Reinforcement Learning-Assisted Ferroelectric Domain Wall Design Using a Machine Learning Phase-Field Surrogate

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Precise control of ferroelectric domain walls (DWs) is a pivotal challenge for advancing DW-based memory device technologies. While recent advancements in scanning probe microscopy-enabled automated experiments have improved the efficiency of tip control, real-time optimization of tip trajectories for configuring arbitrary domain structures remains a significant hurdle.

In this study, we propose a reinforcement learning (RL) framework for autonomous DW manipulation, employing a three-dimensional machine learning phase-field surrogate model to accelerate environment dynamics [1]. An overview of the proposed methodology is depicted in Figure 1, illustrating the agent's interaction with the environment to configure DWs via tip-induced switching.

Initially, we explore a single-goal RL strategy, wherein the agent adjusts the DW configuration to match a specific DW target by controlling the tip's spatial position and applied bias on the film surface. Subsequently, we extend the approach with a goal-augmented RL strategy, enabling the agent to generalize across diverse target configurations and optimize tip trajectories in real time for arbitrary targets without requiring retraining. Furthermore, we demonstrate the agent's capability to design domain structures at the patch level, facilitating precise polarization control in large-scale systems. The framework is also adapted to directly optimize ferroelectric properties in an inverse design context rather than focusing on specific DW configurations, as illustrated in Figure 2, where the DW area under a virtual top electrode region is optimized.

Overall, this RL framework marks a substantial step forward in real-time design and control of ferroelectric DWs.

References

[1] Alhada–Lahbabi, K., Deleruyelle, D. Gautier, B. Machine learning surrogate for 3D phase-field modeling of ferroelectric tip-induced electrical switching. *NPJ Computational Materials* **10**, 197 (2024).

Figures

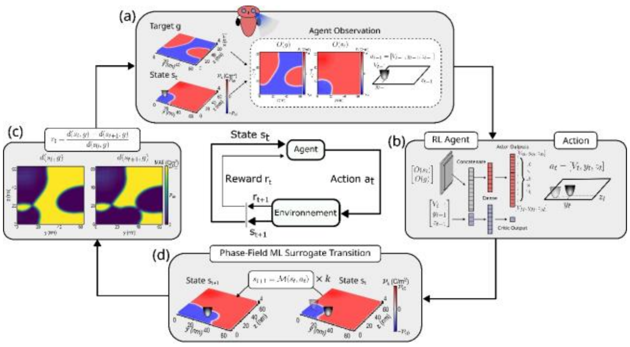

Figure 1. Overview of the RL Framework for Tip-Assisted Domain Wall Control. (a) At each timestep, the agent observes the environment (current state, domain wall target surface, prior action) and (b) selects an action consisting of tip offset and location. (c) A reward is then assigned based on the agent's progress toward achieving the target configuration, following the transition of the environment simulated by the machine learning-based phase-field surrogate model (d).

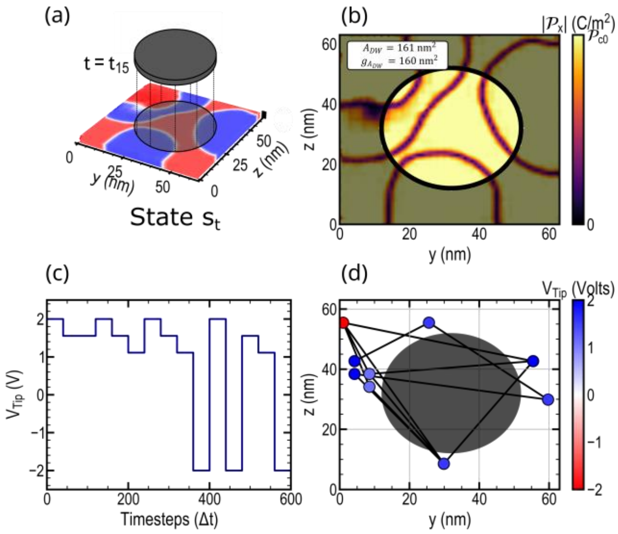

Figure 2. Domain Wall Inverse Design for Resistivity Optimization. (a) Final microstructure state after 15 moves, including a schematic of a conceptual top electrode region. (b) Out-of-plane polarization amplitude, with the DW region used to compute the highlighted DW area, below the electrode. The agent achieves a final DW area under the electrode of A = 161 nm², closely matching the target area g= 160 nm², (c) Tip bias profile V(t) over time. (d) Tip trajectory [y(t), z(t)] on the film surface. The virtual electrode region, marked in black, is excluded from permissible tip positions.