

Mesoscale Modeling of Materials Microstructures: From Nanocrystalline Alloys to Additive Manufacturing Processes

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The response of materials systems to a wide range of external stimuli is a direct manifestation of their inherent characteristic microstructural features (e.g., interfaces, grains, phases, dislocations). Thus, it is of great importance to fundamentally understand microstructure in order to predict its role on the macroscopic properties and performance of materials, and ultimately develop innovative ones with increased functionality. In this presentation, which is delivered in two parts, we cover the development of mesoscopic models aimed at unraveling the role of microstructure on the evolution of materials systems in two applications, namely, nanocrystalline alloys and additive manufacturing processes.

The first part of the talk is focused on nanocrystalline (NC) materials and their instability against grain growth processes even at low service temperatures, an effect that hinders their use in extreme environments. Grain boundary (GB) solute segregation has been recently proposed as a route to thermally stabilize the grain structures of NC materials. With the aid of a mesoscale model, we examine GB solute segregation and its role on the stabilization of NC alloys. Regimes are identified, where the reduction in GB energy, and thus the driving force for grain growth, is significant. The discussion will then move to immiscible NC alloys, where the enhanced stability is a manifestation of the competing effects of GB segregation, bulk phase precipitation, and particle pinning mechanisms.

In the second part of the talk and based on a diffuse interface model, we examine solid-state sintering in direct ink write additive manufacturing processes. The framework is capable of accounting for bulk thermodynamics, free energies of grain boundaries and free surfaces; and capturing various mass transport mechanisms. Quantitative analysis of the roles of particle size/distribution, equilibrium dihedral angles, and interfacial anisotropy on the microstructural evolution is presented. With the aid of several statistical measures, the evolution of the pore space and densification rates are quantified in order to establish a microstructure/morphology map in terms of the processing parameters.

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