Machine Learning-Driven Automated Scanning Probe Microscopy

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Machine learning (ML) has rapidly become an indispensable part of materials science research, which is capable of accelerating fundamental and applied research. Since the invention of scanning probe microscopy 35 years ago, it has become a mainstay of the field of materials science. However, until now, the search for interesting functionalities in microscopy experiments has relied on human operators to identify objects of interest and/or explore physical mechanisms, e.g., human operators make decisions for subsequent experiments according to the previous experiments, prior information, and knowledge.

Here, we implemented task-specific ML algorithms, including deep kernel learning (DKL), deep convolutional neural network (DCNN), and hypothesis (Hypo) learning in SPM, which enable ML-driven automated SPM to learn objects of interest and/or explore physical mechanisms in materials in an automated manner. First, the DKL actively learns the relationship between structural elements in microscopy images and properties encoded in spectroscopic data during real-time experiments. This method discovered a larger hysteresis opening near 180° domain walls due to the larger polarization mobility in the vicinity of the 180° walls in a $PbTiO_3$ sample. Second, the DCNN converts the real-time microscope image into a semantically segmented image of objects of interest, then a pre-defined workflow will drive the microscope to investigate these objects systematically. Third, Hypo-learning aims to establish the best physical hypothesis for the material's behavior during operating experiments. We investigated the ferroelectric domain switching mechanism in a $BaTiO_3$ thin film using this method and found that the domain switching is determined by the kinetics of the domain wall motion. We implemented these approaches in SPM here, however, these approaches can be adapted to apply to a wide range of characterization and synthesis experiments.