Graduate Student Research Seminar

Fall 2021

Unraveling the Role of Grain Boundary Anisotropy in Sintering

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3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

Sintering is a thermal processing technique used to consolidate particle compacts into structures by heat or pressure without melting. It is broadly used in optical, catalytic, electronic, and structural applications. In recent years, the sintering of nanoscale particles has received considerable attention, as it leads to reduced sintering temperatures and faster processing times. In crystalline nanoparticles, the high surface area to volume ratio amplifies the role of the grain boundaries in densification (i.e., elimination of internal pores) and coarsening (i.e., surface smoothing and grain growth) processes. Grain boundaries are internal interfaces that separate differently oriented crystalline grains.

Atomistic simulations are used to investigate the sintering behavior of a series of [001] tilt GBs in Ni over 200 ns using the two-particle geometry. The interface free energy and self-diffusion for these GBs are first calculated. Then, several microstructural and topological features, such as particle rotation, local interface curvatures, particle neck growth, and shrinkage rates are tracked as a function of time and GB type. Our results show a direct correlation between the GB energy and the boundary's self-diffusion coefficient. Further, our simulations reveal considerable variations in particle neck growth and shrinkage rates as a function of GB type, and suggest faster sintering kinetics with increased GB misorientation angle. In broad terms, our approach provides future avenues to employ particle orientations and resultant GB types as a strategy to fabricate sintered materials with controlled nanostructured features.

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