High-throughput screening of compositionally-graded Al-Cr-Fe thin films using machine learning techniques

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Exploring a large amount of different mixture combinations with little guiding theory is a significant challenge in the discovery of applicable multinary alloy phases. High-throughput experimentation on compositionally-graded thin films can allow for rapid characterization of multinary alloys. Machine learning techniques can then be leveraged to dissect useful information from reams of structure data. In this study, compositionally-graded Al-Cr-Fe films were deposited on silicon wafers and annealed at 800°C. Synchrotron x-ray diffraction (XRD) and energy dispersive x-ray spectroscopy data was collected along the wafers. The XRD spectra were clustered according to similarity and mapped onto an Al-Cr-Fe ternary. Several clustering algorithms were executed with two commercial packages and with the scikit-learn Python module. Dimensionality reduction was explored as a preprocessing technique. An adaptation of the graph-based endmember extraction and labeling (GRENDEL) algorithm was then used to control cluster connectivity. Results from the various clustering algorithms were compared quantitatively to a calculated isotherm. Methods for testing the plausibility of cluster assignments within the same dataset were also developed.