Insights into Nanocrystalline Grain Growth through Phase Field Crystal Calculations

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Phase field crystal (PFC) models have been used to describe a wide range of phenomena from grain growth to solidification and dislocation motion in crystals. The strength of the method lies in its ability to follow the atomic scale motion and defect formation that accompanies a process that occurs on diffusive timescales. An introduction to the method will be given. Using the PFC approach, the evolution of the dislocation structure of non-planar grain boundaries, the local atomic displacements of atoms near the boundary, and the long-range strain fields that accompany grain growth have been examined. We find that the atomic-scale structure of the boundary gives rise to qualitatively new grain growth kinetics as well as to both grain rotation and translation. The grain translation is a result of the climb, glide, and interactions of the dislocations that comprise the grain boundary, as well as dislocation interactions at trijunctions. Finally, the effect of temperature and vacancy concentration on grain growth will be discussed.