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## Numerical modeling of microstructure evolution during laser additive manufacturing of a nickel-based superalloy

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## Abstract

A multi-scale model that combines the finite element method and stochastic analysis is developed to simulate the evolution of the microstructure of an Nb-bearing nickel-based superalloy during laser additive manufacturing solidification. Through the use of this model, the nucleation and growth of dendrites, the segregation of niobium (Nb) and the formation of Laves phase particles during the solidification are investigated to provide the relationship between the solidification conditions and the resultant microstructure, especially in the morphology of Laves phase particles. The study shows that small equiaxed dendrite arm spacing under a high cooling rate and low temperature gradient to growth rate (G/R) ratio is beneficial for forming discrete Laves phase particles. In contrast, large columnar dendrite arm spacing under a low cooling rate and high G/R ratio tends to produce continuously distributed coarse Laves phase particles, which are known to be detrimental to mechanical properties. In addition, the improvement of hot cracking resistance by controlling the morphology of Laves phase particles is discussed by analyzing the cracking pattern and microstructure in the laser deposited material. This work provides valuable understanding of solidification microstructure development in Nb-bearing nickel-based superalloys, like IN 718, during laser additive manufacturing and constitutes a fundamental basis for controlling the microstructure to minimize the formation of deleterious Laves phase particles.

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## 1. Introduction

The laser additive manufacturing process, as an alternative to traditional multi-pass welding and thermal spray technologies, uses lasers as a concentrated heat source to fabricate coatings with a perfect metallurgical bond to substrates. The process is particularly of interest in the rapid component manufacturing and repairing fields due to its high efficiency and relatively low cost. Materials that have been used in laser additive manufacturing include

nickel-based superalloys [1–4] and steels [5–8]. The IN 718 superalloy is a precipitation-strengthened Nb-bearing nickel-based alloy with excellent mechanical properties [9–11]. One of the most outstanding microstructural features of as-deposited IN 718 coatings by laser additive manufacturing is the distribution of Nb-rich Laves phase particles in the austenitic matrix [12–17]. Unfortunately, it was also confirmed that the presence of Laves phase particles dramatically reduces the performance of the IN 718 alloy, e.g. in terms of the tensile ductility, ultimate tensile strength, fracture toughness and fatigue life [18]. Therefore, one of the challenges in improving the performance of IN 718 coatings is by controlling the Laves phase particles.

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A large number of research works have been implemented to search for an effective method to control Laves phase particles in IN 718 superalloy. The most widely used method is homogenization heat treatment. Qi et al. [19] completely removed Laves phase particles from laser clad Inconel 718 coatings by employing the homogenization heat treatment. Huang et al. [20] also reported the tendency of a decrease in the volume fraction of Laves phase particles with respect to an increase in the homogenization heat temperature in welded cast IN 718 alloy. Although heat treatment is an efficient method to remove Laves phase particles, the problems associated with microfissuring, recrystallization and grain growth in the heat-affected zone, and distortion of the processed parts, also arise at the same time. When those concomitant problems are not tolerable in practice, it is necessary to search for other methods to control the Laves phase particles. With this purpose in mind, several interesting research works have been carried out. For example, Manikandan et al. [21] and Ram et al. [22] found that a high cooling rate obtained by replacing the constant current with a pulsed current in gas tungsten arc (GTA) welding is beneficial to reducing the amount of Laves phase particles in the welded IN 718 alloy. Radhakrishna and Rao [23] also found that reducing the heat input in GTA welding is beneficial in suppressing the formation of Laves phase particles. They also attributed the reason to the high cooling rate obtained in low heat input welding processes. Based on those reports, it can be concluded that the formation of Laves phase particles can be controlled by changes in the solidification conditions, e.g. cooling rate, by varying the processing parameters. Therefore, fully understanding the evolution of the microstructure during solidification is highly beneficial.

It is very difficult to directly observe the evolution of the microstructure by experimental technology due to the rapid solidification of the deposited coatings. An alternative method for studying this problem is by using numerical simulation. Wang and Beckermann [24,25] proposed a solute diffusion model aimed to predict the transition of columnar to equiaxed dendritic structures in metal casting. Nastac and Stefanescu [26-28] mapped the morphology and segregation pattern in cast dendritic alloy by using a stochastic model. Yin and Felicelli [29] combined the finite element method (FEM) and cellular automaton (CA) together to investigate the dendrite arm spacing of a coating for the laser-engineered net shaping (LENS) process. Dong and Lee [30] also developed a coupled finite difference-CA model to predict the microstructure of the Al-Cu alloy. However, limited work has been carried out to investigate the IN 718 alloy coatings.

The general objective of this work is to investigate the evolution of the microstructure in the IN 718 coating fabricated by laser additive manufacturing. The specific objective is to study the influence of solidification conditions on the formation of Laves phase particles, and illustrate a way to control Laves phase particles by optimizing the solidification conditions in laser additive manufacturing. In the present work, the control of the morphology of Laves phase particles is paramount, because the mechanical performance of Nb-bearing nickel-based superalloys, like IN 718, is significantly influenced by the presence and morphology of Laves phase particles. A multi-scale model that couples the FEM and stochastic analysis is developed to simulate solidification. The nucleation and growth of dendrites, segregation of Nb and formation of Laves phase particles during the solidification of the IN 718 superalloy are predicted by using the model. The dependence of Laves phase particle formation on solidification conditions is numerically simulated and the results are compared with experimental observation. Improvement in the hot cracking resistance by controlling the morphology of Laves phase particles is also discussed. The work presented herein offers a comprehensive understanding of microstructure development during the solidification of Nb-bearing nickel-based superalloy processed by the laser additive manufacturing method. It is firmly believed that this work is useful for research that aims to improve the performance of the IN 718 coating by controlling Laves phase particles in laser additive manufacturing.

## 2. Model description and experimental details

A multi-scale model is developed in this work by using a model that couples FEM and a stochastic analysis. FEM is employed to calculate the transient temperature field during the deposition of one layer of IN 718 alloy coating onto a IN 718 alloy substrate in a macro-scale domain, and the stochastic analysis which is based on the solidification theory is applied to compute the evolution of the microstructure during solidification in a micro-scale domain. In order to verify the simulation and illustrate the dependence of the microstructure on the solidification conditions, two IN 718 alloy coatings with dimensions of 3 mm in width and 0.6 mm in height were deposited by the laser additive manufacture onto IN 718 alloy substrate, using a diode laser (808 nm wavelength) system with a coaxial powder jet. The spherical powder of IN 718 alloy with an average size of  $\sim 100 \,\mu\text{m}$ , which was produced by the plasma rotation electrode process (PREP), was used in laser additive manufacturing. The laser power values used were 1 kW and 3.5 kW. The laser spot dimensions were 3 mm in length and 1 mm in width, and the energy was uniformly distributed over the laser spot due to the nature of the diode laser source. The laser scanning speed was  $10 \text{ mm s}^{-1}$ , and the feed rate of the powder was  $15 \text{ g min}^{-1}$ . Pure argon was used as the shielding  $(151 \text{ min}^{-1})$  and carrier gas  $(151 \,\mathrm{min}^{-1})$ . The laser processing parameters resulted in a conduction mode deposition.

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