Contribution ID: **114** Type: **Poster Only**

Building Automated PFM Scientist

Ferroelectric materials exhibit diverse behaviors influenced by local structure, domain configurations, and external stimuli. To support their systematic exploration, an integrated platform has been developed that combines autonomous scanning probe microscopy (SPM), physics-informed measurements, and machine learning-guided decision-making.

In one study, domain wall dynamics in $PbTiO_3$/$KTaO_3$ heterostructures are investigated. Global SPM scans are used to identify candidate regions, followed by autonomous selection of areas containing specific domain wall types. Voltage pulses with varying amplitude and duration are applied in a controlled, repeatable manner across hundreds of sites. This enables statistically robust, spatially resolved insights into domain wall mobility and switching behavior.

In a separate investigation, automated DART-PFM is used to characterize ferroelectric responses in composition-spread libraries, including Sm-doped $BiFeO_3$ (SmBFO) and $Al_{1-x-y}B_xSc_yN$ (AlBScN). High-throughput maps of polarization loops, piezoresponse strength, and domain morphology are obtained. The morphotropic phase boundary in SmBFO is localized, and previously unreported functional transitions are identified in AlBScN.

To enable data-driven materials optimization, a multi-objective Bayesian optimization framework based on deep kernel learning (MOBO-DKL) is implemented. Domain-specific reward functions—such as loop area, net piezoresponse, and domain symmetry—are used to guide measurement selection. Pareto front analyses support simultaneous optimization of competing objectives and discovery of regions with desired functional responses.

Topical Area

AI and data science

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