

THE ROLE OF GRAIN BOUNDARY CHARACTER IN NANOSCALE SINTERING

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Sintering is a materials process that leads to the consolidation of a particle powder compact and the increase in its strength and integrity. During sintering, particle neck regions form and grow leading generally to densification (i.e., elimination of internal pores) and coarsening. In crystalline solids, classic theoretical treatments of sintering yield dynamical scaling laws relating the temporal evolution of a feature of interest (typically particle neck width) to diffusion pathways, materials properties, and operating temperature. Such treatments do not account for the thermodynamic and kinetic roles of grain boundaries (GBs) in sintering processes. Herein, we explore, through classical atomistic simulations, the effects of grain boundary misorientation on nanoscale sintering. The two-particle geometry is used, in which their crystallographic orientations are systematically varied, and their sintering behavior is quantified. Our simulation results clearly demonstrate the paramount role that GBs play in sintering of nanoscale particles. In broad terms, our work provides future avenues to explore the role of GBs in the sintering of nanoscale particles.

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