Numerical Analysis of Microstructure Development during Laser Welding Nickel-based Single-crystal Superalloy 
Part III: Nonequilibrium Solidification Behavior

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Abstract. The thermal-metallurgical modeling of primary $\gamma$ gamma phase nonequilibrium solidification behavior during laser welding nickel-based single-crystal superalloy is further developed through coupling of heat transfer model, multicomponent dendrite growth model and nonequilibrium solidification model to evaluate solidification cracking susceptibility and advance the understanding of the material weldability. The useful relationship among welding conditions (laser power, welding speed and welding configuration), weld pool geometry, dendrite selection, dendrite growth, solidification temperature range, solidification cracking susceptibility and weldability are established for welding conditions optimization and microstructure control. It is indicated that for (001) and [100] welding configuration, solidification cracking susceptibility along the solid/liquid interface is symmetrically distributed about the weld pool centerline. It is crystallographically favorable for mitigation of solidification cracking with bimodal distribution of solidification temperature range. By contrast, for (001) and [110] welding configuration, solidification cracking susceptibility is asymmetrically distributed. The solidification cracking susceptibility of the unfavorable [100] dendrite growth region on the right side of the weld pool is higher than that of [010] dendrite growth region on the left side due to the enlargement of solidification temperature range. The mechanism of asymmetrical crystallography-dependent solidification cracking is proposed. Asymmetrical dendrite growth region induces asymmetrical solidification behavior and solidification cracking susceptibility along the solid/liquid interface, although heat transfer is symmetrical. The overall solidification temperature range of (001) and [100] welding configuration is beneficially narrower than that of (001) and [110] welding configuration throughout the weld pool regardless of heat input. The theoretical predictions agree well with the experiment results. In addition, the promising model is also applicable to other single-crystal superalloys with similar metallurgical properties during laser welding or laser cladding.

1. Introduction
Nickel-based single-crystal superalloys with gamma phase $\gamma$ and gamma prime precipitate $\gamma'$ are widely used in many aerospace and energy industries due to superior performance of high-temperature mechanical properties, microstructure stability and corrosion resistance. Optimum rapid solidification conditions of laser welding are potential for single-crystal nature of material to avoid two typical weld defects of columnar/equiaxed transition (CET) and solidification cracking. The successful defect-free welding is still an increasing challenge. Some attractive ongoing researches are introduced as follows.
Weiping et al [1,2] developed a mathematical model for dendrite growth and microstructure development during the three-dimensional melt pool solidification by laser surface melting single-crystal superalloy CMSX-4 to compute dendrite growth of different substrate orientations. Hunziker et al [3,4] developed a model to numerically analyze the weld defects of centerline grain boundary and solidification cracking during tungsten inert gas (TIG) welding nickel-based superalloy IN718. Anderson et al [5,6] developed the mathematical model by coupling of heat transfer and fluid flow model, dendrite growth model and morphology transition model to simulate the influence of welding parameters on solidification condition and stray grain formation during laser, electron beam and gas tungsten arc (GTA) welding single-crystal superalloy CMSX-4. Wang et al [7] evaluated the effect of grain boundary misorientation on hot cracking susceptibility during laser welding single-crystal superalloy MC2. Rappaz et al [8-11] analyzed microstructure development during electron beam welding single-crystal superalloy. Theoretical prediction of dendrite growth is extended from binary to ternary system on the basis of rapid solidification Kurz-Giovanola-Trivedi (KGT) model with marginal stability criterion. Vitek et al [12-17] evaluated the effect of laser welding conditions (laser power, welding speed and crystallographic orientation) on the stray grain formation and solidification cracking susceptibility of single-crystal superalloy Rene N5 and CMSX-4. Moreover, the γ phase microstructure development, nonequilibrium solute partition and phase transformation phenomena were analyzed through kinetic and thermodynamic modeling under rapid solidification conditions during laser welding single-crystal superalloy CMSX-4 and nickel-based superalloy CM247DS. Moat et al [18] analyzed the effect of laser welding conditions on grain size and crystallographic orientation of laser-deposited Waspaloy. Gauermann et al [19] developed epitaxial laser metal forming to repair single-crystal superalloy CMSX-4. Microstructures development, growth morphology and solidification conditions are closely correlated. Wagner et al [20] analyzed the grain selection mechanisms and dendrite morphology of three single-crystal superalloys (CMSX-4, CM186LC, CMSX-10) during directional solidification casting. Yang et al [21] and Bussac et al [22] analyzed the effect of withdrawal velocity and thermal gradient on dendrite growth crystallography, growth kinetics of dendrite tip and stray grain formation to simulate the dendrite growth during single-crystal superalloy directional solidification casting. Gao Zhiguo and Huang et al [23-25] further developed the metallurgical modeling of nonequilibrium solidification behavior during laser welding nickel-based superalloy. Metallurgical modeling of nonequilibrium grain boundary segregation is also proposed by coupling with nonequilibrium solidification of the weld pool. The objective of this work is therefore to numerically evaluate the effect of laser welding conditions (laser power, welding speed and welding configuration) on crystallography-dependent solidification temperature range under nonequilibrium solidification conditions during single-crystal superalloy weld pool solidification to facilitate the understanding how the metallurgical factors contributes to solidification cracking susceptibility.

2. Mathematical model
 Nickel-based single-crystal superalloy CMSX-4 was used with chemical composition of Ni-9Cr-6.5Al-1Ti-6W-6.5Ta-3Re-0.6Mo-0.1Hf (in wt%). A framework of mathematical model is separately provided for evaluation of solidification cracking susceptibility, and solution procedure are briefly introduced as follows.

2.1. Heat transfer model
 The three-dimensional weld pool shape is calculated by the liquidus isotherm distribution of Rosenthal thick plate solution. The weld pool is subdivided into 12 discrete sections of equal length along the weld pool from the maximum width of the weld pool section 1 (the location where solidification begins) to the end of the weld pool section 12 (the location where solidification terminates).

2.2. Dendrite growth selection model
 The relationship between the dendrite tip growth velocity $V_{\text{hkl}}$ along active crystallographic orientation [hk0] (one of the preferential <100> growth orientations) and the welding speed $V_{\text{w}}$ is derived on the basis of minimum growth velocity or minimum undercooling criterion.
\[ V_{hl} = V_b \frac{\cos \theta}{\cos \psi_{hl}} \]  

(1)

where \( \psi_{hl} \) is the misorientation angle between the solid/liquid interface normal and active [hkl] dendrite growth orientation. \( \phi \) is the angle between the Y-axis and the projection of normal on the Y-Z plane (0≤\( \phi \)≤180º). \( \theta \) is the angle between solid/liquid interface normal and the welding direction (0≤\( \theta \)≤90º).

The crystallography-dependent solidification conditions of temperature gradient \( G_{hl} \) and dendrite growth velocity \( V_{hl} \) are subsequently calculated. Three temperature gradient components \( G_x, G_y \) and \( G_z \) along the solid/liquid interface are mathematically derived by the weld pool geometry.

\[ G_d = \sqrt{G_x^2 + G_y^2 + G_z^2} \]  

(2)

The temperature gradient along the active dendrite growth orientation \( G_{hl} \) is thereby calculated by

\[ G_{hl} = \frac{G_d}{\cos \psi_{hl}} \]  

(3)

2.3. Multicomponent dendrite growth model

Dendrite growth is essentially controlled by the diffusion of Cr and Al in Ni. Constraint dendrite growth kinetics under rapid solidification conditions is derived by Kurz-Giovanola-Trivedi (KGT) model within marginal stability criterion in Ni-Cr-Al ternary system and implicitly solved through numerical iteration at each location with crystallography consideration.

\[ \frac{4\pi^2 \Gamma}{R^3} + 2 \sum_{i=1}^2 \frac{P_{ei} m_i C_{o,i} (1-k_i) \xi_i (P_{ei})}{[1-(1-k_i) \xi_i (P_{ei})]} + G_{hl} = 0 \]  

(4)

where \( \Gamma \) is the Gibbs-Thomson coefficient, \( R \) is the dendrite tip radius, \( P_{ei} \) is the Peclet number for i, \( m_i \) is the liquidus slope, \( C_{o,i} \) is the initial concentration, \( k_i \) is the partition coefficient for element i, \( \xi_i(P_{ei}) \) is the function of Peclet number, \( G_{hl} \) is the average thermal gradient near the dendrite tip along the preferential crystallographic orientation. The steady-state solution distribution of Cr and Al around a parabolic dendrite tip is given by the Ivantsov solution \( \text{Iv}(P_{ei}) \).

2.4. Nonequilibrium solidification model

The crystallography-dependent solidification temperature range is narrower at high dendrite growth velocity under nonequilibrium solidification conditions in order to satisfy the dendrite growth kinetics. Liquidus and solidus temperatures are suppressed below the equilibrium temperature in case of binary system. The solidification temperature range between nonequilibrium liquidus and solidus temperatures \( \Delta T_q \) (the range between subliquidus and subsolidus) is thermodynamically derived by means of linear Ni-Cr and Ni-Al binary phase diagrams on the nickel-rich sides. The well-defined angular relationships \( \theta, \phi, \psi_{hl} (\alpha, \beta, \gamma) \) of transition boundaries, dendrite growth model, nonequilibrium solidification model are provided in the literature [5,8,9,24,25] for more details. The material properties of single-crystal superalloy CMSX-4 are available in the literature [8,15,26,27].

3. Results and discussion

Effect of laser welding configuration on solidification temperature range along the solid/liquid interface during single-crystal superalloy weld pool solidification is shown in figure 1. Active crystallographic orientation plays a predominant role in solidification behavior and dendrite selection simultaneously. Wide solidification temperature range provides a metallurgical driving force for solidification cracking. Transition boundaries between different dendrite growth regions are delineated. The weld pool shape is approximately elliptical in (a). \( \phi \) is symmetrical about the weld centerline and the weld width decreases from section 1(\( \theta \) close to 90º) to 12 (\( \theta \) close to 0) (0≤\( \phi \)≤180º) in (d). For (001) and [100] welding configuration in (b) and (e), the distribution of solidification temperature range is symmetrical about the weld pool centerline in the section 1-12. Symmetrical dendrite growth crystallography leads to symmetrical distribution of solidification temperature range. The solidification temperature range increases from section 1 to 12. There are four dendrite growth regions.
[100],[010],[001] and [001]. Solidification temperature range in [001] dendrite growth region is narrower. Solidification temperature range in the [100] dendrite growth region is significantly maximum due to equiaxed dendrite formation of morphology instability. Solidification temperature range at the transition boundary is wider.

![Figure 1](image)

Weld pool geometry (a), φ distribution (d), dendrite selection (e), solidification temperature range (b) in the (001) and [100] welding configuration. Dendrite selection (f), solidification temperature range (c) in the (001) and [110] welding configuration.

**Figure 1.** Effect of laser welding configuration on solidification temperature range along the solid/liquid interface during single-crystal superalloy weld pool solidification (laser power 5kW and welding speed 1m/min).

By contrast, for (001) and [110] welding configuration in (c) and (f), the distribution of solidification temperature range is asymmetrical because of asymmetrical dendrite growth crystallography. There are three [100],[010] and [001] dendrite growth regions, and centerline grain boundary is between [010] and [100] dendrite regions. The size of [100] dendrite growth region in (001) and [110] welding configuration is broadened than that of in (001) and [100] welding configuration to detrimentally widens the solidification temperature range. The solidification temperature range in [100] dendrite growth region on the right of weld pool (90º<φ<180º) is larger than that in [010] dendrite growth region on the left side (0<φ<90º). Therefore, there is difference in solidification cracking susceptibility. Although the same heat input exerts in the weld pool, the asymmetrical solidification behavior is induced by different solidification conditions in the both sides of weld pool. These results are consistent with the foregoing results of stray grain formation in part I and dendrite trunk spacing in part II. Solidification temperature range, stray grain formation, dendrite size and centerline grain boundary are four contributing metallurgical factors for solidification cracking susceptibility.
Figure 2. Effect of laser welding configuration on solidification temperature range along the solid/liquid interface during single-crystal superalloy weld pool solidification (laser power 5kW and welding speed 4 m/min)

The effect of increasing welding speed on solidification temperature range along solid/liquid interface is shown in figure 2. Crystallography-dependent solidification temperature range and microstructure development depend on weld pool geometry and welding configuration. Temperature gradient and dendrite growth velocity along the solid/liquid interface both increase with high welding speed. For [100] welding direction on (001) substrate orientation, the size of [100] dendrite growth region on the top surface center of weld pool is reduced to suppress solidification temperature range, and the distribution of solidification temperature range becomes narrower. The angle θ sufficiently decreases with steep solidification interface at the rear of the weld pool because of weld pool shape elongation to stabilize the [010]/[100], [001]/[100] and [010]/[100] dendrite transition boundaries. [001] dendrite growth region is larger than other regions. By contrast, for [110] welding direction on (001) substrate orientation, the size of vulnerable [100] dendrite growth region in the right side of weld pool (90º<φ<180º) is beneficially reduced. [001] dendrite growth region outgrows and almost extends to the top surface. The discrepancy of crystallography-dependent dendrite growth results in nonuniform solidification behavior. Therefore, the two typical weld defects of solidification cracking and centerline grain boundary are reduced to improve weldability through the amelioration of solidification behavior. Solidification temperature range alone solid/liquid interface increases with misorientation of dendrite growth. The higher welding speed of low heat input is used, and the narrower solidification temperature range occurs. (001) and [100] welding configuration is less...
susceptible to solidification cracking than that of (001) and [110] welding configuration due to narrow solidification temperature range.

Weld pool geometry (a), $\phi$ distribution (d), dendrite selection (e), solidification temperature range (b) in the (001) and [100] welding configuration. Dendrite selection (f), solidification temperature range (c) in the (001) and [110] welding configuration.

**Figure 3.** Effect of laser welding configuration on solidification temperature range along the solid/liquid interface during single-crystal superalloy weld pool solidification (laser power 2kW and welding speed 1m/min)

The effect of decreasing laser power on solidification temperature range is shown in figure 3. For [100] welding direction on (001) substrate orientation, the size of [100] dendrite growth region decreases with low laser power. Low laser power increases the steep temperature gradient and decreases the dendrite velocity growth along the solid/liquid interface throughout the weld pool to avoid morphology transition. Moreover, as solidification approaches the centerline ($0^\circ$ from $90^\circ$ at the fusion boundary to 0 at the weld pool centerline), the maximum solidification temperature range near the top surface center is reduced with low laser power. By contrast, for [110] welding direction on (001) substrate orientation, crystallography-dependent solidification behavior induces the discrepancies of solidification temperature range in both sides of weld pool, and thereby low laser power tends to reduce the vulnerable region of [100] dendrite growth. Two type of quite different solidification behavior on the left and right sides of weld pool coexist from the beginning of solidification (section 1) to the end of solidification (section 12). Low heat input (low laser power and low welding speed) favors narrow solidification temperature range because of less morphology transition to reduce the metallurgical driving force for solidification cracking and control weld pool solidification and microstructure development. Although low laser power further improves the weldability, laser power cannot be sufficiently decreased because of incomplete melting. It is necessary for sufficient laser power to melt the substrate and satisfy weld penetration requirement and epitaxial dendrite growth.
Weld pool geometry (a), $\phi$ distribution (d), dendrite selection (e), solidification temperature range(b) in the (001) and [100] welding configuration. Dendrite selection (f), solidification temperature range(c) in the (001) and [110] welding configuration.

**Figure 4.** Effect of laser welding configuration on solidification temperature range along the solid/liquid interface during single-crystal superalloy weld pool solidification (laser power 2kW and welding speed 4 m/min).

The effect of increasing welding speed on solidification temperature range at low laser power is shown in figure 4. The shallow and elliptical weld pool shape is less susceptible to solidification cracking. For [100] welding direction on (001) substrate orientation, the size of unfavorable [100] dendrite growth region is significantly reduced and less dendrite morphology transition takes place to mitigate the metallurgical driving force for solidification cracking. The solidification temperature ranges along the solid/liquid interface throughout the weld pool are suppressed. Optimum low heat input (low laser power and high welding speed) facilitates single-crystal nature of solidification conditions that promotes the morphology stability in the weld pool to completely prevent solidification cracking. It is imperative to ameliorate solidification behavior within narrow solidification temperature range to prompt faster solidification. By contrast, for [110] welding direction on (001) substrate orientation, the stray grain formation, centerline grain boundary formation and solidification cracking susceptibility are simultaneously reduced with high welding speed, once [100] dendrite growth region is diminished. Low heat input is useful to minimize solidification cracking and improve the weldability. It clearly elucidates why asymmetrical solidification cracking occurs at the right side of weld pool due to misorientation of morphology transition, and how optimum weld conditions minimize the solidification cracking susceptibility at the expense of shallow weld pool shape. The theoretical predictions of dendrite selection and growth on (001) substrate orientation along either [100] or [110] welding direction are verified by the experiment results [1,2,5]. Moreover, asymmetrical solidification cracking susceptibility agree well with the experimental results in (001) and [110] welding configuration [14,28,29]. Theoretical analysis provides unprecedent insight into the
nonequilibrium solidification behavior and dendrite growth crystallography. There is an impetus to suppress the metallurgical driving force of the final stage of solidification at the rear of the weld pool through welding conditions optimization for successful crack-free weld.

4. Conclusions

The mathematical model is further developed for multicomponent single-crystal superalloy weld pool solidification to evaluate solidification cracking susceptibility over a wide range of solidification conditions during laser welding nickel-based single-crystal superalloy. Welding conditions (laser power, welding speed and welding configuration), weld pool geometry, dendrite selection, morphology transition, solidification behavior and solidification cracking susceptibility are closely correlated. The following useful conclusions can be drawn from this work.

- Symmetrical distribution of dendrite growth regions about the weld pool centerline leads to symmetrical distribution of solidification temperature range and solidification cracking susceptibility along the solid/liquid interface in (001) and [100] welding configuration, while asymmetrical dendrite growth region results in asymmetrical distribution of solidification temperature range and solidification cracking susceptibility along the solid/liquid interface in (001) and [110] welding configuration.
- The two typical weld defects of centerline grain boundary formation and solidification cracking are prevented because of narrow solidification temperature range in (001) and [100] welding configuration with appropriate low heat input that provides the potential advantage of single-crystal nature of the material.
- Asymmetrical solidification cracking predominantly occurs in [100] dendrite growth region in the (001) and [110] welding configuration because of anomalous nonuniform solidification of the weld pool.
- The overall solidification temperature range along the solid/liquid interface in (001) and [100] welding configuration is beneficially narrower than that of (001) and [110] welding configuration, and therefore suppresses the [100] dendrite growth region in favor of [001] dendrite growth region.

5. References

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Acknowledgement
The project was financially supported by the Anyang Institute of Technology (Grant No. BSJ2019031).