Mesoscale Modeling of Materials Microstructures: From Sintering Kinetics to Grain Boundary Segregation

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Hetergeneous materials systems hold the key to the future development of a wide range of technologies. A key strategy in designing such systems is the manipulation of various micro- and/or nano-scale features yielding non-equilibrium structures, which tend to evolve in time in response to a wide range of perturbations. In this talk, which is delivered in two parts, we cover the development of mesoscopic models aimed at unraveling the role of interfaces on the microstructural evolution of materials systems.

In the first part 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 (GBs) 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 model parameters.

The second part of the talk is focused on grain boundary (GB) solute segregation as a route to mitigate thermally driven grain growth processes in nanocrystalline metals and stabilize their grain structures. Regimes are identified, where the reduction in GB energy, and thus the driving force for grain growth, is significant. The discussion will then focus on immiscible alloys, where the enhanced thermal stability is a manifestation of the competing effects of GB segregation and bulk phase separation.

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