Phase field model development for microstructure prediction in additive manufacturing and post-processing

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ABSTRACT

Complex microstructures are obtained in multi-component aerospace alloys such as alloy 718 during powder bed laser fusion additive manufacturing process. The as-built microstructure is dendritic with well-developed primary and secondary arms along with segregation of solutes in the inter-dendritic space. Heat transfer and fluid flow models were used to compute the steady state temperature gradient and an average value of the solid-liquid (s-l) interface velocity that were used as input for the phase field simulations. A multi-fidelity and multi-scale Bayesian Framework has been demonstrated to calibrate parameters for phase field model. The simulations show that the solidification morphology is sensitive to the spacing between the columnar structures. Spacing narrower than a critical value results in continued growth of a columnar microstructure, while above a critical value the columnar structure evolves into a columnar dendritic structure through the formation of secondary arms. These results are discussed in terms of the existing columnar to dendritic transition (CDT) theories. The measured interdendritic Nb concentration, the primary and secondary arm spacing is in reasonable agreement with experimental measurements performed on the nickel-base superalloy IN718.These alloys require post-processing heat treatment in order to recover the mechanical properties through precipitation hardening. Conventional heat treatment schedules developed for wrought 718 alloy has to be modified in order to optimize the properties of the AM processed material. Simulation tools are being developed to predict the precipitation in AM material during post-processing and design a customized heat treatment for the alloy. A mathematical approach has been developed in ORNL phase field code in MEUMAPPS-SS to extend the single-phase Kim-Kim-Suzuki model to the simultaneous precipitation of two-phases from the matrix. The simulations will employ a phase field model and take advantage of the HPC capabilities at ORNL.

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