Material Informatics Approach for Composition Reconstruction in Irradiated Fe-Cr-Al Alloys

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Neutron and ion irradiation results in spinodal-like instabilities manifested in the form of periodic composition fluctuations in alloys due to the inverse Kirkendall effect. Enrichment and depletion of certain species in various regions of the alloy is a characteristic feature of this phenomenon. The local composition changes occur at a length scale on the order of the dislocation interaction distances, thus leading to spatial variations in dislocation mobility and elastic modulus over short distances. The collective deformation behavior of the material is expected to be highly affected by this composition heterogeneity. In order to capture such local effects in dislocation dynamics, it will be necessary to reconstruct the composition field in 3D and assess the local changes in dislocation mobility and modulus as a function of composition. In this work, a data-driven approach to analyzing the local composition changes in an FeCrAl alloy is presented, wherein composition data acquired from experimental techniques such as energy dispersive x-ray spectroscopy (EDS) can be reconstructed on a finite dimension grid. We use frequency representation of the data to determine auto-correlations and cross-correlations between different phases. These 2-point correlations serve as an input to a trial microstructure having the nominal uniform distribution of the composition. The methodology for the reconstruction has been tested on two model FeCrAl alloys, namely C35M (nominally Fe-13%Cr-5%Al) and C37M (nominally Fe-13%Cr-7%Al).