Automated Phase Mapping for Large-Scale X-ray Diffraction Data Using a Graph-Based Phase Segmentation Algorithm

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Abstract: The creation of composition–processing–structure relationships currently represents a key bottleneck for data analysis for high-throughput experimental (HTE) material studies. Here we propose an automated phase diagram attribution algorithm for HTE data analysis that uses a graph-based segmentation algorithm and Delaunay tessellation to create a crystal phase diagram from high throughput libraries of X-ray diffraction (XRD) patterns. We also propose the sample-pair based objective evaluation measures for the phase diagram prediction problem. Our approach was validated using 278 diffraction patterns from a Fe–Ga–Pd composition spread sample with a prediction precision of 0.934 and a Matthews Correlation Coefficient score of 0.823. The algorithm was then applied to the open Ni–Mn–Al thin-film composition spread sample to obtain the first predicted phase diagram mapping for that sample.