Numerical Analysis of Solidification Behavior during Laser Welding Nickel-based Single-crystal Superalloy Part IV: Optimization of Thermo-metallurgical Factors

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Abstract. Important metallurgical factors, such as alloying aluminum redistribution, supersaturation and undercooling of dendrite tip around solid/liquid interface, are separately optimized to alleviate stray grain formation and columnar/equiaxed transition (CET) with series of welding conditions and provide a very efficient method for microstructure control through modification of growth kinetics of dendrite tip under nonequilibrium solidification conditions of ternary Ni-Cr-Al molten pool. Asymmetrical (001)/[110] welding configuration is inferior to symmetrical (001)/[100] welding configuration, because overall area-weighted alloying redistribution, supersaturation and undercooling of dendrite tip throughout the solid/liquid interface of weld pool are consistently severer to exacerbate solidification behavior and microstructure development and incur morphology instability of columnar/equiaxed transition. High heat input, such as combination of higher laser power and slower welding speed, monotonically increases aluminum enrichment, supersaturation and undercooling of dendrite tip near solidification interface to simultaneously deteriorate nucleation and growth of stray grain formation and weaken columnar dendrite morphology, while low heat input, such as combination of lower laser power and faster welding speed, decreases solute buildup, relieves supersaturation and beneficially suppresses dendrite tip undercooling to minimize equiaxed dendrite morphology in the crack-susceptible region, and thereby facilitate single-crystal epitaxial growth with decrease of thermo-metallurgical factors for columnar/equiaxed transition in order to provide prerequisite for optimization of welding conditions. Favorable solidification conditions are obtainable with preferential crystallographic orientation to eliminate columnar/equiaxed transition under which the epitaxy of single-crystal metallurgical properties across fusion boundary of substrate is predominantly promoted to essentially reduce stray grain formation in (001)/[100] welding configuration, and is kinetically capable of significant reduction of microstructure anomalies and nonuniform solidification behavior. The useful relationship among welding conditions, alloying aluminum redistribution, supersaturation and undercooling of dendrite tip is properly established within dendrite stability range through thorough analysis. In addition, the validation of theoretical predictions is fairly reasonable by the experiment results. It is worth that the contributions of kinetics-related solidification phenomena with advancement of solid/liquid interface are imposed altogether to understand why stray grain formation occurs on the basis of controlling mechanism of minimum undercooling or minimum velocity by the reproducible methodology procedure.
1. Introduction
Laser welding or cladding successfully enable repair of nickel-based single-crystal turbine blades in the aircraft and power generation industries and are advantageous over precedent technologies, such as TIG and electron beam welding, because of dominant microstructure amelioration, by which weld is free of crack. Numerous nucleation and growth of stray grain formation are unacceptable, and the insidious phenomena of dendrite growth kinetics is challenging for epitaxial growth of single-crystal metallurgical properties in the defect-free weld. Available recent research and applicable methods are briefly introduced in the following part. Arulmurugan et al. [1] analyzed the solidification behavior of ternary Ni-Cr-Mo superalloy 686 during gas tungsten arc welding (GTAW). Xueyuan et al. and Strondl et al. [2,3] analyzed the effect of NiAlHf coating and alloying powder on solidification behavior, microstructure development and solidification cracking susceptibility of single-crystal superalloy by electron beam physical vapor deposition and electron beam melting. Mang et al., Shi et al. and Gerald et al. [4-6] analyzed the solidification behavior and microstructure development of Inconel 718 during selective laser melting. Wenzhe et al. [7] analyzed the effect of TiC nanoparticles on microstructure refinement of nickel-based superalloy Inconel 738LC during laser power bed fusion. Ramakrishnan et al. and Karsten et al.[8,9] analyzed the solidification behavior and microstructure development of Inconel 738 by direct laser metal deposition and selective laser melting. Ojo et al.[10,11] analyzed the solidification behavior and intergranular liqation cracking of heat-affected zone of nickel-based superalloys TMS-75, TMS-75+C and IN718 during electron beam welding and tungsten inert gas (TIG) welding. Dinda et al. and Inaekyan et al. [12,13] analyzed the dendrite morphology and solidification cracking susceptibility of Ni-based superalloy Inconel 625 during laser-aided direct metal deposition and laser powder bed fusion. Hongfei et al. and Ramakrishnan et al. [14,15] analyzed the microstructure development of new Ni-Fe based superalloy and Haynes 282 with Haynes 282 filler wire during gas tungsten arc welding and direct laser metal deposition. Devendranath et al. and An et al. [16,17] analyzed the effect of heat treatment on microstructure development of Inconel X750 and GH4169 superalloys during activated flux tungsten inert gas (A-TIG) welding. Yao et al. and Yuchao et al. [18,19] analyzed solidification behavior, microstructure development and solidification cracking susceptibility of Ni3Al-based single-crystal superalloy IC21 and 713ELC through optimization of multiple process parameters during selective electron beam melting. Taoshen et al., Wenhua et al. and Sang et al.[20-22] analyzed the microstructure development of dissimilar materials Ni-based superalloys IC10/GH3039 and tantalum/GH3128 during laser welding and electron beam welding. The motivation of this work is thus to predict single-crystal growth conditions in order to eliminate morphology instability through efficient combinations of laser power, welding speed and welding configuration.

2. Mathematical Model
2.1. Heat Transfer Model
Symmetrical profiles of steady-state solid/liquid interface, which is independent on welding configuration, are separately calculated by Rosenthal solution with different combinations of laser power and welding speed on the basis of relevant thermalphysical properties of nickel-based single-crystal superalloy CMSX-4. The solidification interface contour of liquidus temperature is superimposed after discretization of transverse section in longitudinal direction. The predictions of weld pool geometry are comparable with experiment results.

2.2. Transition of Dendrite Growth Model
Three components of solidification conditions ahead of solid/liquid interface, especially temperature gradient and dendrite growth velocity, are subsequently determined by the derivative of molten pool geometry in X,Y and Z axes for each condition. The weld pool geometry and solidification conditions are interdependent to aid understanding of growth crystallography of single-crystal properties. Competitive dendrite growth regions activate discernable transition boundaries, which are limited by available mechanism of minimum velocity or minimum undercooling. Outline boundaries of
preferential <100> crystallographic orientations are controlled by two factors, molten pool geometry and welding configuration.

2.3. Ternary Ni-Cr-Al Dendrite Growth Model
Because diffusions of Cr and Al in Ni are significant for dendrite growth, Kurz-Giovanola-Trivedi (KGT) model provides more opportunities for microstructure control through modification of growth kinetics ahead of dendrite tip across solidification interface to simultaneously meet the calculation requirement of crystallography-dependent alloying aluminum redistribution and supersaturation.

\[
\frac{4\pi^2 \Gamma}{R^2} + 2 \sum_{i=1}^{2} \frac{P_{ei} m_i C_{0,i} (1 - k_i) \xi \left( Pe_i \right)}{[1 - (1 - k_i) Iv(Pe_i)]} + G_{hkl} = 0
\]

where \( \Gamma \) is the Gibbs-Thomson coefficient, \( R \) is the dendrite tip radius, \( Pe_i \) is the Peclet number for \( i \), \( m_i \) is the liquidus slope, \( C_{0,i} \) is the initial concentration for \( i \), \( k_i \) is the partition coefficient for \( i \), \( \xi(\text{Pe}_i) \) is a function of the Peclet number, \( Iv(\text{Pe}_i) \) is the Ivantsov solution (\( i = \text{Cr or Al} \)) and \( G_{hkl} \) is the average temperature gradient near the dendrite tip.

2.4. Minimum Dendrite Tip Undercooling Model
Morphology instability of columnar/equiaxed transition strongly depends on the mechanism of dendrite tip undercooling. For metallic alloys solidification, the thermal undercooling is much smaller and only constitutional undercooling and curvature undercooling are considered in the calculation of dendrite size and morphology. Any reduction of dendrite tip undercooling results in planar interface growth with decrease of diffusion driving forces for nucleation and growth of stray grain formation.

2.5. Overall area-weighted average model
Finally, overall area-weighted solid aluminum concentration \( \overline{C_{Al}} \) is calculated by

\[
\overline{C_{Al}} = \frac{\sum_{k=1}^{12} A_k \overline{C_{Al,k}}}{\sum_{k=4}^{12} A_k}
\]

where \( k \) is 1-12 transverse-section discretization of weld pool solidification interface with controllable the same distance along longitudinal axis. \( A_k \) and \( \overline{C_{Al,k}} \) are outer surface area of solid/liquid interface and average solid aluminum concentration for each part, separately. Similarly, the area-weighted average supersaturation of liquid aluminum \( \overline{\Omega} \) and minimum dendrite tip undercooling \( \Delta T^\gamma \) are consistently calculated with consideration of growth crystallography.

3. Results and Discussion
Interrelationship of laser power, welding speed and overall area-weighted solid aluminum concentration of diffusion-controlled dendrite growth with different welding configurations is shown in figure 1. For (001)/[100] welding confirmation in (a), the range of area-weighted solid concentration of aluminum is order of 5.47-5.55%. High heat input with combination of higher laser power and slower welding speed, within which the solidification conditions (lower temperature gradient and slower dendrite growth velocity) are unfavorable, monotonically increases more aluminum enrichment ahead of solid/liquid interface than that of low heat input with combination of lower laser power and higher welding speed, within which the solidification conditions (steep temperature gradient and faster dendrite growth velocity) are favorable, to promote solute diffusion and deteriorate crack-susceptible microstructure development. It is energetically preferable for alloying aluminum redistribution to predominantly enrich in the \( \gamma \) phase. The lower heat input is initiated, the smaller enrichment of alloying aluminum, narrower solidification temperature range,
insignificant columnar/equiaxed transition and subsequent finer dendrite size are spontaneously incurred to facilitate nonequilibrium solidification behavior and kinetically improve resistance to solute redistribution and vice versa. The flexible relationship among heat input (laser power and welding speed), welding configuration and solid aluminum concentration is acquired by optimization procedure of solidification conditions around solid/liquid interface for suppression of alloying aluminum buildup within solubility to thoroughly evaluate nucleation and growth of stray grain formation, and thus provide alternative way for microstructure control with symmetrical growth crystallography. The concise dependency of overall aluminum concentration on heat input is consistent with distributions of stray grain formation, dendrite trunk spacing and solidification temperature range of previous theoretical results under similar solidification conditions.

(a) Restriction of (001)/[100] crystallographic orientation
**Figure 1.** Interrelationship of laser power, welding speed and overall area-weighted solid aluminum concentration of diffusion-controlled dendrite growth with different welding configurations.

For comparison, (001)/[110] welding configuration in (b), the area-weighted solid aluminum concentration is order of 5.55-5.60%. Welding configuration is more significant contributing factor to redistribution of alloying aluminum, while heat input is less preferred. (001)/[110] welding configuration more enriches overall redistribution of alloying aluminum than that of (001)/[100] welding configuration with various combinations of laser power and welding speed. (001)/[100] welding configuration geometrically contributes to favorable solidification conditions ahead of solidification interface with symmetrical crystallography of microstructure development, while (001)/[110] welding configuration dominates unfavorable solidification conditions with asymmetrical crystallography of microstructure development. Therefore, appropriate solidification conditions of two factors, such as low heat input and (001)/[100] welding configuration, beneficially minimizes the overall aluminum concentration with increase of kinetic driving forces for epitaxial growth of molten pool to suppress columnar/equiaxed transition rather than other factors, such as high heat input and (001)/[110] welding configuration. It is imperative to control welding conditions to prevent the crystallography-dependent microstructure instability and completely alleviate solidification cracking during laser welding. Reliable alloying redistribution is numerically analyzed on the basis of minimum undercooling or minimum velocity criterion to predict diffusion-controlled anomalies of solidification behavior and provide guideline for successful crack-free weld and single-crystal dendrite growth.

Interrelationship of laser power, welding speed and overall area-weighted supersaturation of liquid aluminum of diffusion-controlled dendrite growth with different welding configurations is shown in figure 2. For (001)/[100] welding confirmation in (a), the range of liquid aluminum supersaturation is
In order to optimize growth kinetic of dendrite tip by supersaturation of liquid aluminum, welding configuration is of significance during single-crystal molten pool solidification to predominantly determine distributions of either symmetrical or asymmetrical microstructure development. When (001)/[100] and (001)/[110] welding configurations are compared, smaller overall supersaturation of liquid aluminum in symmetrical (001)/[100] welding configuration is attributable to preferential crystallographic orientation and crystallographically suppresses nucleation and growth of stray grain formation for columnar/equiaxed transition, which is an important contributing factor to weldability improvement. The relationship between heat input and supersaturation of liquid aluminum is consistent each other in two welding configurations. For low heat input and (001)/[100] welding configuration, this combination is particularly beneficial to amelioration of solidification behavior and microstructure control through alloying redistribution rather than combination of high heat input and (001)/[110] welding configuration. For comparison, (001)/[110] welding configuration in (b), the range of liquid aluminum supersaturation is order of 0.94-0.96. Favorable heat input (lower laser power and faster welding speed) is low enough to mitigate supersaturation of liquid aluminum and simultaneously minimize growth kinetics of dendrite tip for nucleation and growth of stray grain formation, refine dendrite growth and advance stable morphology of solidification interface under nonequilibrium solidification conditions, while undesirable heat input (higher laser power and slower welding speed) monotonically worsens supersaturation of liquid aluminum and incurs severe columnar/equiaxed transition and microstructure anomalies to deteriorate weldability without relief of supersaturation in the residual liquid. Solidification cracking susceptibility is evaluated by welding conditions optimization to minimize the aluminum enrichment in the γ phase and potentially improve weldability. The reasonable correlation of heat input, welding configuration and supersaturation of liquid aluminum possesses appropriate understanding of anomalous solidification behavior and crack-susceptible microstructure development of single-crystal superalloy, and thereby provides deep insight into thermo-metallurgical factors for essential columnar dendrite morphology growth at solidification interface.

(a) Restriction of (001)/[100] crystallographic orientation
Interrelationship of laser power, welding speed and overall area-weighted minimum dendrite tip undercooling of diffusion-controlled dendrite growth throughout the molten pool interface with different welding configurations is shown in figure 3. For (001)/[100] welding configuration in (a), the range of overall minimum dendrite tip undercooling is order of 0.4-0.6°C. The overall undercooling of dendrite tip ahead of solidification interface monotonically increases with either high laser power or slow welding speed. High heat input with combination of higher laser power and slower welding speed widens dendrite tip undercooling and contributes to microstructure degradation, instead, feasible low heat input with combination of lower laser power and faster welding speed modifies driving forces of solidification behavior to minimize columnar/equiaxed transition, improve weldability and promote multicomponent microstructure development of the single-crystal superalloy without nucleation and growth of stray grain formation. Optimum welding conditions (low heat input and (001)/[100] welding configuration) is more beneficial to crystallographic alleviation of columnar/equiaxed transition under nonequilibrium solidification conditions than that of insidious welding conditions (high heat input and (001)/[110] welding configuration), and is kinetically capable of further reduction of thermo-metallurgical factors for microstructure anomalies and solidification cracking. This tendency is fairly consistent with other phenomena ahead of solid/liquid interface, especially alloying aluminum redistribution and supersaturation of liquid aluminum under different solidification conditions.
Figure 3. Interrelationship of laser power, welding speed and overall area-weighted minimum dendrite tip undercooling of diffusion-controlled dendrite growth with different welding configurations.
For comparison, (001)/[110] welding configuration in (b), the range of overall minimum dendrite tip undercooling is order of 0.8-1°C. The lower heat input (smaller laser power and faster welding speed) is chosen, the narrower undercooling of dendrite tip, smaller aluminum concentration and lower aluminum supersaturation ahead of solidification interface are simultaneously satisfied to mitigate morphology transition and stray grain formation. When compared with (001)/[100] welding configuration, the anomalous solidification behavior and microstructure development are kinetically driven by wider dendrite tip undercooling ahead of solidification interface in (001)/[110] welding configuration under different combinations of laser power and welding speed. Appropriate welding configuration is more significant contributing factor for weldability improvement than heat input. In addition, the calculation results, such as crystallography-dependent transition of dendrite growth region within γ phase, are verified by the weld morphology of experiment results in a feasible way to properly understand the microstructure development by the metallurgical driving forces of solidification behavior [23,24]. The mechanism of obtainable microstructure amelioration through controllable kinetic factors is conveniently proposed. The kinetic calculation of diffusion-controlled dendrite growth facilitates understanding of metallurgical driving forces at the solid/liquid interface behind phenomena of anomalous microstructure development to eliminate nucleation and growth of stray grain formation through beneficial solidification conditions and thereby provides further challenges of solidification behavior improvement with an efficient method for successful defect-free weld. The useful results also provide prerequisite for optimization of welding conditions and solidification cracking resistance together.

4. Conclusions
The welding conditions, such as laser power, welding speed and welding configuration, solidification conditions, such as temperature gradient and dendrite growth velocity, and kinetic driving forces, such as aluminum redistribution, supersaturation and undercooling of dendrite tip are closely correlated through numerical analysis during nonuniform solidification of ternary Ni-Cr-Al single-crystal superalloy, and is therefore indispensable towards appropriate solidification conditions optimization to minimize microstructure degradation through solidification behavior amelioration in the fusion zone. Besides, beneficial results are subsequently concluded.

- The aluminum redistribution, supersaturation and undercooling of dendrite tip ahead of solidification interface are strongly dependent on crystallographic orientation of dendrite growth instead of heat input.
- When compared with (001)/[110] welding configuration, overall crystallography-dependent aluminum redistribution, supersaturation and undercooling of dendrite tip in (001)/[100] welding configuration is significantly smaller to efficiently mitigate metallurgical factors for stray grain formation.
- The larger heat input is chosen, the severer overall area-weighted aluminum redistribution, supersaturation and undercooling of dendrite tip ahead of solidification interface are monotonically imposed and vice versa.
- Under nonequilibrium solidification conditions, high heat input, either higher laser power or slower welding speed, is kinetically detrimental to columnar/equiaxed transition, while viable low heat input, either lower laser power or faster welding speed, is potentially beneficial to microstructure development and weldability improvement, and promotes epitaxial growth of single-crystal superalloy properties.

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