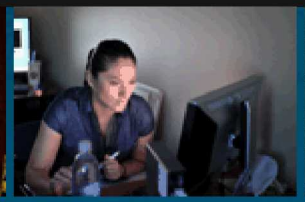
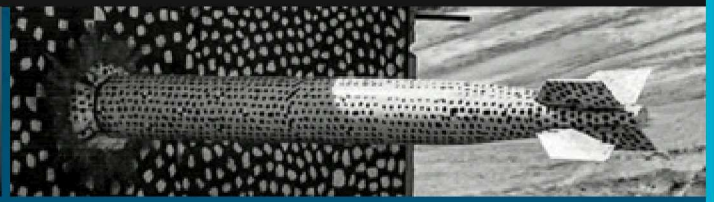
This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

SAND2018-6453C

# Phenomenological Modeling of Nonlinear Behavior in Ferroelectric Materials





WMRIF Early Career Scientist competition

June 18th, 2018

PRESENTED BY

Wen Dong

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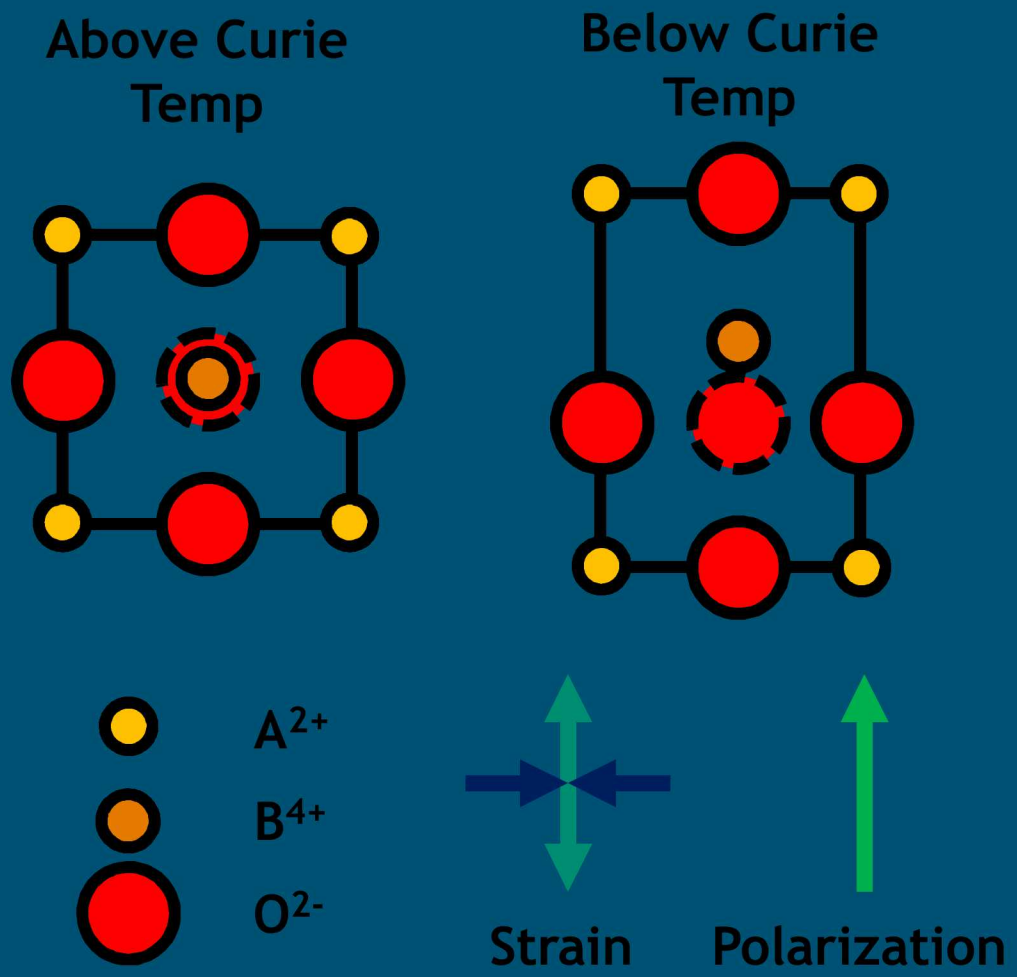
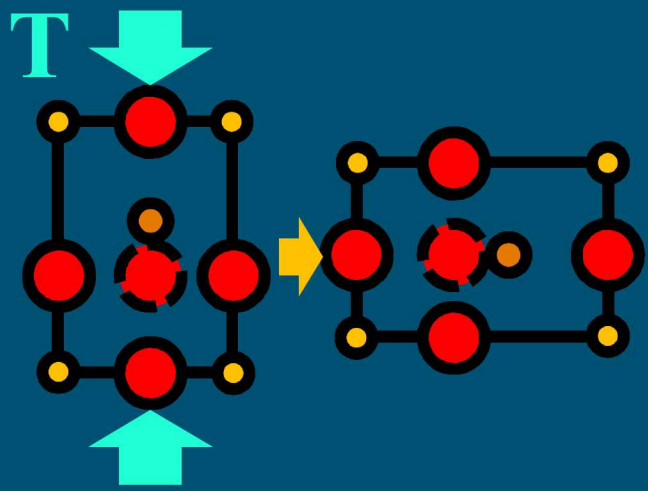
# Overview

- Background: Ferroelectric Ceramics and PZT95/5
- Micromechanical Approach
- Switching Criteria
- Simulation of PZT95/5

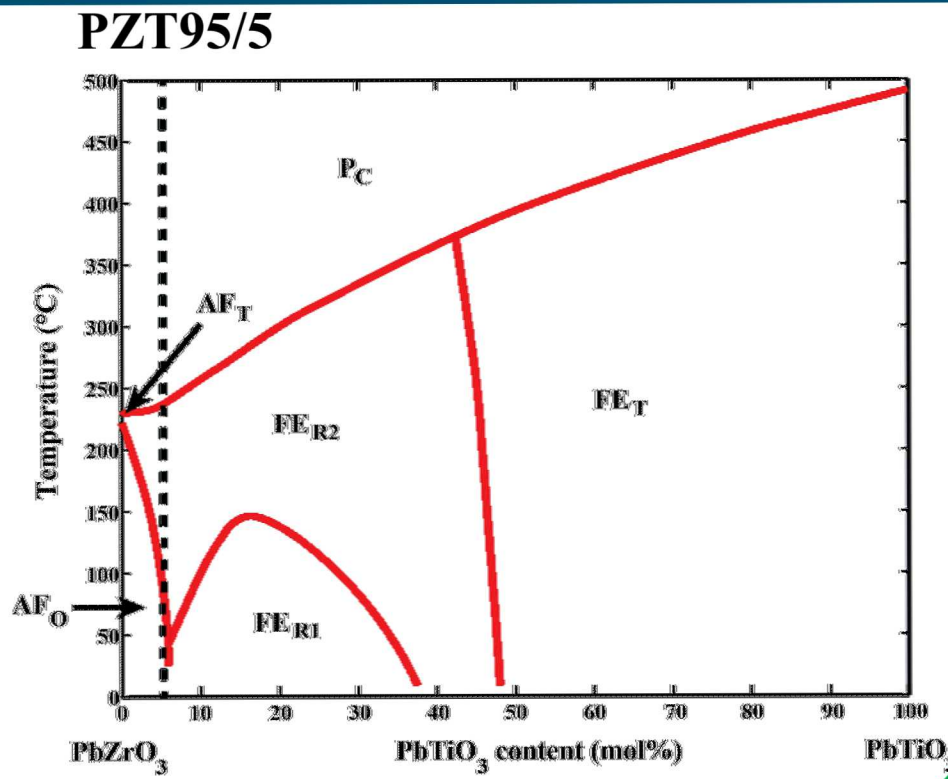
# Ferroelectrics - Perovskites

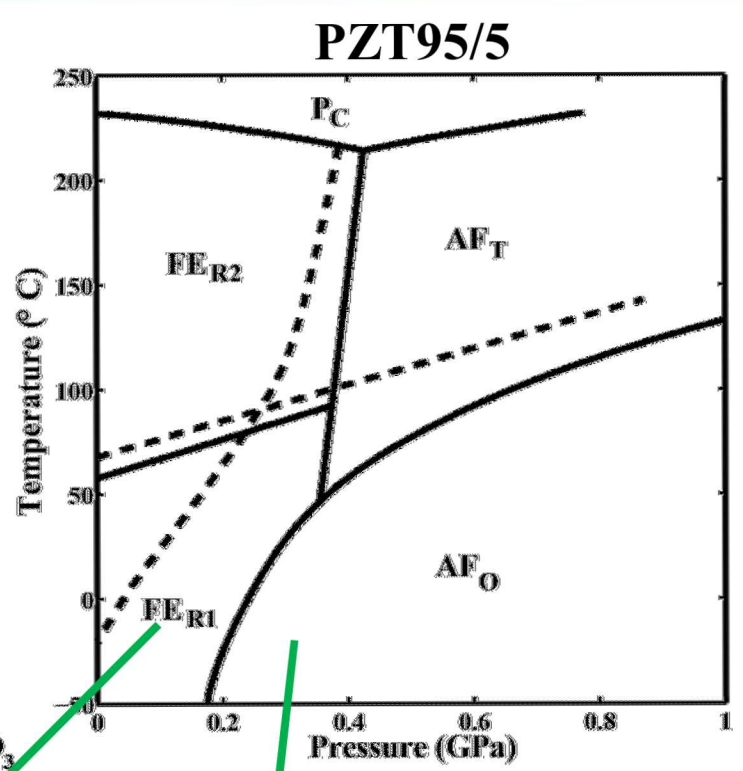


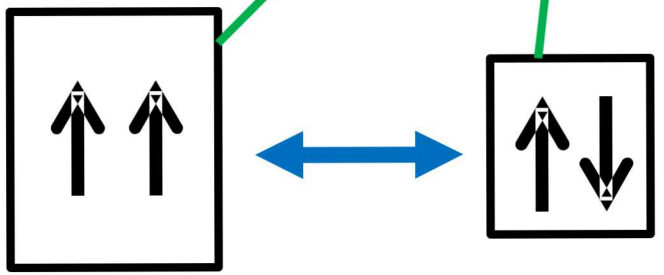

- Cubic above Curie Temp
- Shift of ions positions below Curie temperature causes spontaneous polarization and strain.
- Orientation of polarization and strain is associated with phase.
- Switching between polarization orientations can be induced by electric field or stress (Domain-switching).



# Ferroelectrics – PZT95/5

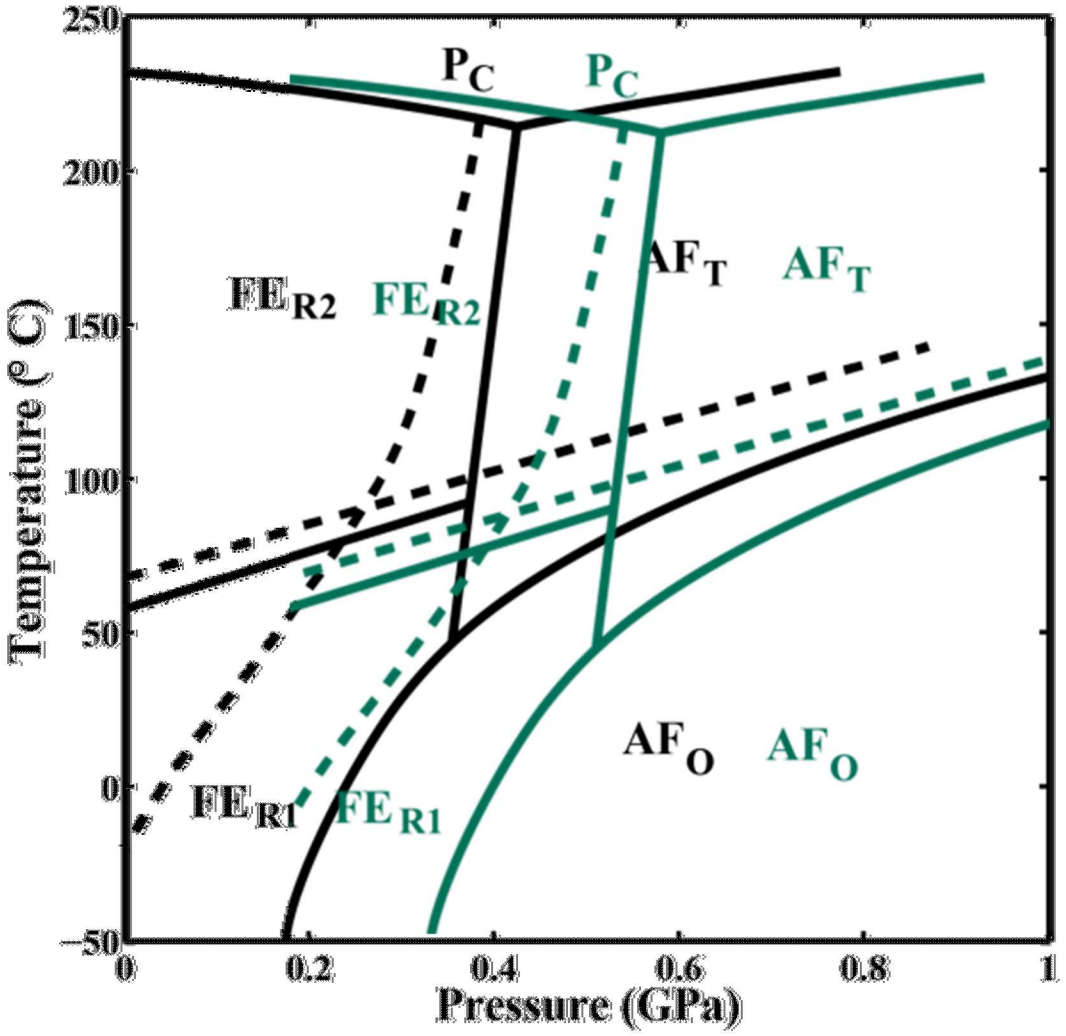


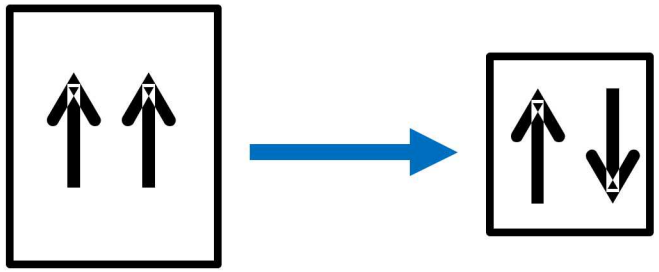



Jaffe et. al. 1971
Fritz and Keck 1978

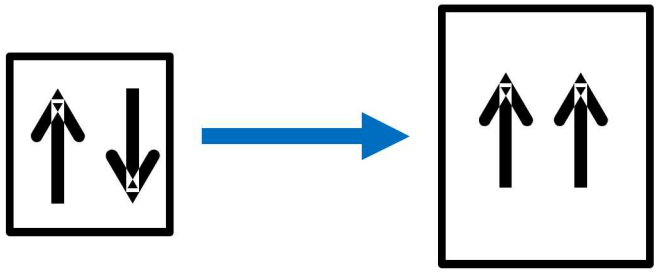
# Ferroelectrics – PZT95/5



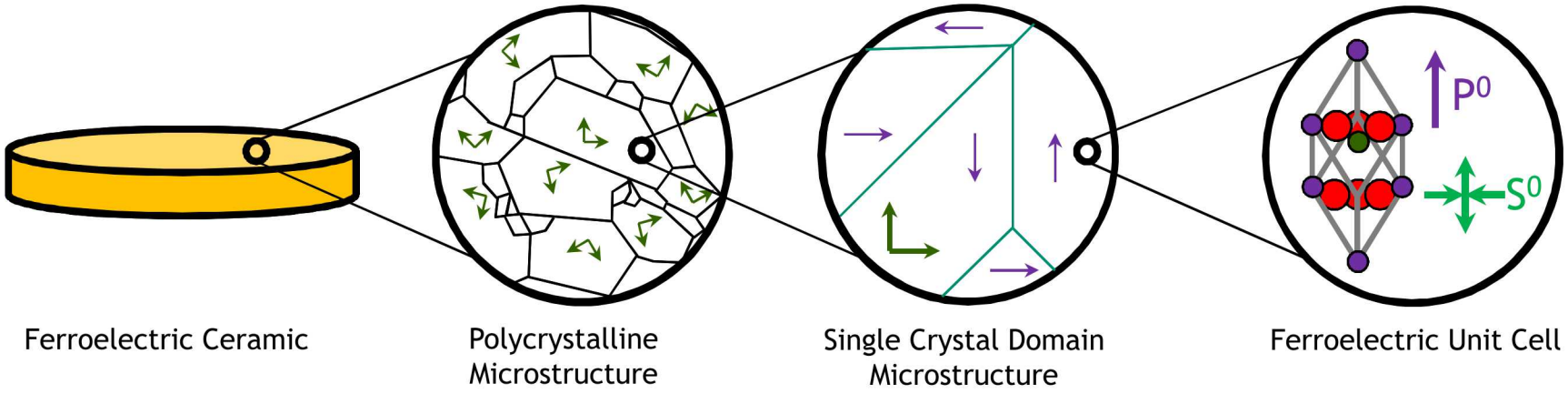

Application of pressure stabilizes antiferroelectric phase



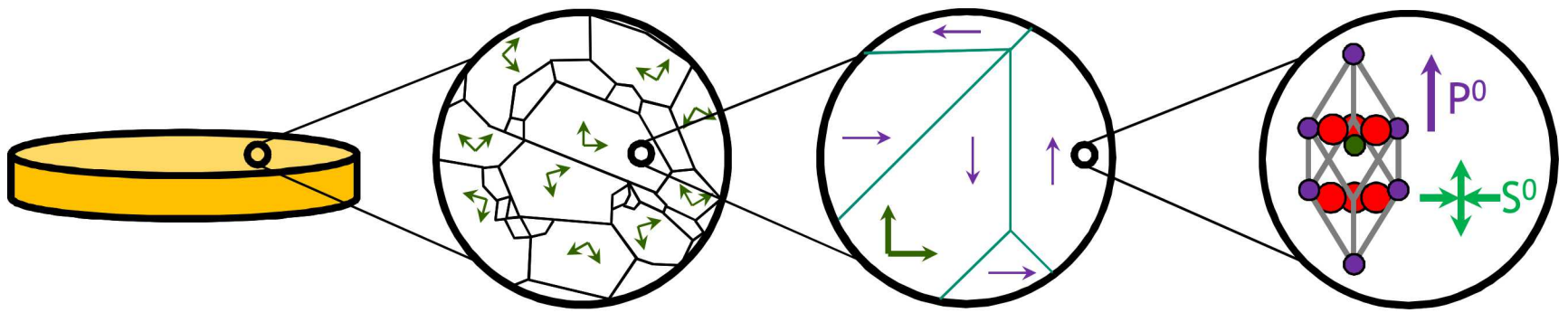
Application of electric field stabilizes ferroelectric phase



# Ferroelectrics - Ceramics

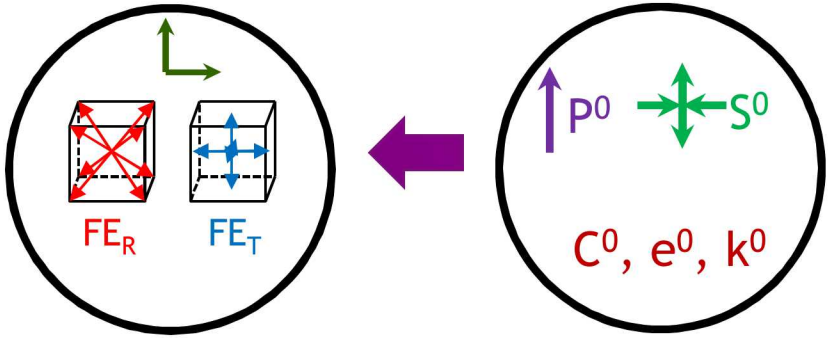


# Micromechanical Approach – Domain Structure




Phase properties are rotated for each domain-variant.

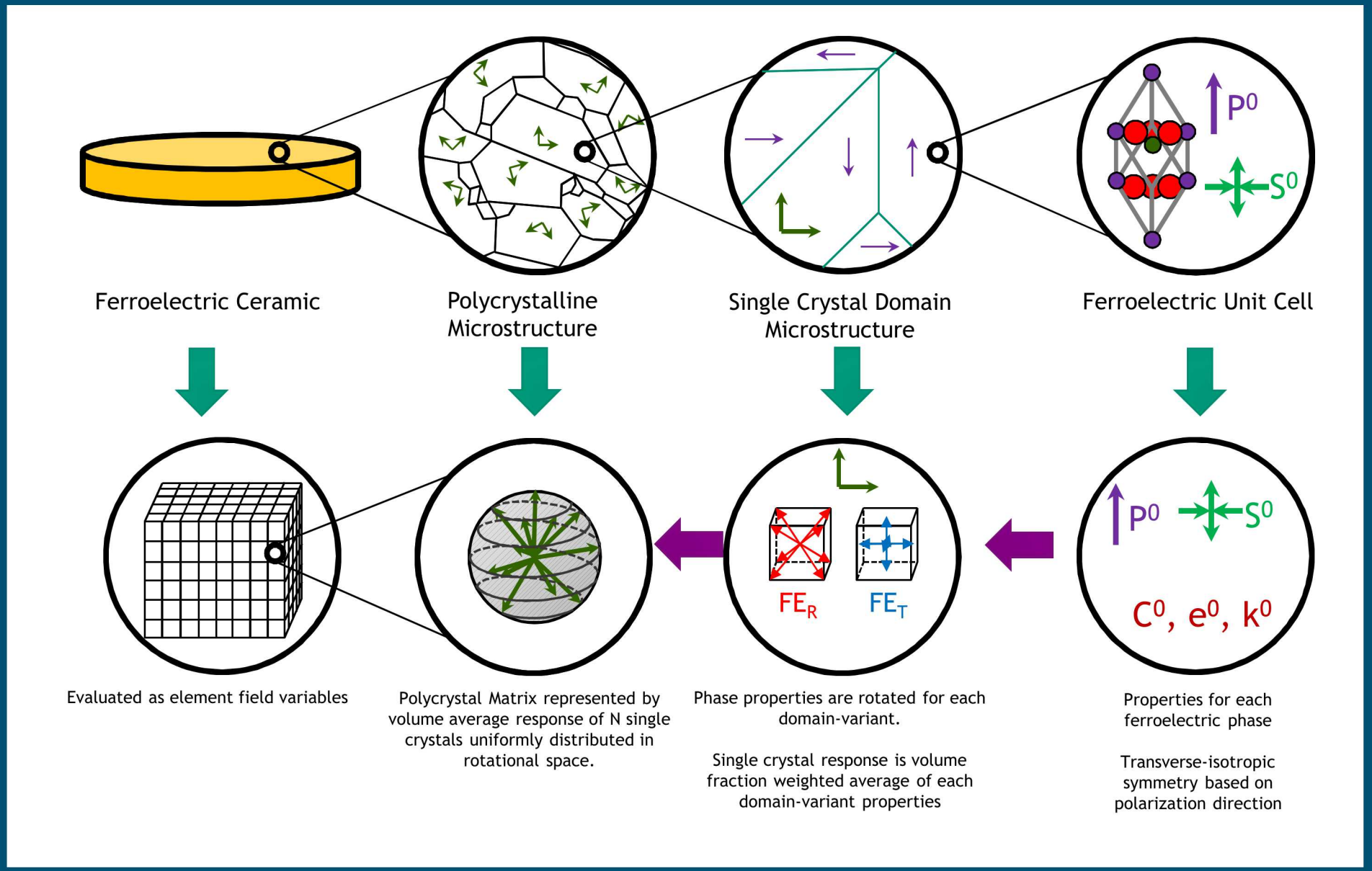
Single crystal response is volume fraction weighted average of each domain-variant properties




Properties for each ferroelectric phase

Transverse-isotropic symmetry based on polarization direction

# Micromechanical Approach – Grain Structure



# Switching Criteria - Energy Dissipation

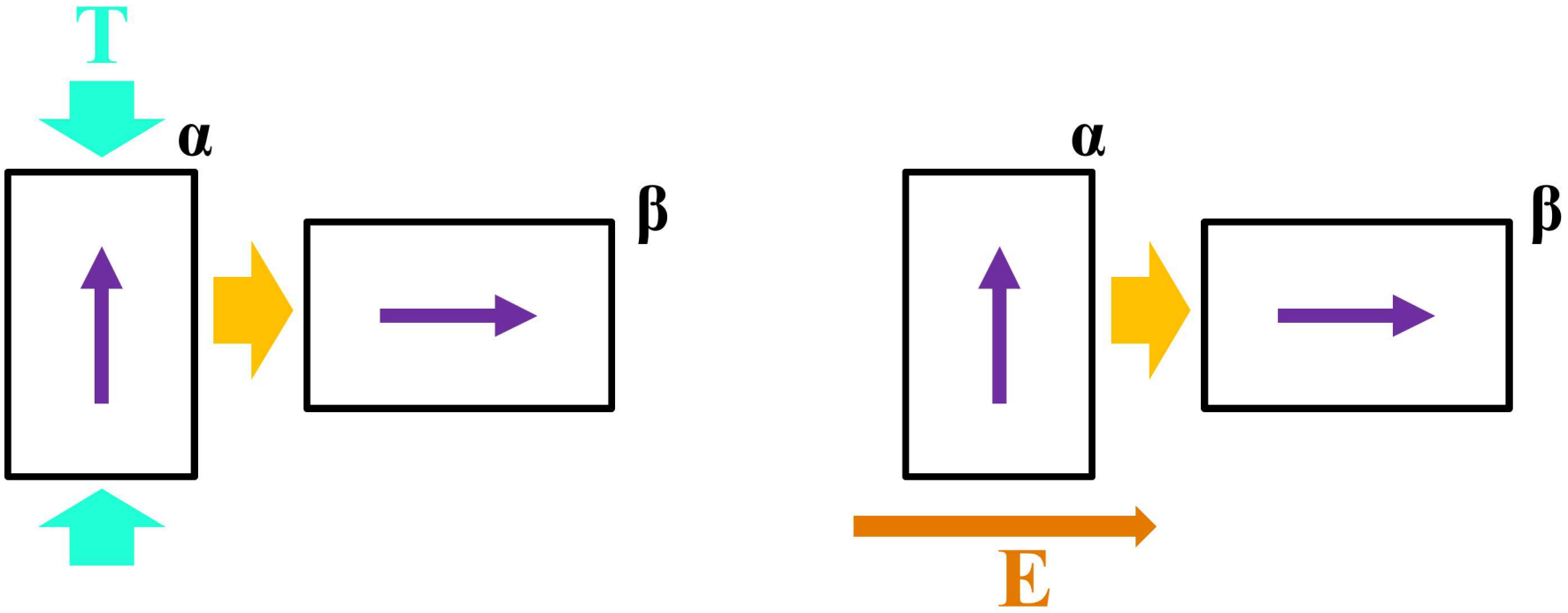
$$g^{\alpha\to\beta} > 0$$

$$g^{\alpha\to\beta} = T : \Delta S^{\alpha\to\beta} + E \cdot D^{\alpha\to\beta} - B^{\alpha\to\beta}$$

Driving force of Transformation

Work performed by the transformation

Energy barrier for transformation



# Switching Criteria - Distributed Switching Criteria

Needed to capture:
Second order (continuous) transitions
Defects/inhomogeneity in the material

Relative volume fractions of β in α-β system

$$\Phi^{\alpha\to\beta} = \frac{v^{\beta}}{v^{\alpha} + v^{\beta}}$$

Deviation of driving force of transformation from switching criteria

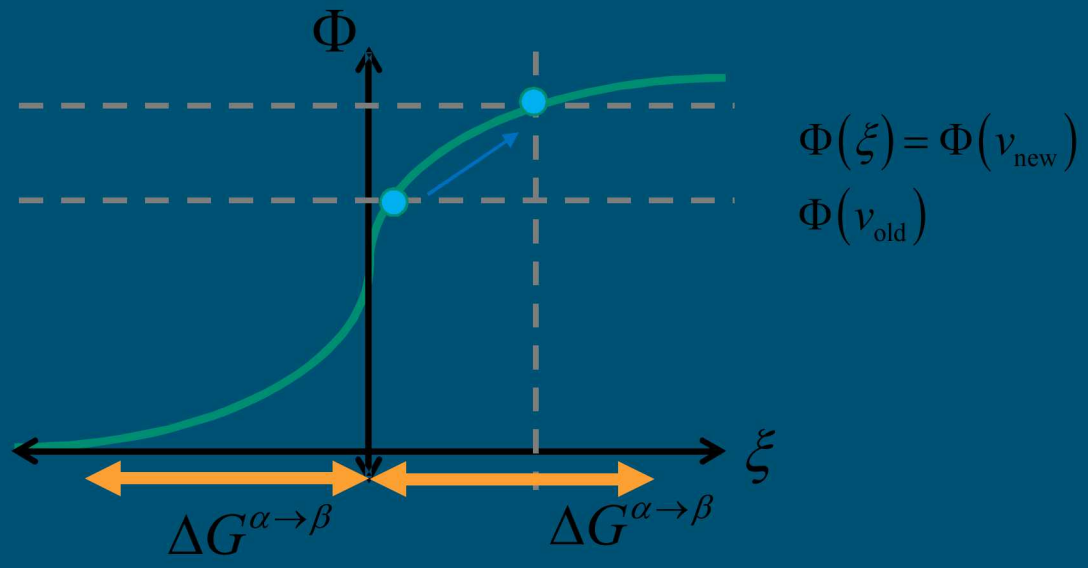
$$\xi^{\alpha\to\beta} = \frac{g^{\alpha\to\beta}}{\Delta G^{\alpha\to\beta}}$$

In the variant α to β transformation, if

$$\Phi(\xi) > \Phi(v_{\text{old}})$$

Then the volume fractions are adjusted such that

$$v_{\text{new}} = v_{\text{old}} + \Delta v \qquad \Phi(v_{\text{new}}) = \Phi(\xi)$$

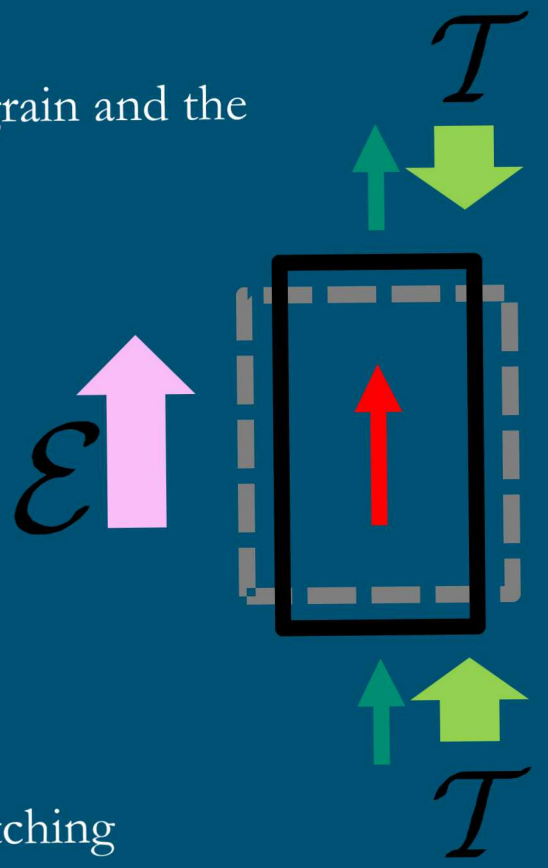


# Switching Criteria - Intergranular Interactions

Remnent polarization and strain difference between each grain and the matrix.

$$\Delta \mathcal{P} = \overline{\mathcal{P}}_m^{\text{Grain}} - \overline{\mathcal{P}}_m^{\text{Matrix}}$$

$$\Delta \mathcal{S}_{ij} = \overline{\mathcal{S}}_{ij}^{\text{Grain}} - \overline{\mathcal{S}}_{ij}^{\text{Matrix}}$$




Incompatibility stresses and electric fields

$$\mathcal{E}_m = \left(\kappa_{mn}^{\text{Matrix}}\right)^{-1} \Delta \mathcal{P}_n$$

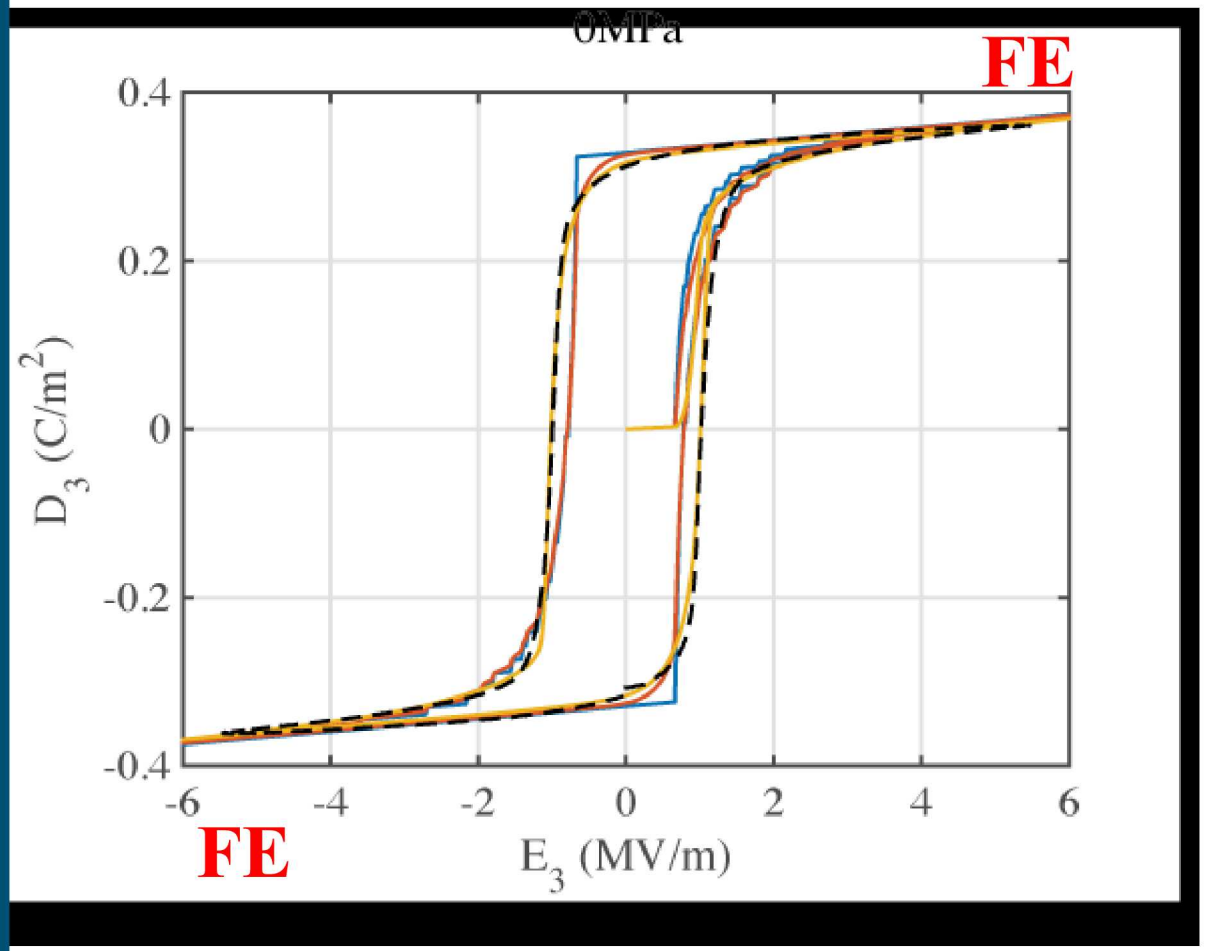
$$\mathcal{T}_{ij} = c_{ijkl}^{\text{Matrix}} \Delta \mathcal{S}_{kl}$$

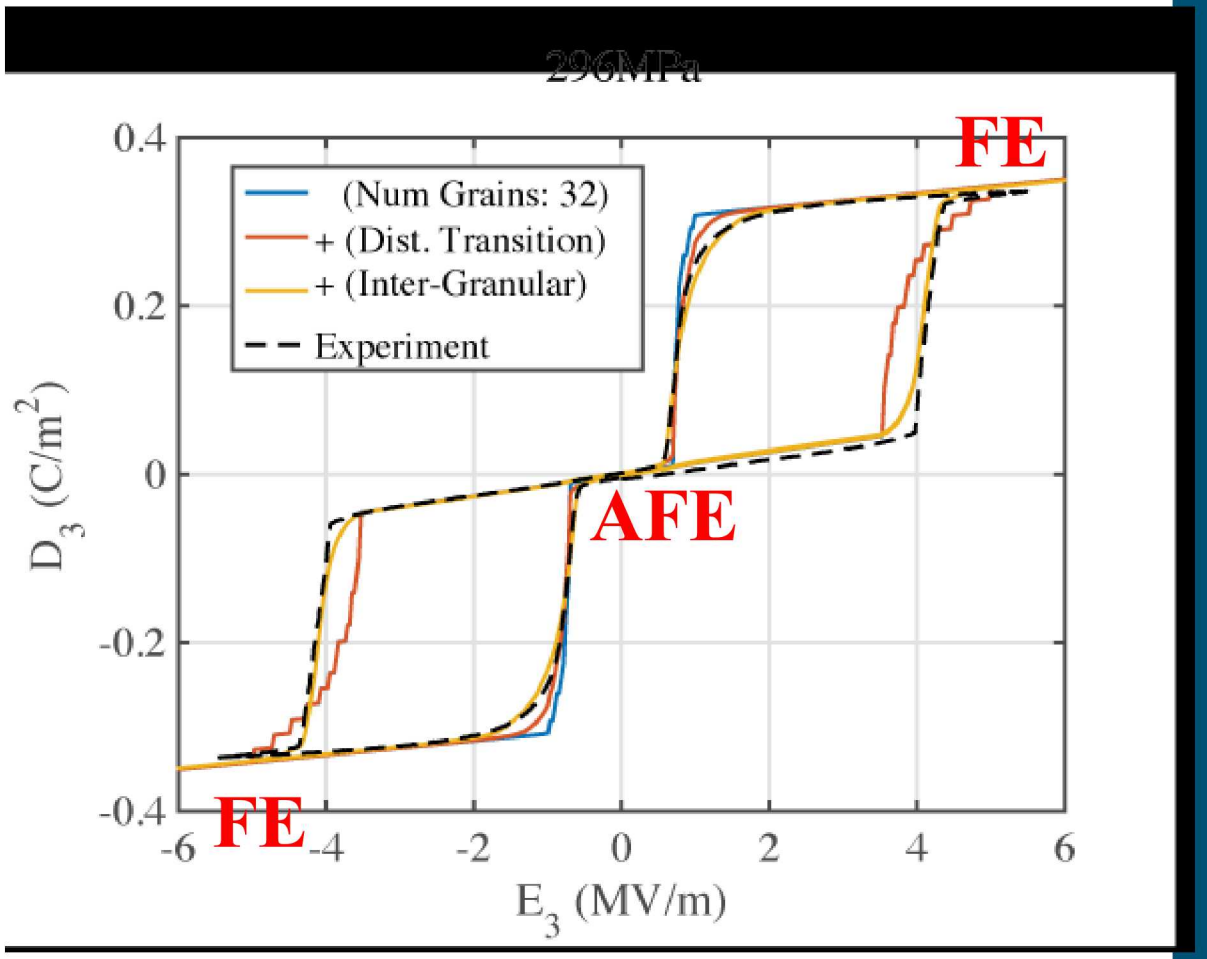
Local corrected stresses and electric fields used by the switching criterion

$$E_m^{\text{Local}} = E_m^{\text{Matrix}} + f_E \mathcal{E}_m$$

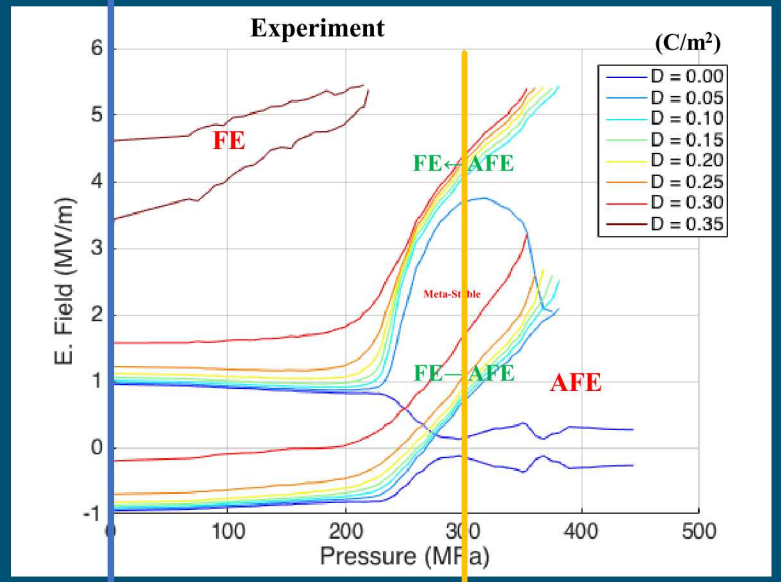
$$T_{ij}^{\text{Local}} = T_{ij}^{\text{Matrix}} + f_M \mathcal{T}_{ij}$$

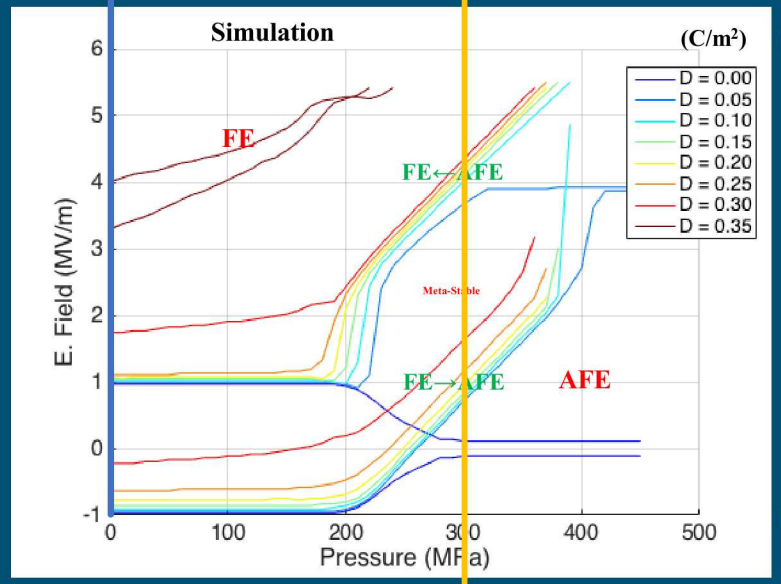
# Simulation of PZT95/5 – Hysteresis Loops

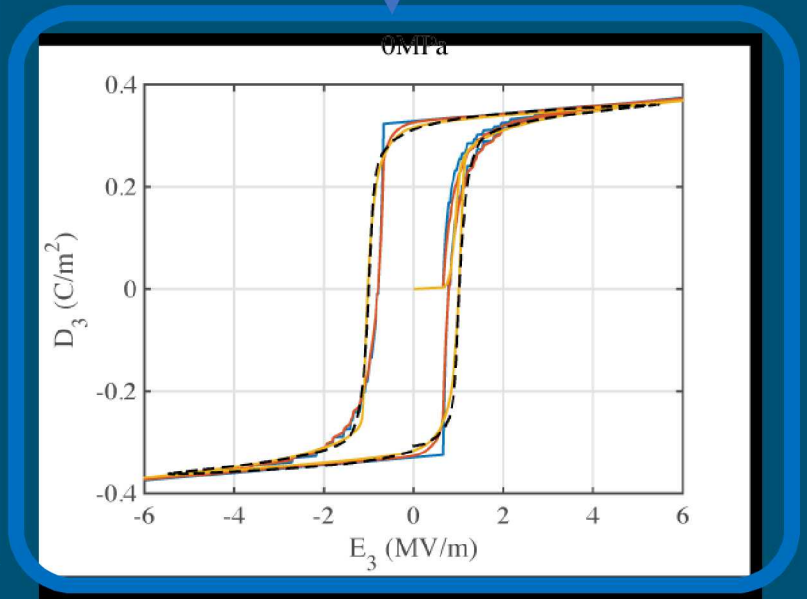


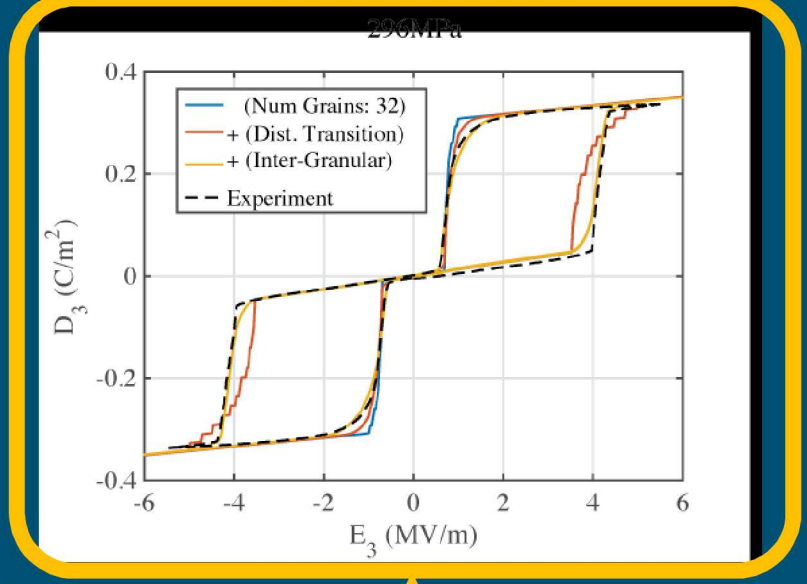



# Simulation of PZT95/5 – Phase Diagrams

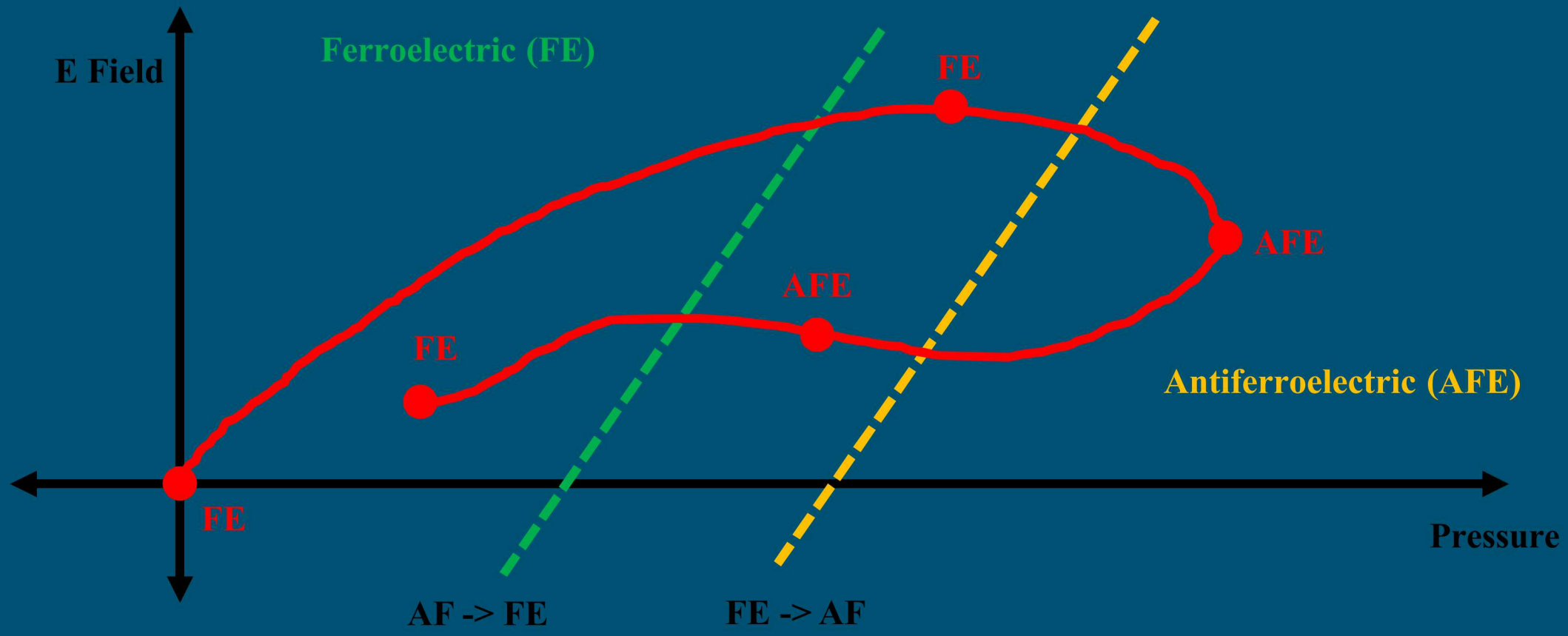


# Simulation of PZT95/5 – Advantages



# Conclusion

Micromechanical approach is used to capture the heterogeneous characteristics of ceramic PZT95/5 without resolution of the microstructure.

Energy based switching criteria are used to govern both domain-switching and phase transformation transitions.

Distributed-transitions and Inter-granular interactions allow for improved capture of hysteresis behavior.

The combination of these techniques results in a model that successfully captures the domain-switching and phase transformation phenomena in ferroelectric ceramics as demonstrated in PZT95/5.