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Analysis of Grain Boundary Character with Dream3D

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The use of the Dream3D package for analyzing the crystallographic character of grain boundaries is described. By segmenting the grains and inserting a triangular surface mesh along the boundaries, the grain boundary structure can be discretized. Each triangle has its own normal, which is transformed into the coordinates of the grain on either side of the boundary. The combination of lattice misorientation across the boundary and the local normal provides the five parameters required to completely specify the grain boundary character. The ensemble of such datapoints represents the grain boundary character distribution (GBCD), which can be binned to make contour plots. Each plot typically is made for a single misorientation such that the variation in population is shown for all inclinations i.e. variations of the grain boundary normal. Analysis of the grain boundary character distribution (GBCD) reveals the expected inverse relationship between populations and energies, with sharp peaks for certain Coincidence Site Lattice (CSL) types in fcc metals. In most materials, however, the dominant influence over grain boundary energy is from the variation in energy of the two surfaces that make up the boundary. The high fractions of $\Sigma 3$, $\Sigma 9$ and related CSL types observed in fcc metals is dominated by the occurrence of annealing twins, i.e. $\Sigma 3$ boundaries with {111} on both surfaces.