Application of Phase Field Methods to Additive Microstructures in Metals

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ABSTRACT

As part of the broader NIST effort in the materials science of additively manufactured metals, we are employing phase field techniques to better understand the unique microstructural aspects of additive manufacturing. Phase field methods are widely applied because of their ability to capture complex morphogical and topological change in evolving microstructures, but the method is computationally demanding. A number of different formulations are possible, with different sets of advantages and challenges.

We will discuss our experience applying three types of phase field models to different aspects of additive manufacturing:

- **A dilute, binary anti-trapping model in the rapid solidification regime.** We have simulated the microstructures that form along the melt pool boundary during laser powder bed fusion of Inconel and T-6Al-4V alloys. Solidification conditions were estimated from a finite element model calibrated to *in situ* experimental thermal imaging of the melt pool. The observed cellular microstructures exhibit quantitative agreement with experiment for the cell spacing, secondary arm spacing, and microsegregation. These microsegregation patterns illuminate the origin of the deleterious phases that can arise during post-build heat treatment of additive alloys.

- **A multi-component, multi-phase solid-state model coupled with CALPHAD-based thermodynamics.** We performed phase field simulations of solid-state precipitation in a ternary Cr-Nb-Ni analogue to Inconel 625, a nominally single-phase 13-component superalloy, with an initial microsegregation profile based on electron microscopy of additively manufactured parts and 1D computational kinetic simulations of dendritic solidification. The phase field results demonstrate preferential nucleation in the enriched last-solidified interdendritic region. We will discuss competitive growth and ternary reversion in the context of diffusion-controlled relaxation of these enriched regions toward the nominal system composition.

- **An amplitude expansion structural phase field crystal model.** This technique enables the study of atomic-scale phenomena at diffusive time scales in an idealized multiphase crystalline material. Starting from a planar single crystal, directional solidification transitions to cellular growth due the Mullins-Sekerka instability. Under some conditions, simulations exhibit a simultaneous onset of localized crystal rotation and injection of geomatrically-necessary dislocations from the cell roots, leading to low-angle grain boundaries between the cells. This behavior may help explain the origin of the high residual stresses in additive metals.