Unsupervised and semi-supervised classification of order-disorder phase transitions in oxides

Arman H. Ter-Petrosyan, Jenna A. Bilbrey, Christina M. Doty, Bethany E. Matthews, Sarah M. Akers, Steven R. Spurgeon

Recent advances in data analytics have provided new avenues for determining process-structure-property linkages in materials. In particular, machine learning (ML) techniques have increased the efficiency of classifying microscopy images for the purposes of material characterization, as well as a mechanism for low-level instrument control for automated microscopy [1]. In this work, we build upon the few-shot learning implementation developed by Akers et al. [2], which has been demonstrated to rapidly and accurately classify features in micrographs using only a handful of representative examples. The pyChip classifier [3] is one such model that implements this functionality and has proven to be useful in classifying images of several different kinds of materials. Building upon the pyChip classifier, we incorporate uncertainty quantification into the classification by using overlapping sliding windows to form the chips. In addition, we show that replacing the previous encoders trained on ImageNet with one trained on microscopy images (MicroNet [4]) improves the classification performance.

We then couple the embeddings extracted from MicroNet with tools from graph theory to perform unsupervised classification of structural motifs within a micrograph. Chips with similar structural motifs will lie close to one another in embedding space, while dissimilar motifs will be farther apart. Therefore, we can use the cosine distance between embeddings to quantify the similarity of two chips. The pairwise similarities of all chips in an image can be represented as a complete weighted network graph, where each vertex represents a chip and edges are placed between each pair of vertices, weighted by the embedding distance between the pair. Groupings of similar chips, corresponding to regions of distinct structural motifs in the full image, can be found by applying standard community detection algorithms used in the field of graph theory. In addition to classification, the relationship between clusters can be measured based on the connectivity of the graph. For example, as shown in Figure 1, unsupervised clustering identifies a disordered region that is intermediate to the STO and Pt/C layers.

Figure 1: Graph analytic models can intelligently describe the defective interface in STO.
Incorporating the results of both the supervised and unsupervised ML methods will help establish trends in analyzing microscopy data which can be exploited for further development of classification models. We suggest that microscopy experiments be automated in the future using a combination of these techniques to enable high-throughput analyses.

References


