The 2019 Interdisciplinary Materials and Physics

Research Experience for Undergraduates

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Phase-Field Simulations: Anisotropic Misfit Strain Phase Diagram of $K_{0.5}Na_{0.5}NbO_3$ Thin Films

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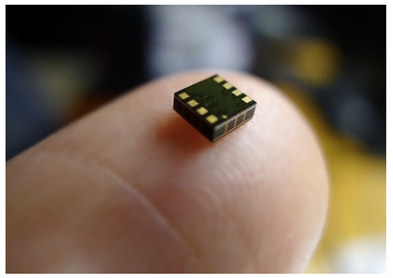
Why is this important?

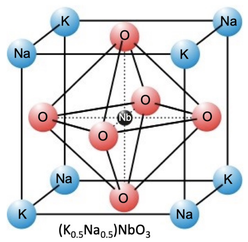
Piezoelectric materials are useful for their ability to convert mechanical deformations into electrical charge. One of the most popular piezoelectric materials is lead zirconate titanate (PZT), however, more demand has pushed for the study of environmentally-friendly lead-free materials such as $K_{0.5}Na_{0.5}NbO_3$ (KNN). This particular study concentrates on the domain structures of KNN thin films under various anisotropic strains, and the present work can prove useful in developing nanodevices with enhanced piezoelectric effects.



Source: Chirp Microsystems

Fig. 1
Micro-electromechanical system (MEMS)-based ultrasonic sensor sitting atop a person's fingertip.

Background Theory and Methods



$$\frac{\partial P_i(\boldsymbol{x},t)}{\partial t} = -L\frac{\delta F}{\delta P_i(\boldsymbol{x},t)}$$

Fig. 2
Perovskite structure of KNN (left) and Ginzburg-Landau (TGDL) equation (right).

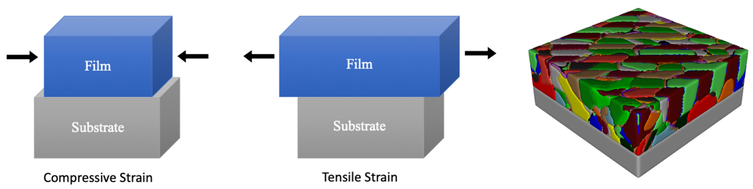


Fig. 3
Diagram depicting strain of thin films on a substrate (left) and sample domain structure using phase-field simulations (right).

Anisotropic Strain Phase Diagrams

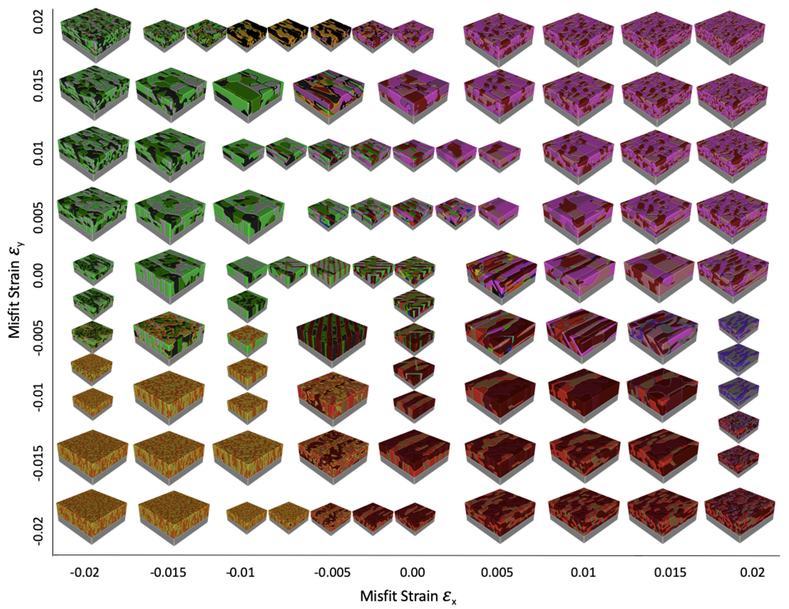


Fig. 4
Domain structures organized according to respective lateral anisotropic misfit strains.

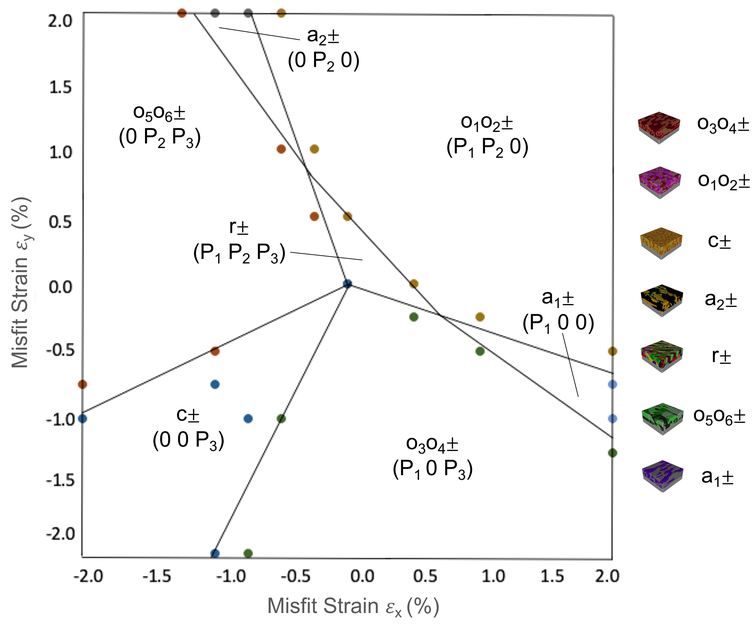


Fig. 5
Anisotropic misfit strain phase diagram of KNN thin films produced using phase-field methods.

Phase-Field vs. Thermodynamic Analysis

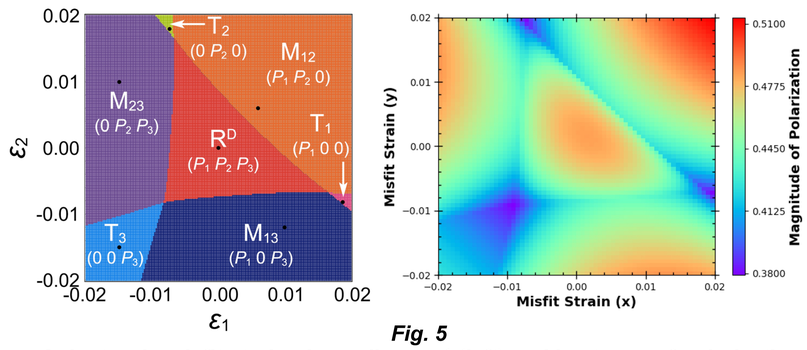


Fig. 5
Anisotropic misfit strain phase diagram[1] (left) and heat map of polarization magnitude[2] (right) created through thermodynamic analysis.

Future Work: Herringbone Structures

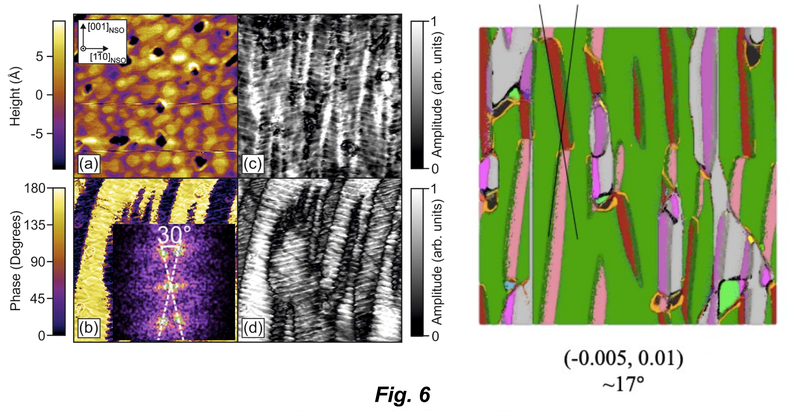


Fig. 6
Herringbone structures of $K_{0.9}Na_{0.1}NbO_3$ thin films through experimental analysis[3] (left) and phase-field simulation depicting a possible herringbone structure (right).

Acknowledgements

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[1] M. J. Zhou, J. J. Wang, L. Q. Chen, C.W. Nan, J. Appl. Phys. **123**, 154106 (2018).
[2] Zorn, J. *μ-Thermo*; Pennsylvania State University: State College (2019).
[3] M. Schmidbauer, D. Braun, T. Markurt, M. Hanke, J. Schwarzkopf, Nanotechnology **28** 24LT02 (2017).

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