DEEP LEARNING OF PHASE-FIELD SIMULATED DOMAIN STRUCTURE OF FERROELECTRICS FOR REFLECTARRAY ANTENNAS

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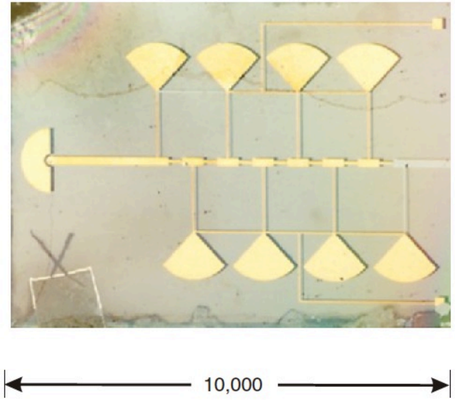
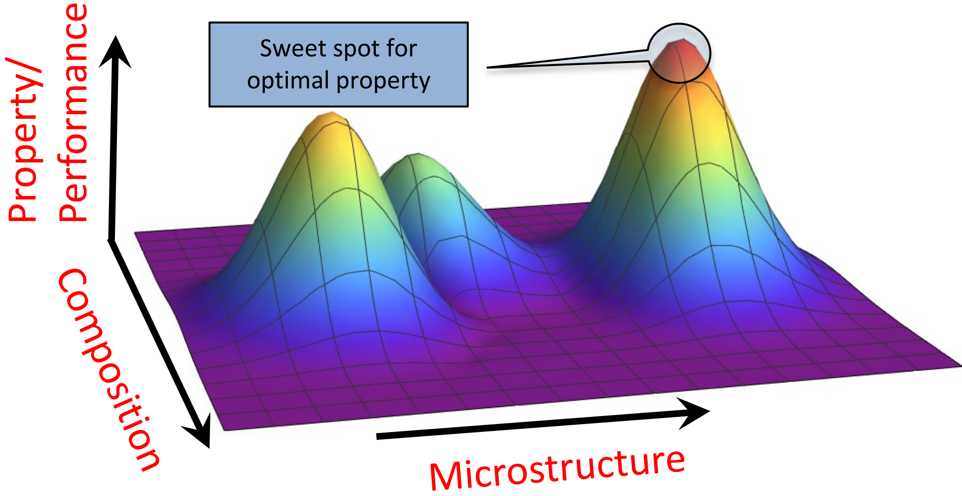
University of Idaho
College of Engineering

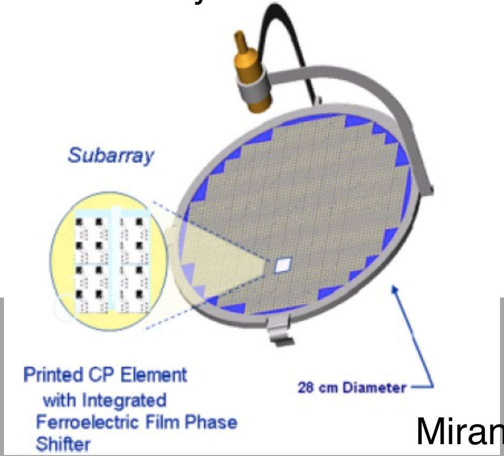
Materials Design for Ferroelectric Reflectarray Antenna

Coupled Microstrip Phase Shifter (CMPS)





Electronically Steerable Reflectarray Antenna

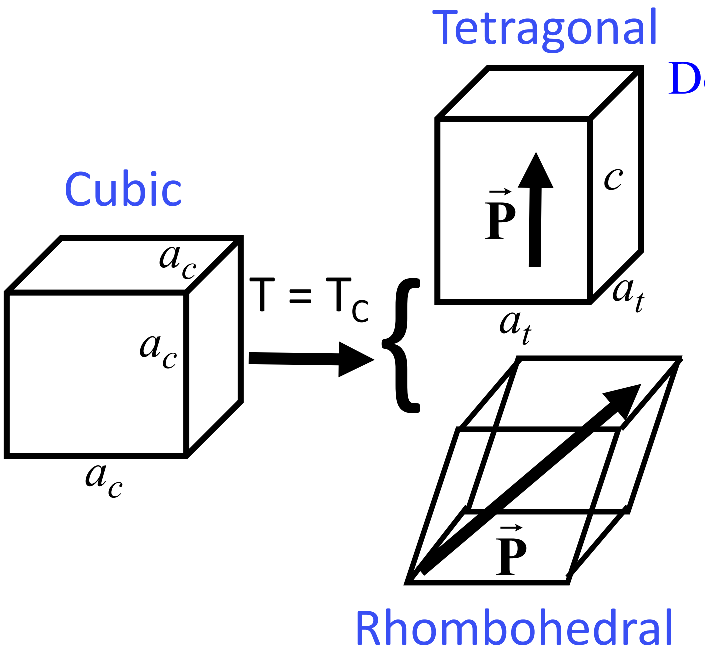


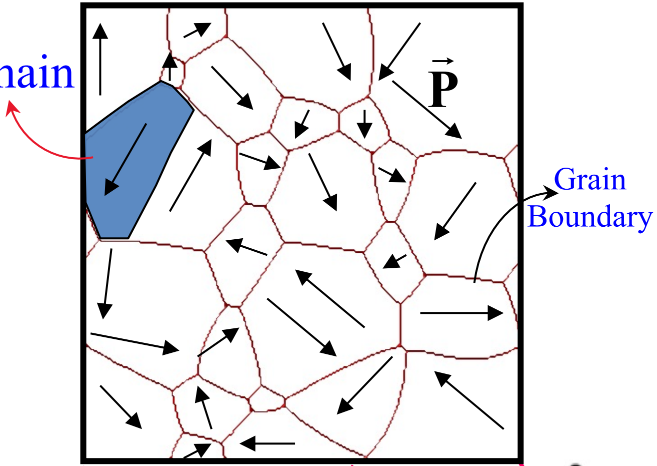
Potential Ferroelectric Compositions Investigated:

- $SrTiO_3$
- $Ba_xSr_{1-x}TiO_3$
- $(Pb,La)(Zr,Ti)O_3$
- $PbSr\ TiO_3$
-

Miranda et al. J. Am. Ceram. Soc., 91 [6] 1864–1868 (2008)

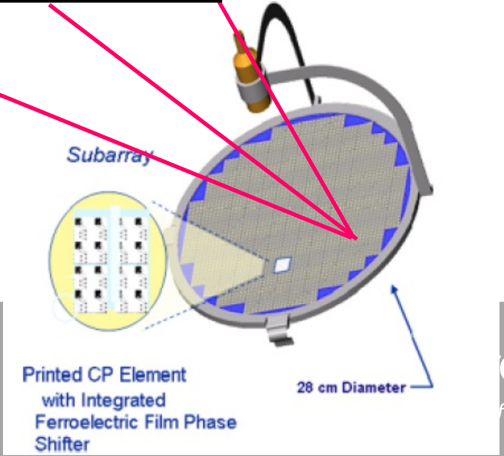
Microstructure/Domain Structure in Ferroelectrics





Inhomogeneities Affecting Polarization Switching in Ferroelectrics

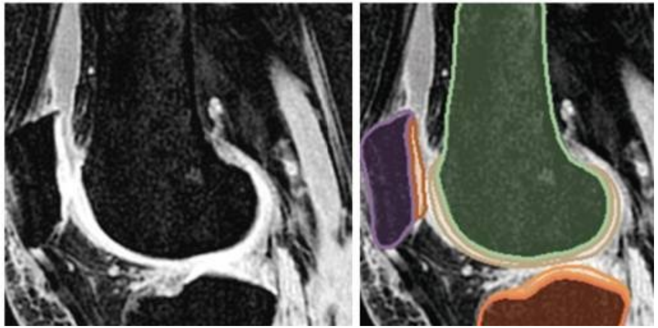
- Grain boundaries
- Twin domains
- Free surfaces
- Domain walls
- Dislocations



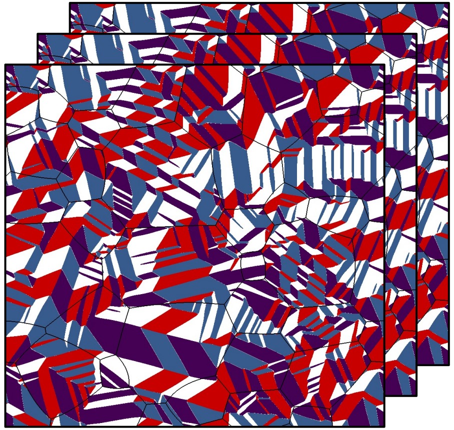
Macroscale device level

DEEP LEARNING

Self-driving Cars



Smarter Healthcare



Microstructure Optimization

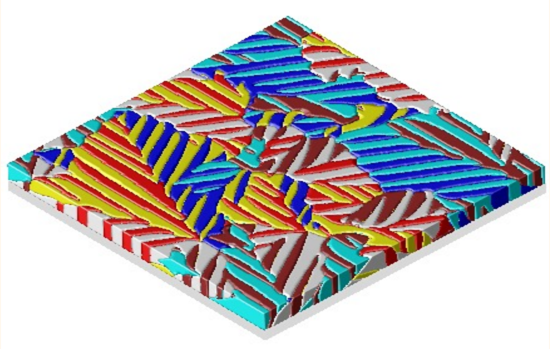
Deep learning can quantitatively analyze patterns in image

Would need tens to hundreds of 1,000s of carefully labeled microstructures

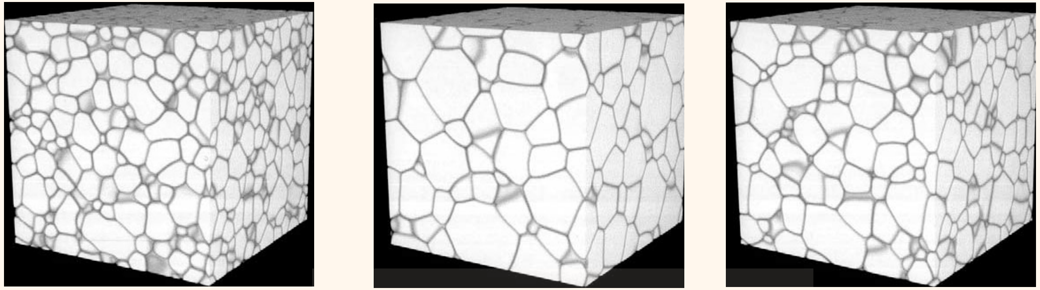
Unlike most experiments, phase-field simulations can generate thousands of microstructures within weeks to months time

Phase-field Simulations of Microstructures

Ferroelectric Domain Structure



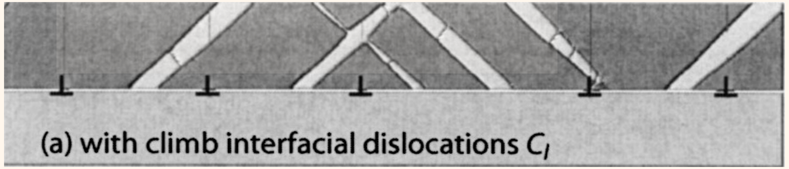
Choudhury and Chen, 2009
Journal cover *J. Am. Ceram. Soc.*



Grain Growth

Krill and Chen, *Acta. Mat.* 2002

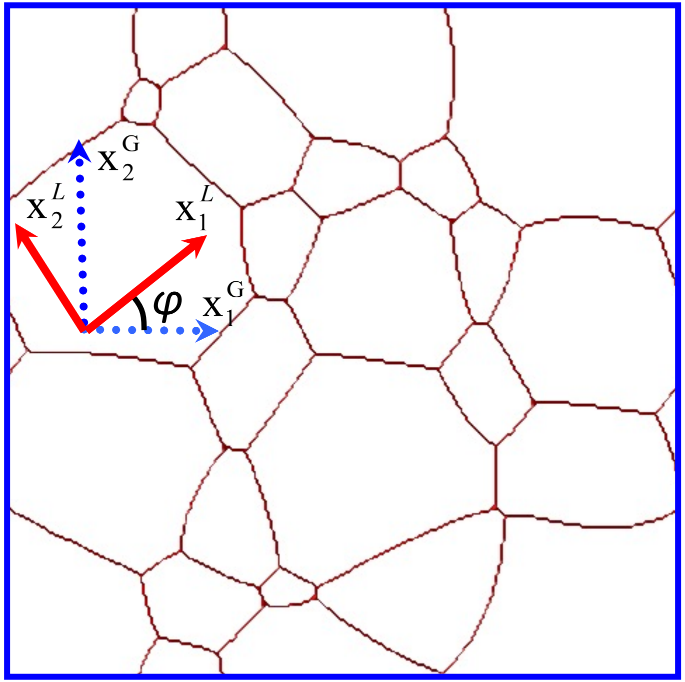
Dislocations



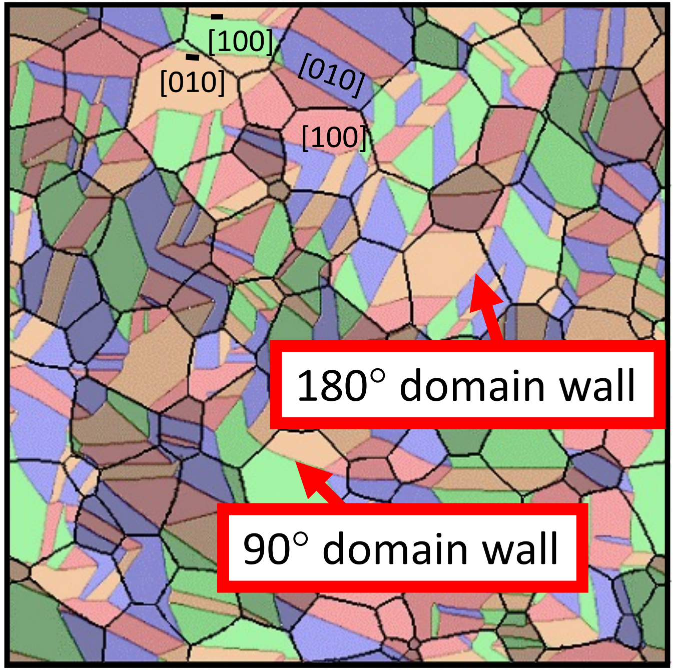
Domain St. in PTO thin films with interfacial dislocations.
Li et. al. *J. Appl. Phys*. 2003

Possible to simulate microstructure when multiple features coexist

Domain Structure in Polycrystalline $PbTiO_3$



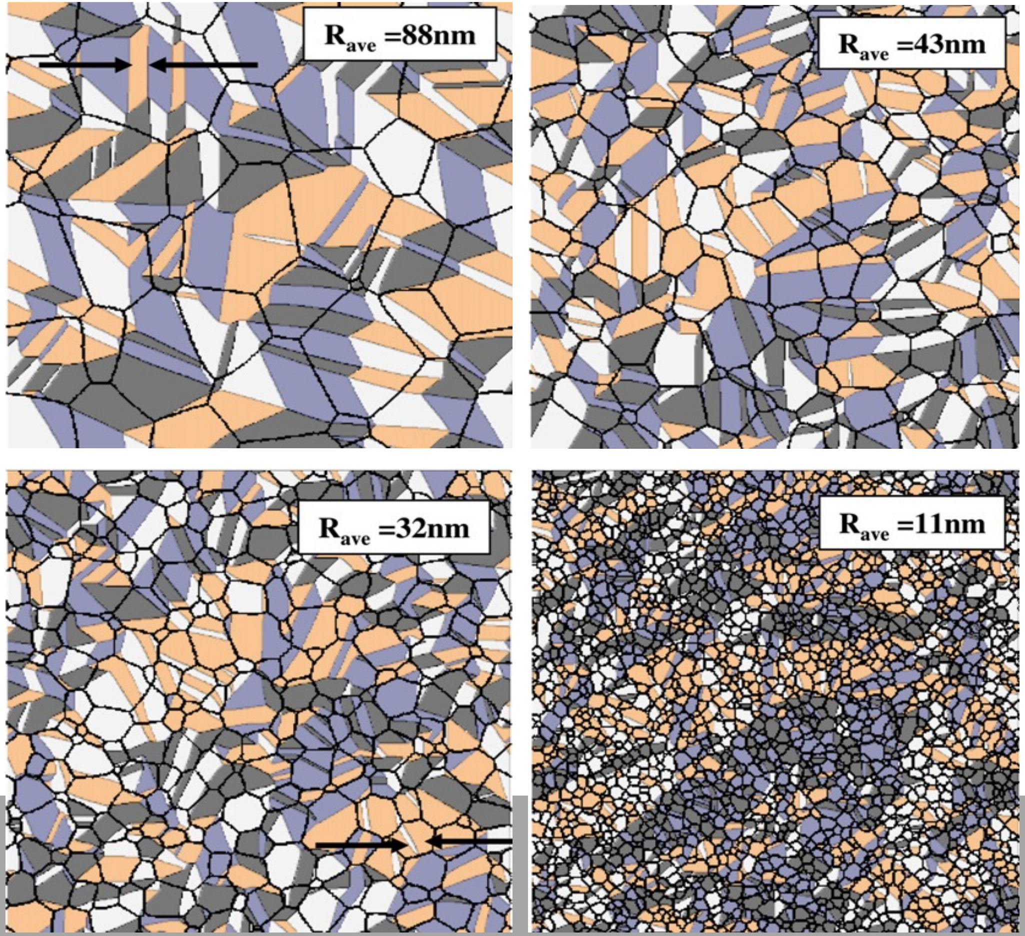
Krill and Chen *Acta Mater.* 50, 3057,2002



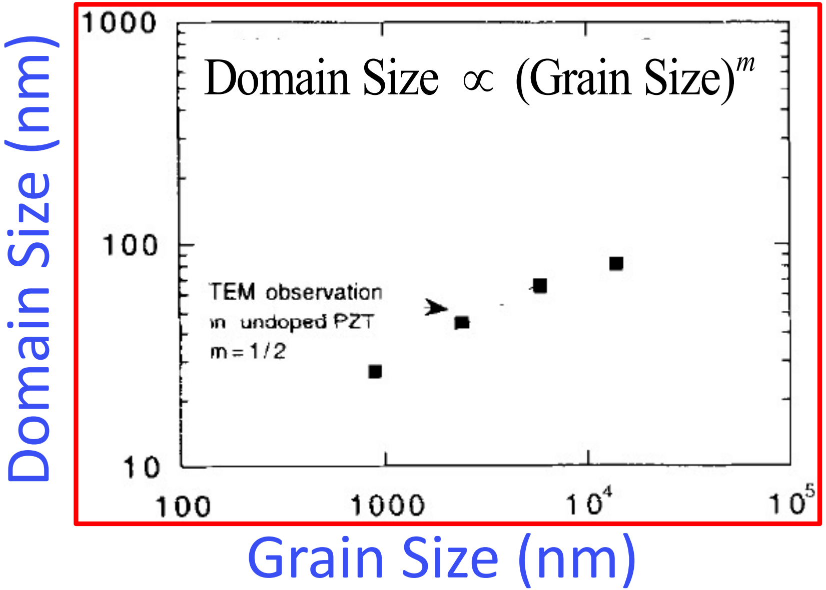
S. Choudhury, et. al *Acta Mater.* 2005

Simulated domain structure of $PbTiO_3$ ceramics with no applied electric field

Effect of Grain Size on Domain Structure in $PbTiO_3$



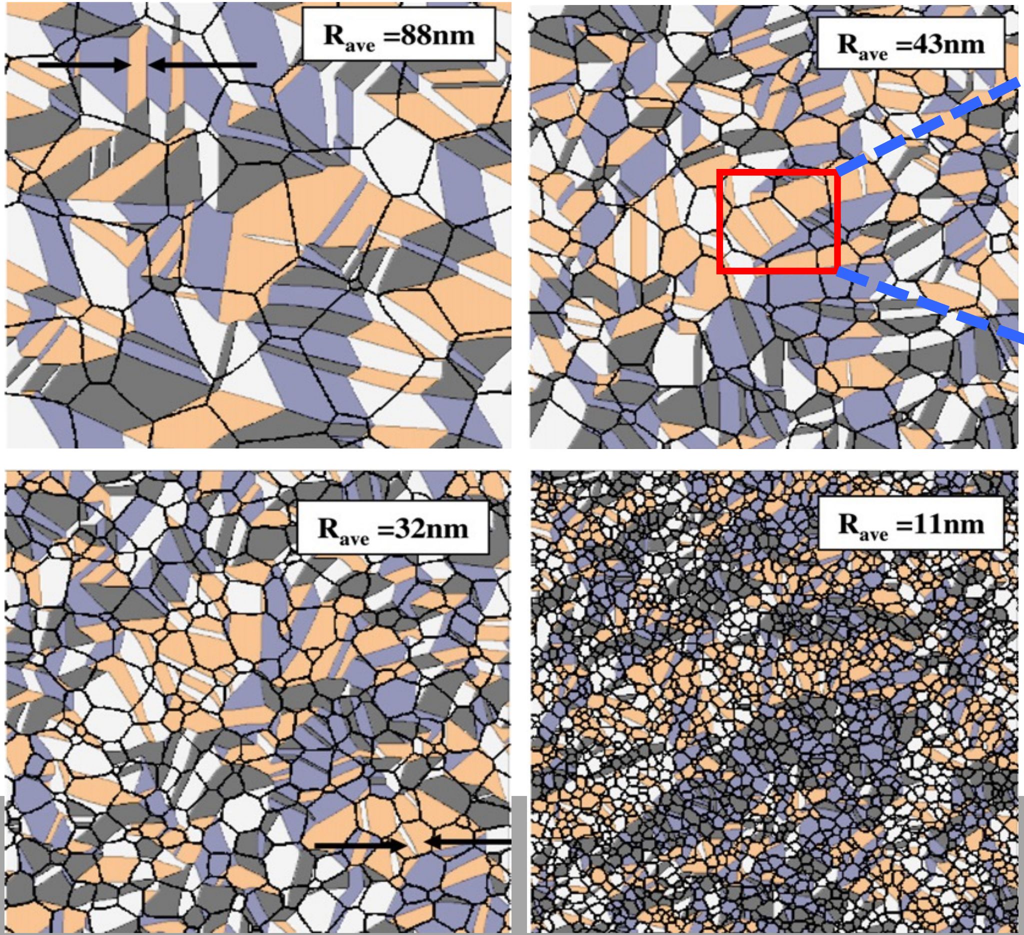
TEM Measured Domain Size



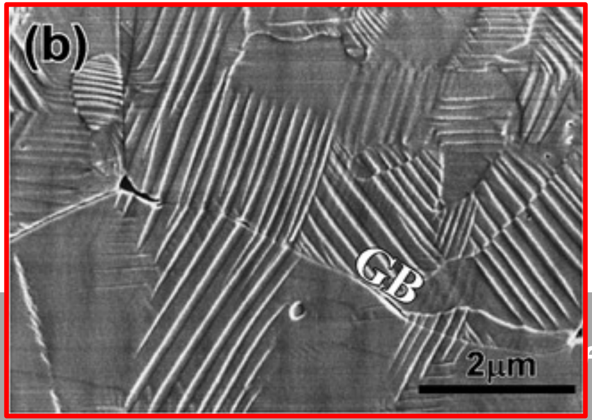
Cao and Randall J *Phys Chem Solids*, 1996

S. Choudhury, et. al *Acta Mater.* 2007

Effect of Grain Size on Domain Structure in $PbTiO_3$



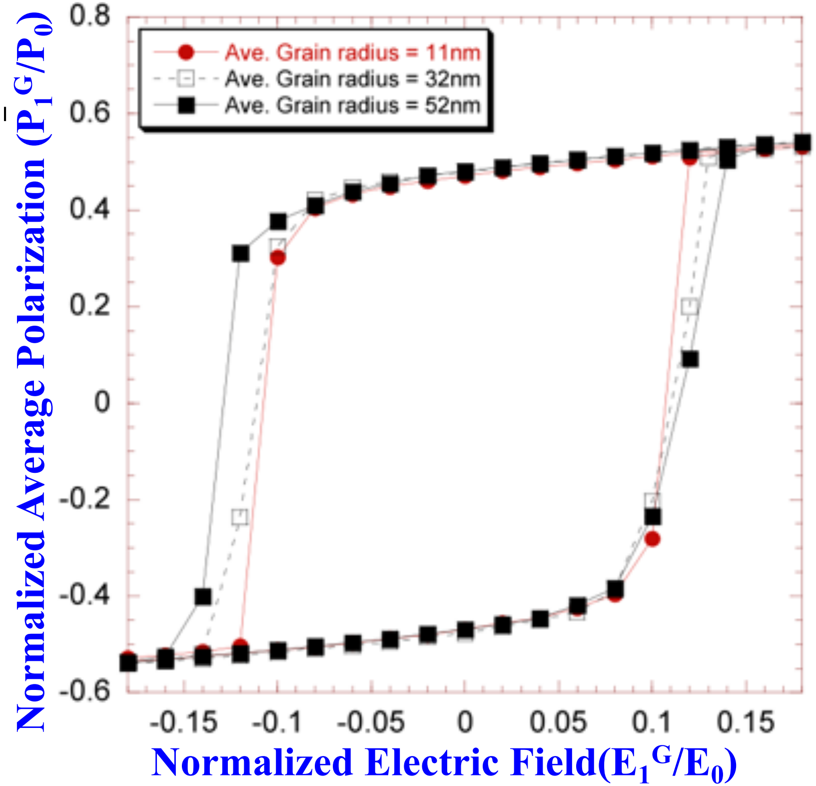
Domain St. of PZT Ceramics



Tsurekawa *et al.*
Scripta Mater., 2007

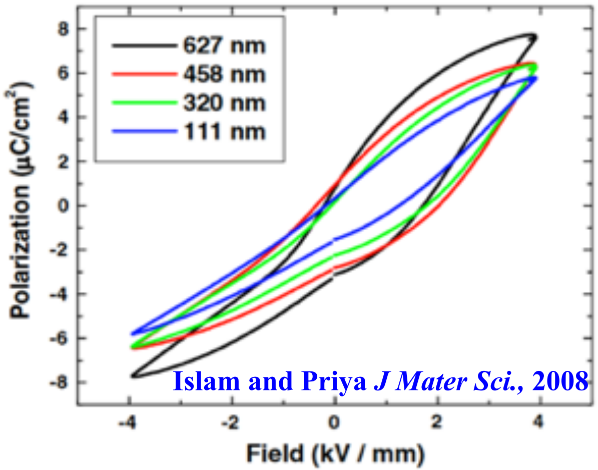
Effect of Grain Size on the Coercive Field in $PbTiO_3$

Phase-field Simulation



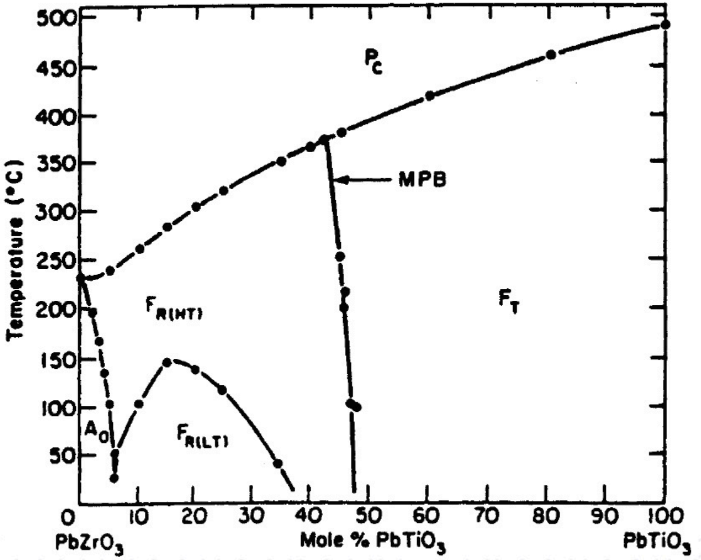
Experimentally Measured

Hysteresis loops of PZT ceramics

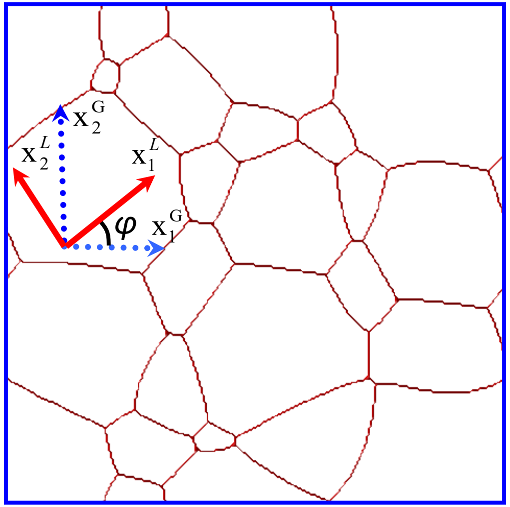


	Grain Size	
	627(nm)	111(nm)
Coercive Field	1.7 (kV/mm)	1.2 (kV/mm)

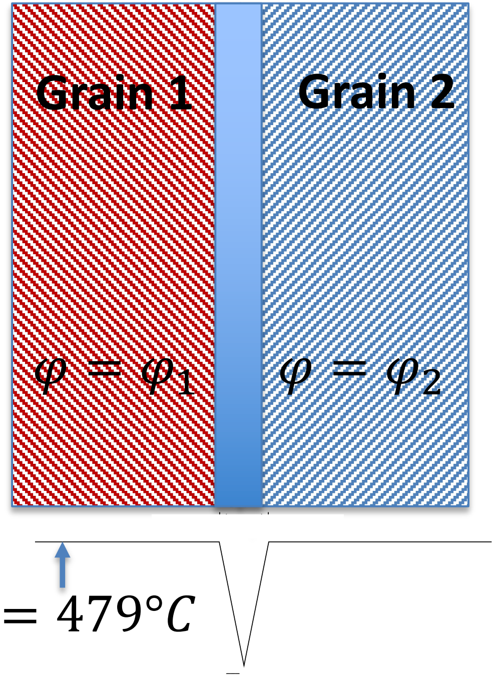
PHASE FIELD SIMULATION OF FERROELECTRIC CERAMICS



Phase Diagram of PZT
Jaffe et al. 1971



Grain structure and grain orientation



$T_{bulk} = 479°C$

$T_{gb} = 25 - 479°C$

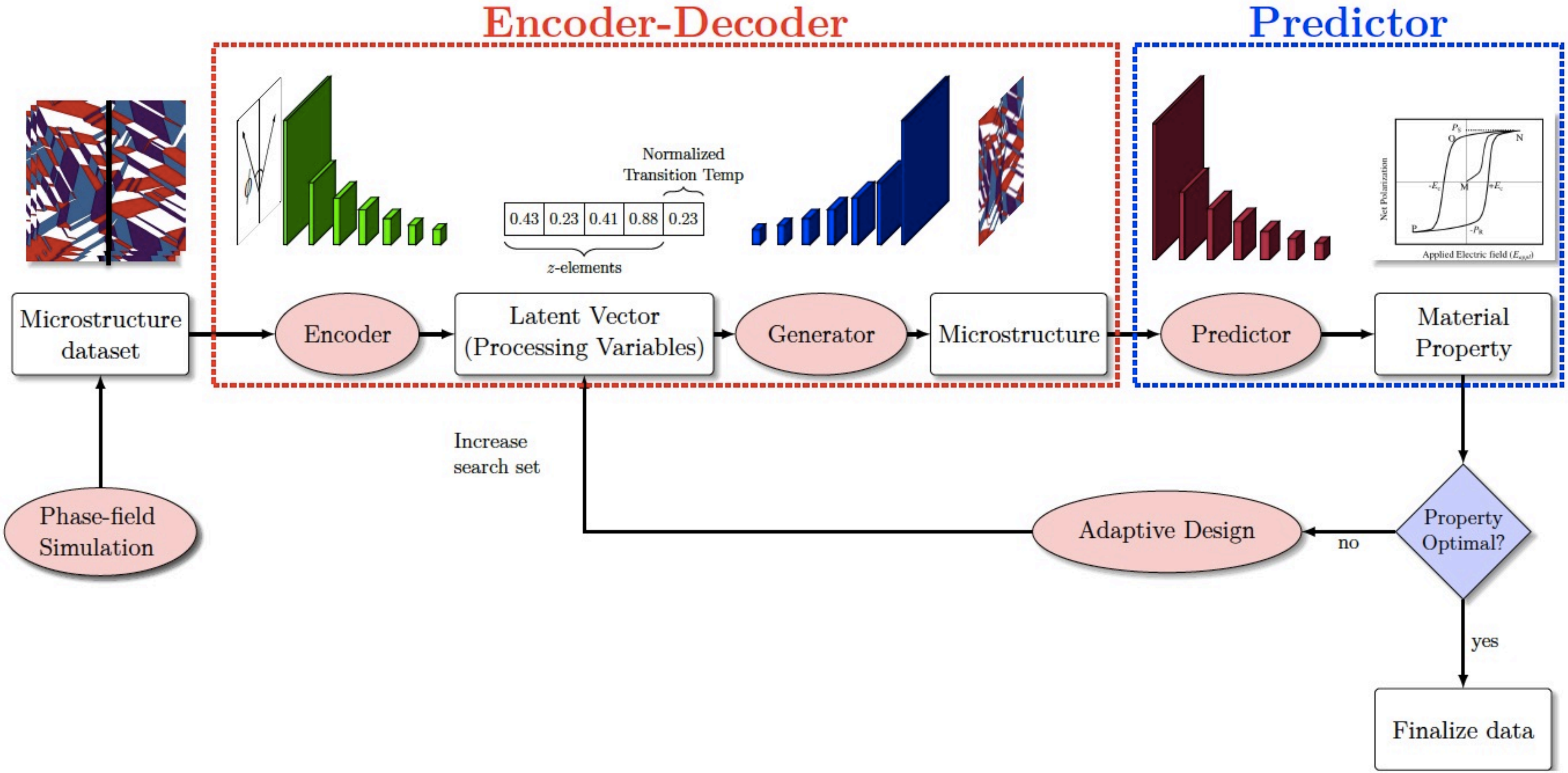
Transition Temperature at G.B

Two processing parameters considered:

(a) Transition temperature are the grain boundary

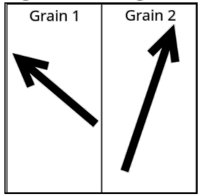
(b) Grain boundary orientation

FLOWCHART OF THE DEEP LEARNING FRAMEWORK

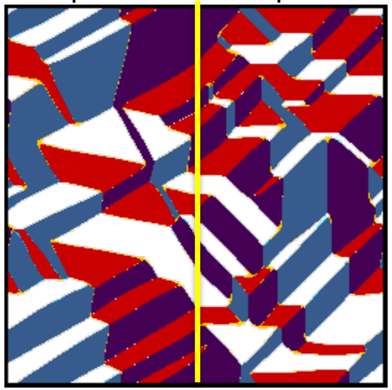


MODEL

grain angles



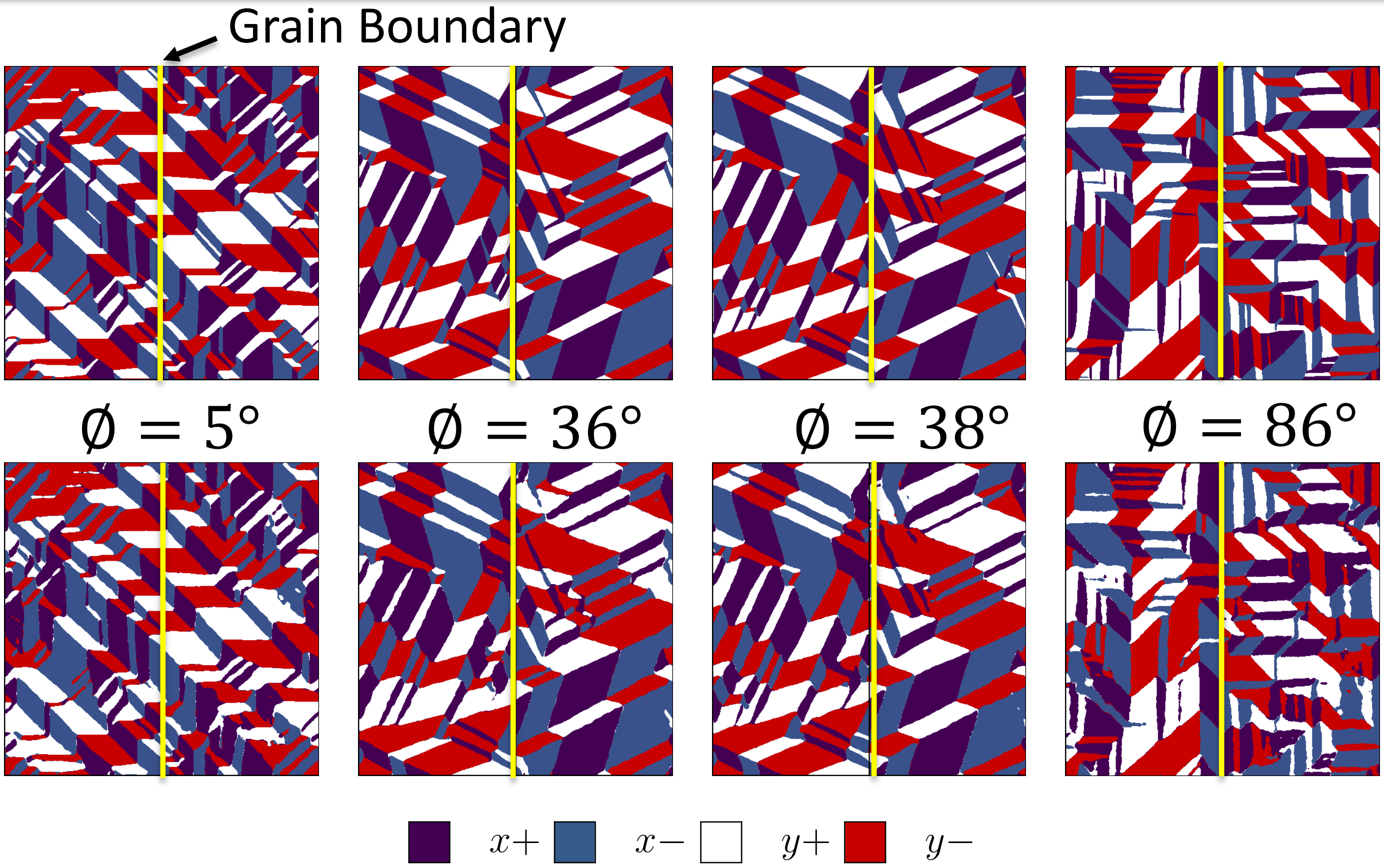
phase-field output



Comparison of Microstructures (T_{GB} =10°C)

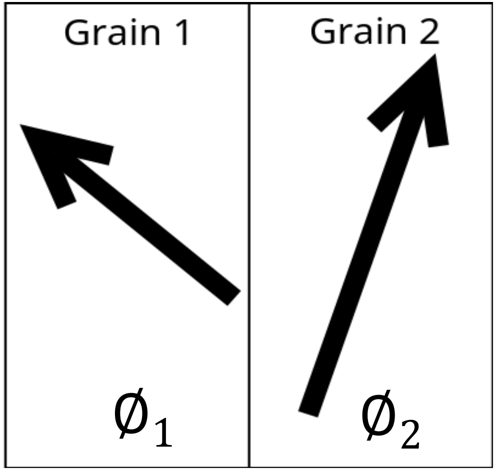
Phase-field Simulated Microstructures

Machine Predicted Microstructures



Quantification of Microstructure Prediction

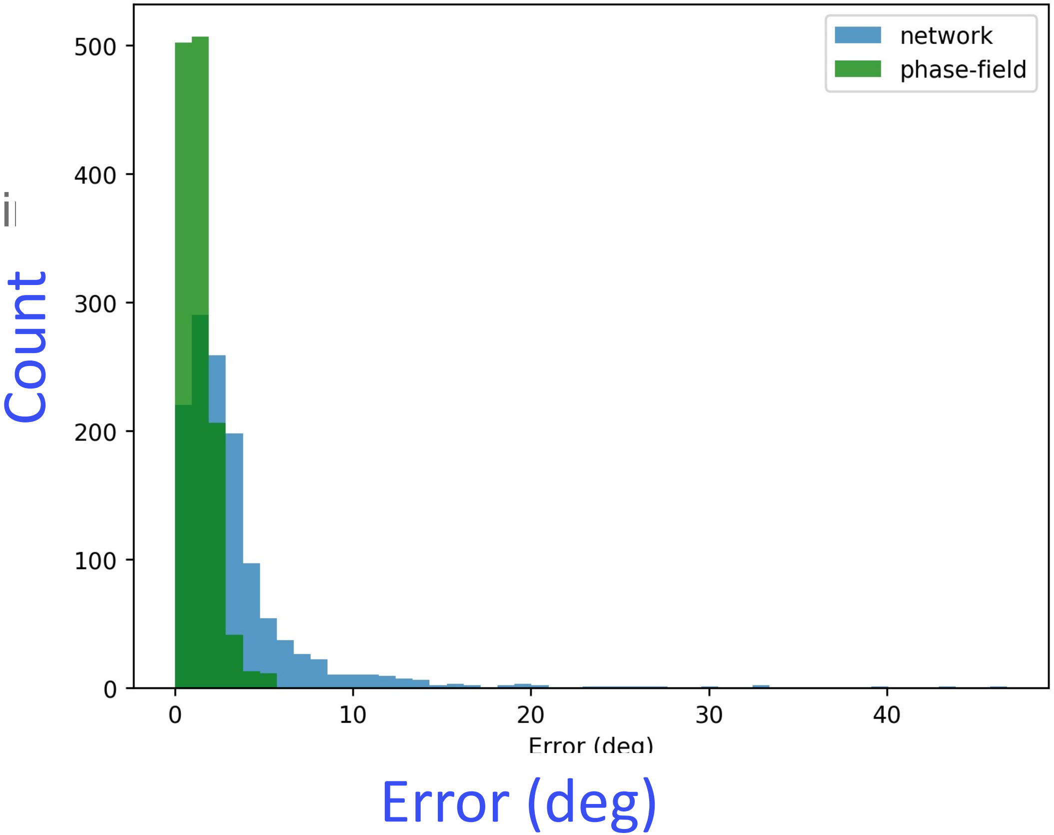
Prediction of Domain Wall Orientation



- The orientation of each grain is defined by, ∅
- For each ∅ domain wall orientation is known
- Our script automatically detects domain wall

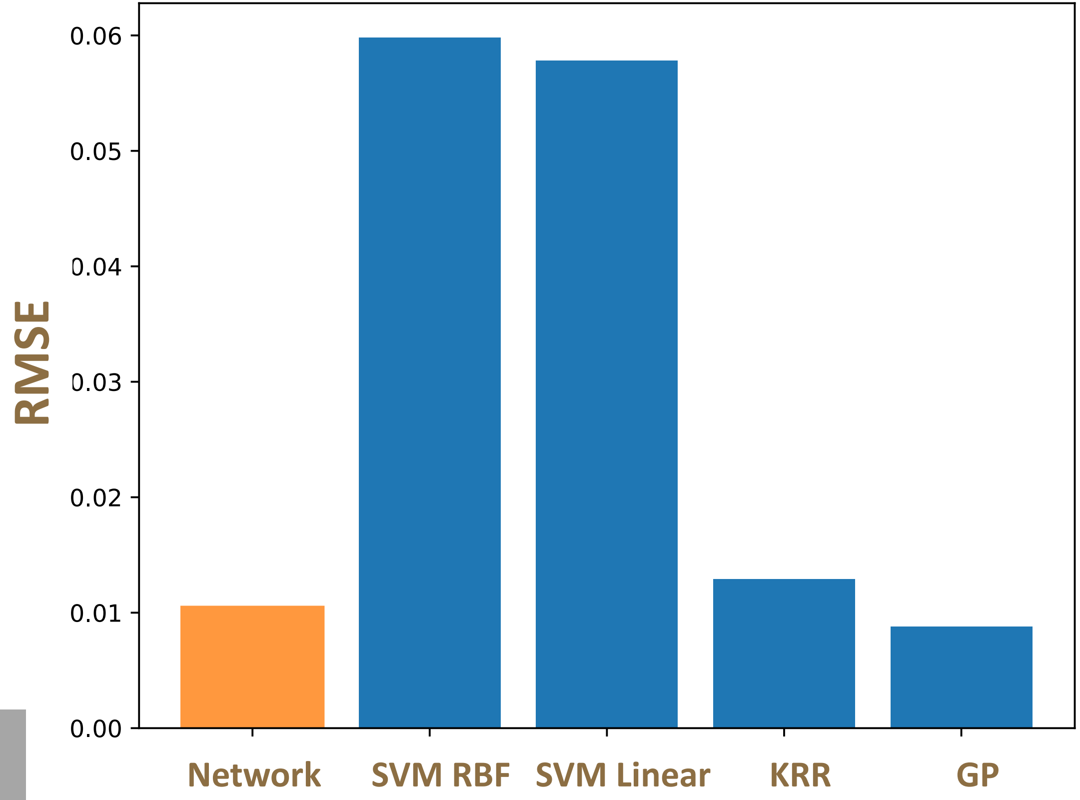
Error in Network Predicted and Phase-field simulated Domain Wall Orientation

- Average angles of same domain wall type within grain
- Average degree deviation from expected domain wall orientation i phase-field simulation:**1.45°**
- Average degree deviation (from expected domain wall orientatior for neural net: **2.87°**
- Average prediction within 1.5° error
- Nearly all cases are within very good estimate of phase-field simulations



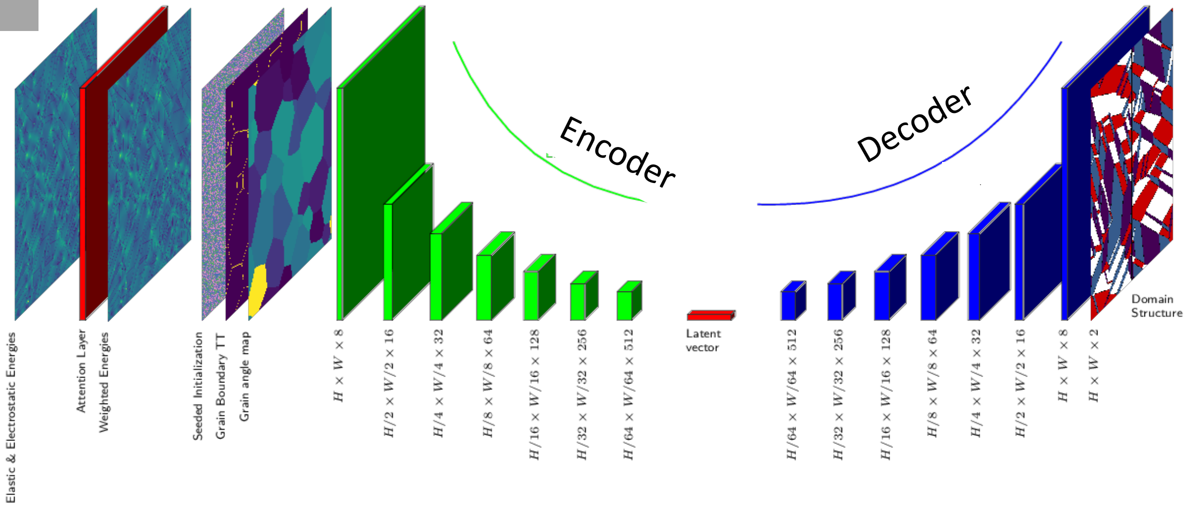
Root Mean Square Error (RMSE) in Predicted Coercive field

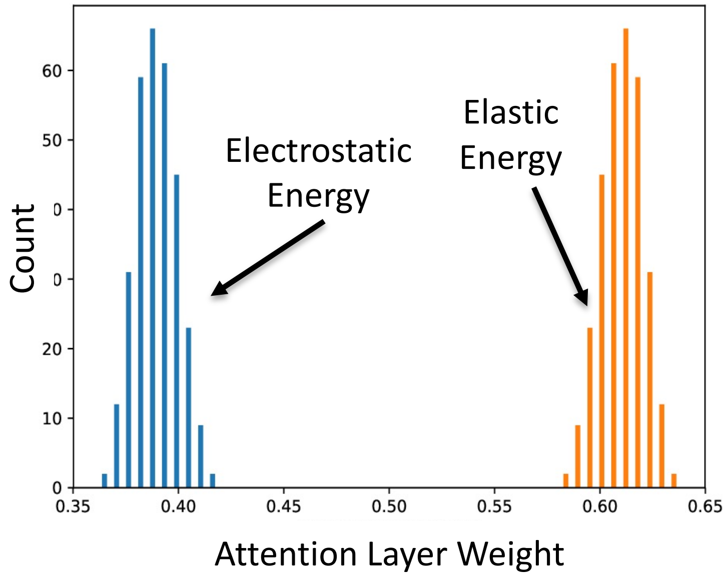
Processing →Microstructure →Property (Coercive Field)



The network prediction of coercive field performs better than those predicted by traditional machine learning on the processing conditions alone.

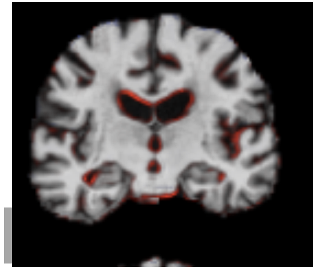
Prediction of Energy Contributions using Attention Layer



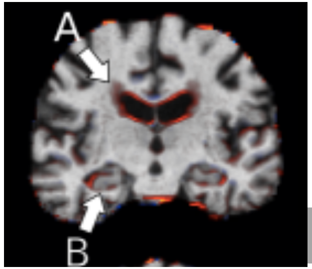


Added an "attention" layer that weights importance of inputs

Network Predicted Brain Scan



Observed Brain Scan



Comparison of regions affected by Alzheimer's disease using attention layer

Baumgartner, C. F et al *IEEE Conference on Computer Vision and Pattern Recognition* (2018).

Network can provide fundamental insights into microstructure evolution

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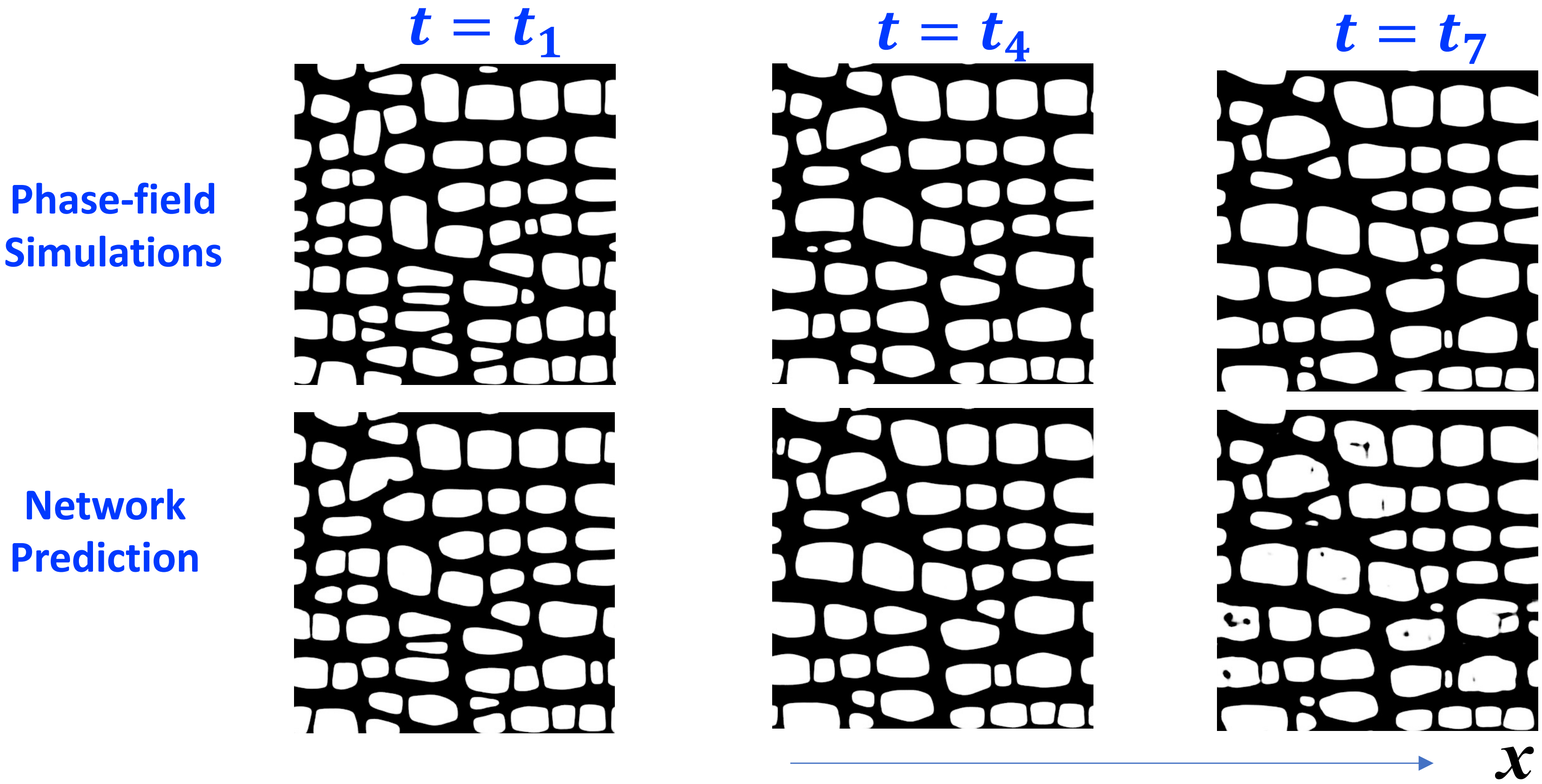
Comparison of the Microstructure Evolution as 0.2% Strain is Applied in the x Direction to an Initial ($t = t_0$) Microstructure using a Encoder-LSTM-Generator network

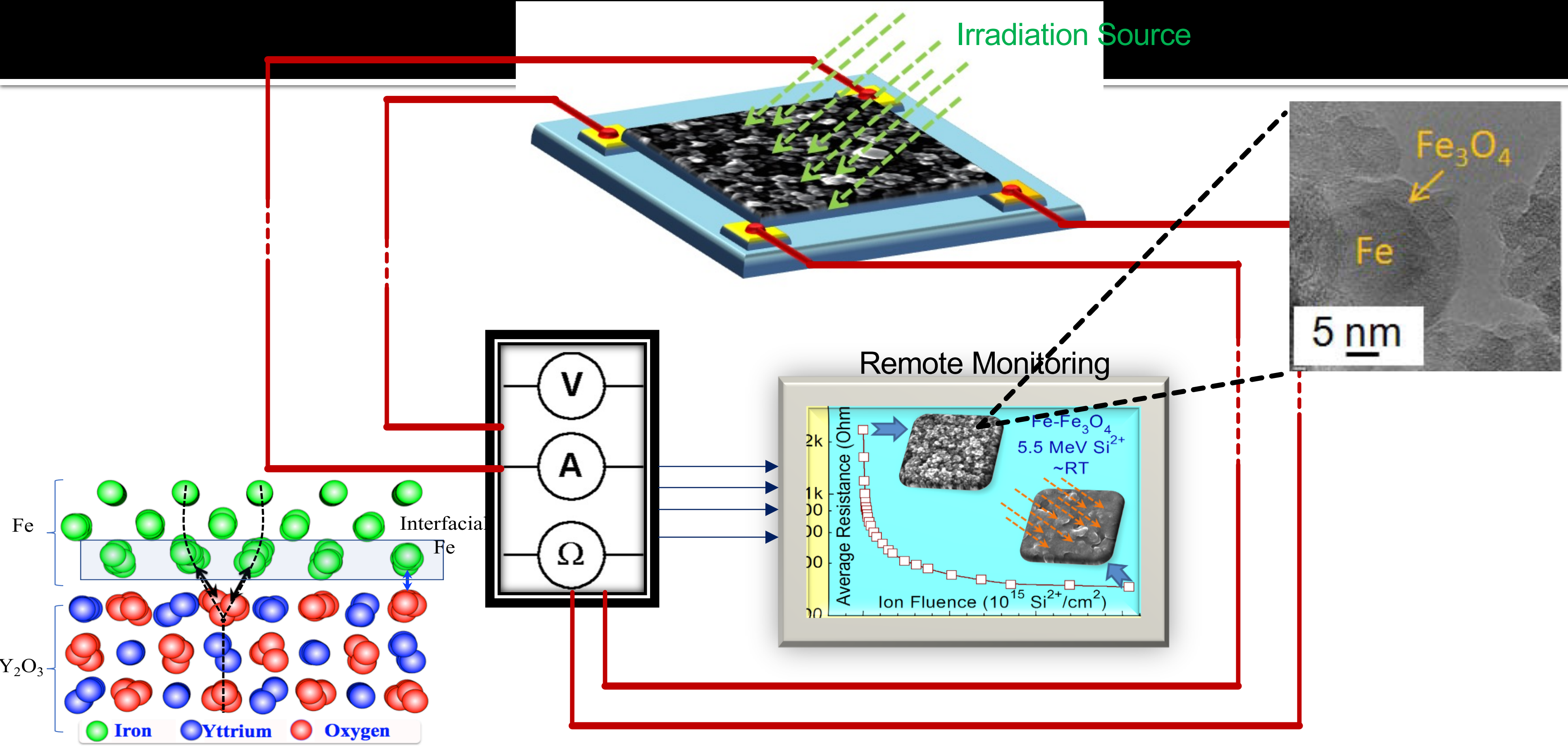


Radiation in Space

Courtesy: Prof. You Qiang (University of Idaho)

- Galactic Cosmic Rays (GCR)
  - Protons
  - Particles (Helium)
  - Positrons
  - Neutron
- Solar Energetic Particles (SEP)
  - Solar Flares
  - Coronal Mass Ejection (CME) – solar winds

Our In-situ Radiation Monitoring Device



S. Choudhury Scientific Reports 2014

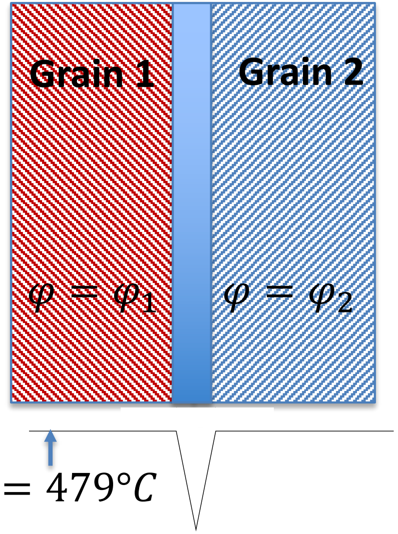
Support: NASA-Idaho EPSCoR Research Initiation Grant

CONCLUDING REMARKS

- Predictive deep learning model is designed for ferroelectric domain structures
- Predicted domains walls match will phase-field model results within 1.5°
- Able to quantify success in learning microstructural properties from phase-field simulations
- Can predict time dependent evolution of microstructures

Acknowledgement: This work was supported financially by a National Science Foundation Graduate Research Fellowship Program under Grant No. 1842399. Part of the calculations were performed at the High Performance Computing Facility at the Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy under Contract No. DE-AC07-05ID14517.

Comparison of Normalized Polarization Magnitude at Grain Boundary



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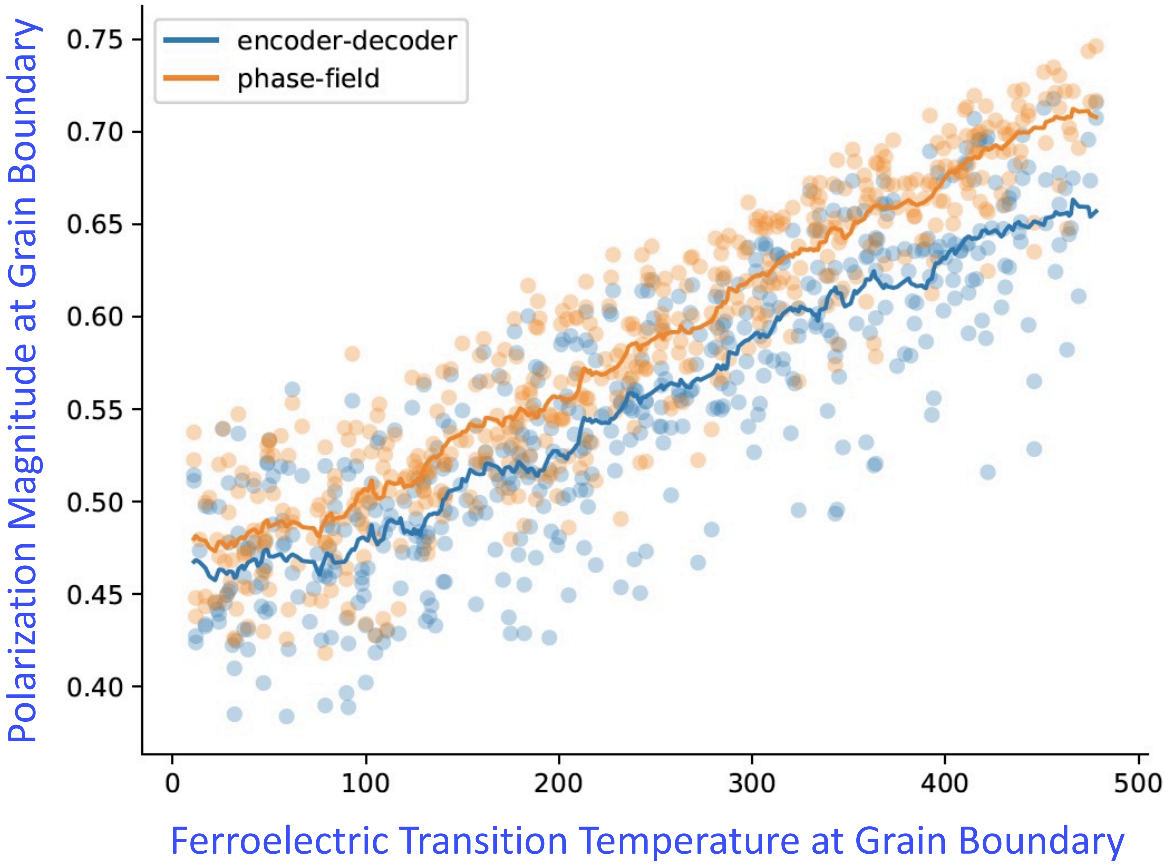
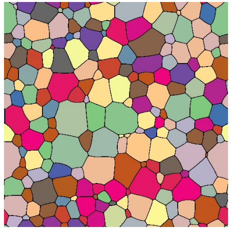
Transition Temperature at G.B

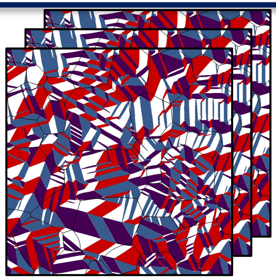


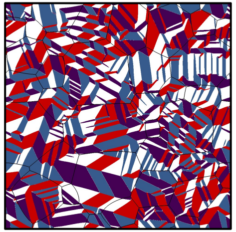
METHOD

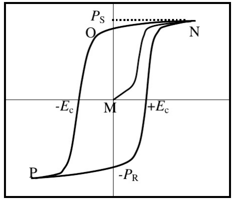
1) Generate samples with phase-field
   - 1,000s of unique samples produced within 2 weeks
2) Use processing conditions to predict ferroelectric domain microstructure of $PbTiO_3$
3) Use domains to predict coercive field property


†

Grain Angles, Processing Conditions → **Machine Learning** → Ferroelectric Domains





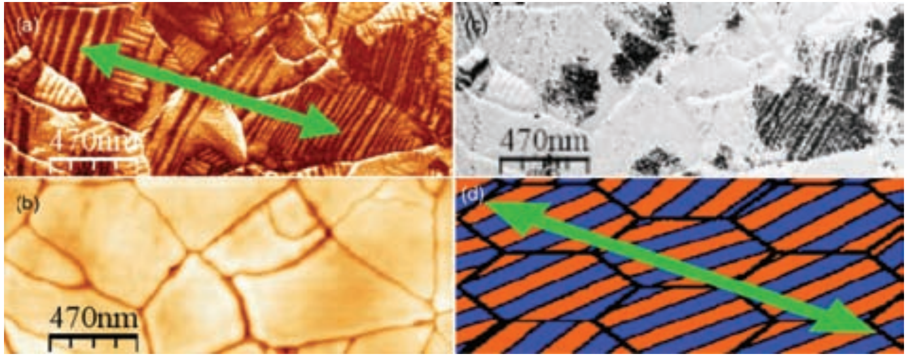


Ferroelectric Domains → **Machine Learning** → Coercive Field

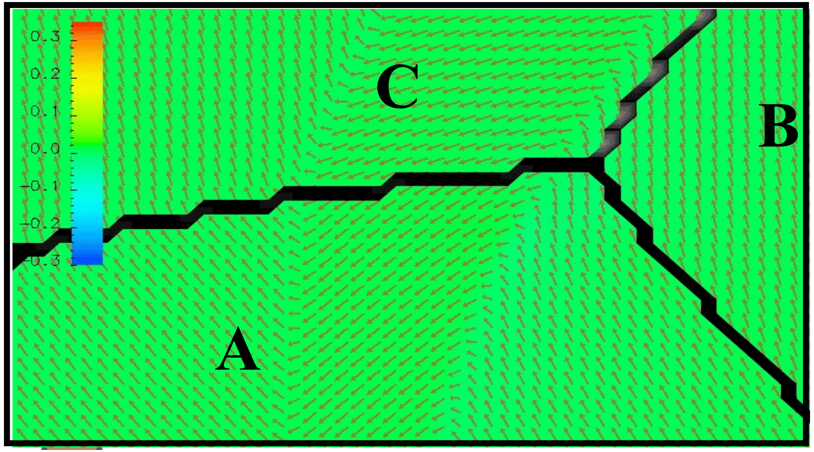
†Grain growth code from C. Krill and L.Q. Chen *Acta. Mat.* **50** 2002

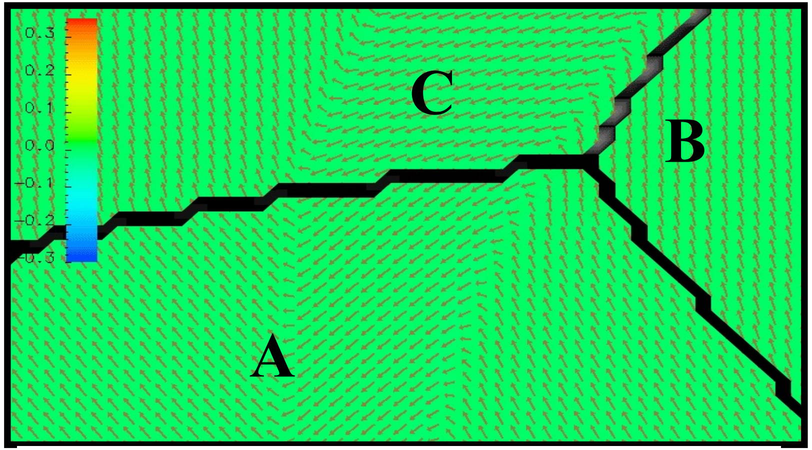
Energetic Contributions toward Domain Formation

Formation of ferroelectric domain structure is governed by a combination of short-range and long-range interaction



Ivry et. al. *Adv. Func. Mater.* (2014)



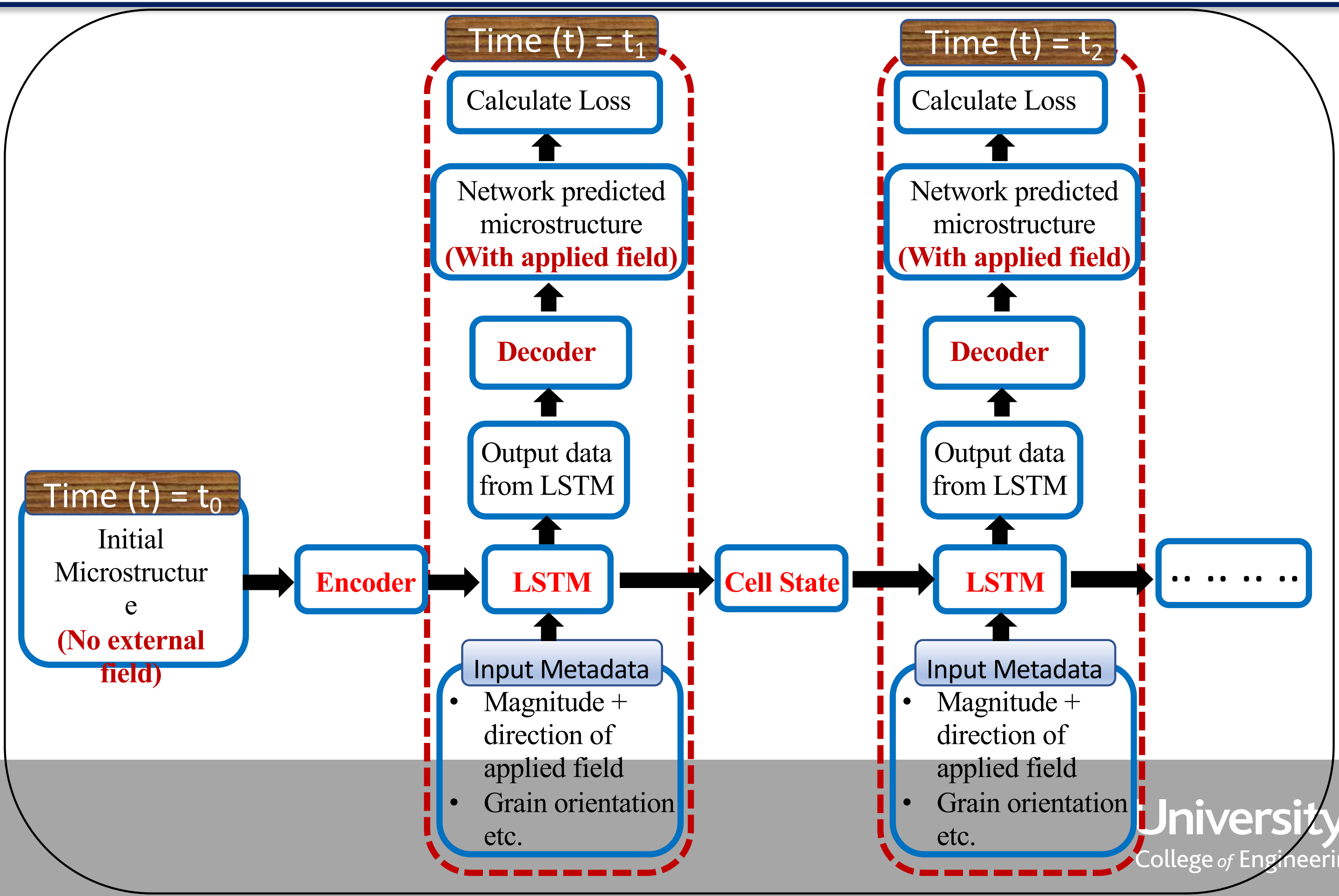


Electric energy distribution **Elastic energy distribution**

daho

What is the role of individual energies toward of microstructure evolution?

Flowchart of the Encoder-LSTM-Generator network



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