Ultrafast and accurate prediction of polycrystalline hafnium oxide ferroelectric hysteresis using graph neural networks

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Polycrystalline hafnium oxide emerges as a promising material for the future of nanoelectronic devices. While phase-field modeling stands as a primary choice tool for forecasting domain structure evolution and electromechanical properties of ferroelectric materials, it suffers from a high computational cost, which impedes its applicability to real-size systems.

Here, we propose a Graph Neural Network (GNN) machine-learning framework to predict the ferroelectric hysteresis of polycrystalline hafnium oxide, with the goal of significantly accelerating computations in contrast to high-fidelity phase-field methods. By leveraging the inherent graph structure of the polycrystalline system and incorporating edge-level feature properties through graph attentional layers, our approach accurately predicts hysteresis behaviors across a broad range of polycrystalline structures, grain numbers, and Landau coefficients.

The GNN framework exhibits high accuracy, with an average relative error of 4%, and demonstrates remarkable computational efficiency with respect to ground truth phase-field simulations, offering speed-ups exceeding a million-fold.

Furthermore, we showcase the transferability of our model to efficiently scale predictions in polycrystals comprising up to a thousand grains, paving the way for effective simulations of real-sized systems. Our approach, by overcoming computational limitations in polycrystalline hafnium oxide, opens doors for accelerating discovery and design in ferroelectric materials.

Figures

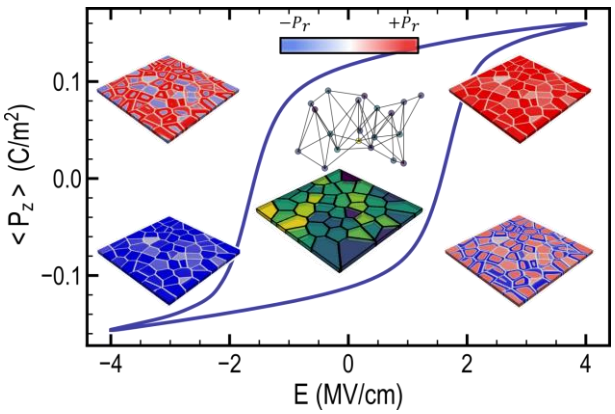

Figure 1. Phase-field modeling of ferroelectric hysteresis in 10 nm thick polycrystalline hafnium oxide thin films, accelerated by Graph Neural Networks.