressure

Phase Transformation in PZT95/5









Isotropic FER to Isotropic AFO. Direct Phase Transformation

Isotropic FER to Anisotropic AFO. Direct Phase Transformation

Isotropic FER to Anisotropic FER to Anisotropic AFO. Domain-Reorientation then Phase Transformation

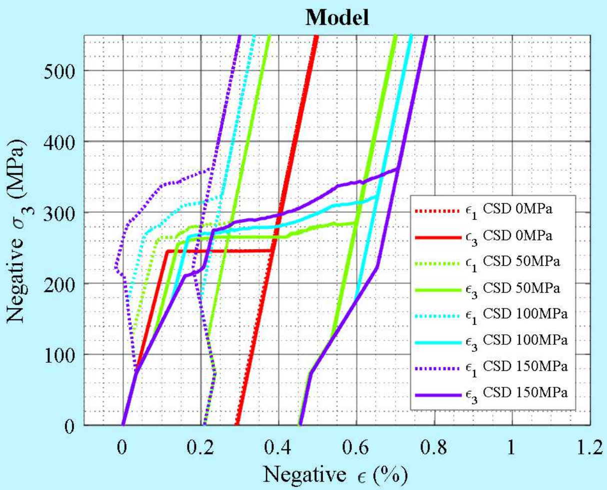
Isotropic Strain-State

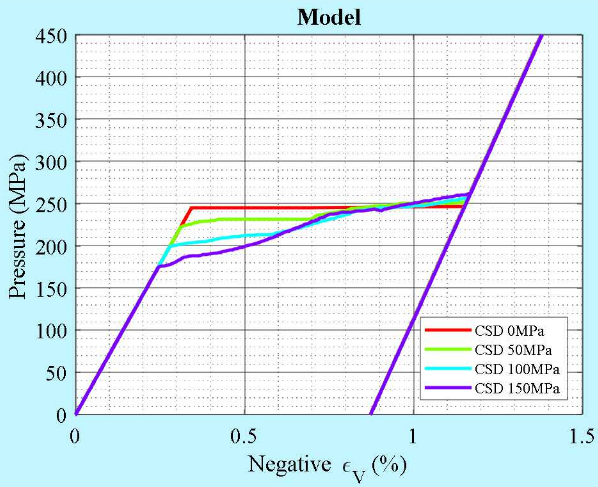
Anisotropic Strain-State

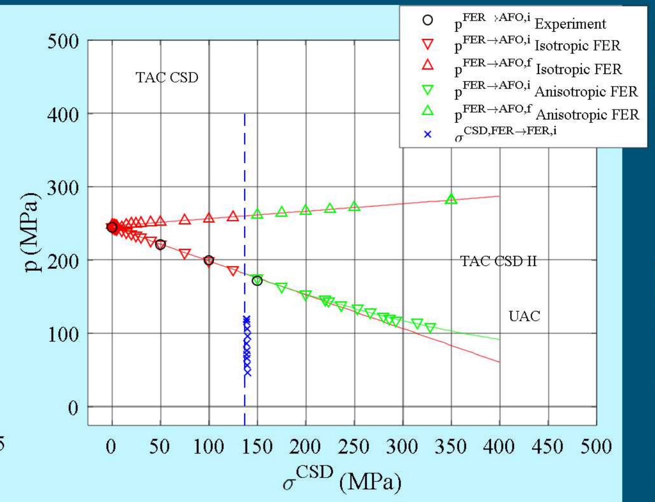
- In each single crystallite grain, there are 11 unique phase variants: 8 unique FER domain orientations and 3 unique AFO strain states.
- Hydrostatic compression causes FER variants to uniformly transform to all AFO variants. Deviatoric stresses cause selective FER-AFO transformations. This leadsd to anisotropic transformation strains.
- This is captured in the material model by energy based switching criteria.

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

Modeling Results







- Material model is capable of accurately capturing phase transformation triaxial loading response in PZT95/5 including
  - Critical transformation stress states
  - Transformation remnant strains
  - Elasticity response
- Material model can also be used to generate FER-AFO phase diagram in hydrostatic-deviatoric stress space.