Graduate Student Research Seminar

Fall 2021

Phase field modeling of grain boundary segregation: Insights from matched asymptotic analysis

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

Abstract

Grain boundaries (GBs) are internal interfaces that separate differently oriented grains in a polycrystalline solid. The interaction of GBs with alloys, or impurities, greatly influences GB dynamical processes, such as grain growth and recrystallization. The preferential segregation of alloys to GBs induces a dynamic drag pressure that hinders GB motion. In this talk, we present a phase field model of GB solute segregation and grain growth in metallic alloys that is based on the time-dependent Ginzburg-Landau formalism. In addition to a solute composition field, the grain microstructure is represented by non-conserved order parameters that vary smoothly, yet sharply across GB regions. Using the method of matched asymptotic expansions with curvilinear coordinates, the phase field dynamical equations are expanded non-dimensionally in close vicinity of GB regions (i.e., inner expansion) and in the bulk (i.e., outer expansion). Solutions of these expansions up to second order are then matched, resulting in a kinetic law describing the migration of doped GBs. The results are then compared with the well-celebrated Cahn's sharp interface model of GB solute drag [Acta Metallurgica 10 (1962) 789-798].

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