Numerical Analysis of Microstructure Development during Laser Welding Nickel-based Single-crystal Superalloy
Part IV: Welding Conditions Optimization

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Abstract. The thermal-metallurgical modeling of columnar/equiaxed transition(CET), multicomponent dendrite growth and nonequilibrium solidification behavior was further developed during single-crystal superalloy weld pool solidification over a wide range of laser welding conditions (laser power, welding speed and welding configuration). It facilitates the unprecedented understanding of the effect of welding conditions on overall stray grain formation, dendrite trunk spacing and solidification temperature range throughout the weld pool. In order to eliminate the solidification cracking through microstructure control, it is imperative to optimize the welding conditions for successful defect-free laser welding. Crystallographic orientation of dendrite growth plays an important role than heat input in microstructure development and solidification cracking susceptibility. Optimum low heat inputs (low laser power and high welding speed) of solidification condition simultaneously prevent stray grain formation, refine dendrite size and mitigate the solidification temperature range to improve the weldability and weld integrity and vice versa. Nonequilibrium solidification behavior of the weld pool suppresses the solidification temperature range and dendrite size, and improves the solidification cracking resistance. The overall stray grain formation, dendrite trunk spacing and solidification temperature range in (001) and [100] welding configuration are beneficially reduced than that of in (001) and [110] welding configuration regardless of heat input. The theoretical predictions agree well with the experiment results. Moreover, this promising model is also available to other single-crystal superalloys with similar metallurgical properties during laser welding or laser cladding.

1. Introduction
γ’ and γ’’ precipitation-strengthened nickel-based single-crystal superalloys are widely used in the aerospace and energy industries for superior mechanical properties, corrosion resistance and microstructure stability at high temperatures. Although laser welding possesses potential advantages over other conventional welding technology, the challenge for successful defect-free welding is weldability issue. Some ongoing research about the microstructure development and solidification behavior during single-crystal superalloys solidification is briefly introduced as follows. Weiping et al.[1,2] developed a mathematical modeling to analyze the effect of substrate crystallographic orientation and melt-pool geometry on dendrite growth and microstructure development during laser surface melting nickel-based single-crystal superalloy CMSX-4. Hunziker et al.[3,4] numerically
analyzed the weld defects of centerline grain boundary formation and solidification cracking by coupling of heat transfer model and multicomponent dendrite growth model during tungsten inert gas (TIG) welding nickel-based superalloy IN 718. Anderson et al.[5,6] evaluated the effect of welding parameters on solidification condition and stray grain formation through heat transfer and fluid flow simulation during gas tungsten arc (GTA), laser and electron beam welding single-crystal superalloy CMSX-4. Rappaz et al.[7-9] numerically analyzed the effect of crystallographic orientation on solidification behavior and dendrite growth under rapid solidification conditions in the Fe-Ni-Cr ternary system during electron beam welding single-crystal superalloy in either [100] or [110] welding direction on (001) substrate orientation. Moreover, a new modeling of heterogeneous nucleation and dendrite growth during solidification was proposed. Vitek et al.[10-12] numerically analyzed the effect of welding conditions(laser welding, laser power and crystallographic orientation of dendrite growth) on the stray grain formation during laser welding nickel-based single-crystal superalloy Rene N5. Moreover, the primary γ phase microstructure development of nickel-based superalloy CM247DS under rapid solidification conditions was analyzed. Wang et al.[13] analyzed the effect of grain boundary misorientation on solidification cracking susceptibility in single- and bi-crystals. Moat et al.[14] analyzed the effect of laser pulse length and duty cycle on the grain morphology and crystallographic orientation during laser deposition Waspaloy powder. Gaumann et al. [15] developed epitaxial laser metal forming to obtain processing-microstructure map for single-crystal superalloy repair. Wagner et al.[16] analyzed the grain selection mechanism and dendrite morphology of three single-crystal superalloys (CMSX-4, CM186LC and CMSX-10) during directional solidification casting. Yang et al.[17,18] analyzed the effect of thermal gradient and withdrawal velocity on stray grain formation and growth kinetics of dendrite tips to simulate dendrite growth during nickel-based single-crystal superalloys casting. The objective of this work is therefore to numerically predict the effect of laser welding conditions on microstructure development and solidification cracking susceptibility through mathematical modeling during single-crystal superalloy weld pool solidification for optimization of solidification conditions (temperature gradient and dendrite growth velocity) and microstructure control.

2. Mathematical model
Nickel-based single-crystal superalloy CMSX-4 was used with chemical composition of Ni-9Co-6.5Cr-5.6Al-1Ti-6W-6.5Ta-3Re-0.6Mo-0.1Hf (in Wt%).

2.1. Heat transfer model
The three-dimensional weld pool shape is calculated by the liquidus isotherm of Rosenthal thick plate solution under steady-state conditions. The weld pool is subdivided into 12 sections of equal length along the X-axis from the maximum weld pool width (where solidification begins) to the end of the weld pool (where solidification terminates).

2.2. Dendrite selection model
On the basis of minimum velocity or minimum undercooling criterion, the relationship between the dendrite growth velocity \( V_{hkl} \) along the solid/liquid interface and welding speed \( V_b \) is geometrically given by

\[
V_{hkl} = V_b \frac{\cos \theta}{\cos \psi_{hkl}}
\]  

(1)

where \( \theta \) is the angle between the solidification interface normal and welding direction, \( \psi_{hkl} \) is the misorientation angle between the solidification interface normal to the active [hkl] crystallographic orientation of dendrite growth, \( \varphi \) is the angle between the Y-axis and projection of \( n \) on the Y-Z plane. Three components of temperature gradient \( G_x \), \( G_y \) and \( G_z \) near the solid/liquid interface are calculated by the derivative of weld pool geometry. The temperature gradient normal to the solid/liquid interface is therefore determined by

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

The temperature gradient along the dendrite growth orientation is given by
\[ G_{hkl} = \frac{G_{sl}}{\cos \psi_{hkl}} \]  

(2)

2.3. Columnar/equiaxed transition model

On the basis of constitutional undercooling criterion, the stray grain formation ahead of solidification front is given by

\[ \frac{G_{hkl}^n}{V_{hkl}} = a \left\{ \frac{-4 \pi N_0}{3 \ln \left(1 - \phi \right) n + 1} \right\}^n \]  

(3)

where \( a \) and \( n \) are material-dependent constants, \( N_0 \) is the nuclei density and \( \phi \) is the fraction of stray grain (\( \phi \geq 0.5 \) for full equiaxed dendrite, \( \phi \leq 0.0006 \) for full columnar dendrite).

Overall area-weighted average stray grain formation \( \phi \) is calculated by

\[ \phi = \frac{\sum_{k=1}^{12} A_k \bar{\phi}_k}{\sum_{k=1}^{12} A_k} \]  

(4)

where \( k \) is cross section 1-12 throughout the weld pool, \( A_k \) and \( \bar{\phi}_k \) are the solid/liquid interface area and average \( \phi \) for each cross section. The area-weighted average dendrite trunk spacing \( \bar{\lambda}_1 \) and solidification temperature range \( \Delta T \) are calculated in the same way with crystallographic orientation consideration.

2.4. Multicomponent dendrite growth model

The primary \( \gamma \) phase dendrite growth is controlled by the diffusion of Cr and Al in Ni for ternary Ni-Cr-Al superalloy. Multicomponent dendrite growth of Kurz-Giovanola-Trivedi (KGT) model is derived by the marginal stability of planar front criterion under rapid solidification conditions.

\[ \frac{4 \pi^2 \Gamma}{R^2} + \frac{2 \sum_{i=1}^2 \frac{P_{ei} m_i C_{0i} (1 - k_i)}{1 - (1 - k_i) Iv(P_{ei})}}{1 - k_i} \xi_i(P_{ei}) \bar{G}_{hkl} = 0 \]  

(5)

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, \( C_{0i} \) is the initial concentration of \( i \), \( k_i \) is the partition coefficient for \( i \) (Cr or Al), \( \xi_i(P_{ei}) \) is function of the Peclet number, \( Iv(P_{ei}) \) is Ivantsov solution, \( \bar{G}_{hkl} \) is the average thermal gradient near the dendrite tip.

2.5. Nonequilibrium solidification model

Nonequilibrium solidification behavior is derived through the linear Ni-Cr and Ni-Al binary phase diagrams on the nickel-rich side in order to satisfy the growth kinetics of dendrite tip within the range of dendrite stability. The solidification temperature range is calculated between subliquidus and subsolidus temperatures. The angular relationship \( (\theta, \phi, \psi_{hkl}) \), \( G_{hkl}, V_{hkl} \), dendrite growth model and columnar/equiaxed transition model are provided in the literature [5-8,10] for more details. The material properties in the calculation are available in the literature [7,10,19,20].

3. Results and discussion
Figure 1. The effect of welding conditions (laser power, welding speed and welding configuration) on the area-weighted average stray grain formation.

The effect of welding conditions (laser power, welding speed and welding configuration) on the area-weighted average stray grain formation is shown in figure 1. For the (001) and [100] welding
configuration in (a), the relationship between laser welding conditions and microstructure development is established. High heat input (high laser power and low welding speed) monotonically increases overall stray grain formation and worsens columnar/equiaxed morphology transition, while low heat input (low laser power and high welding speed) beneficially minimizes stray grain formation to maintain single-crystal nature of the material. The columnar/equiaxed transition occurs in the weld domain \(0.0183 < \phi < 0.0936\), because the magnitude of \(\phi\) exceeds the threshold 0.0066 over the rear of weld pool solidification interface. By contrast, for the (001) and [110] welding configuration in (b), the detrimental columnar/equiaxed morphology transition occurs \(0.166 < \phi < 0.216\). The complexity of stray grain formation is highly sensitive to welding conditions. Irregular and anomalous distribution is elucidated. Although heat input are equivalent on both sides of weld pool, crystallographic orientation plays an important role in stray grain formation than heat input and stray grains are more severe in (b) than in (a). Therefore, this welding configuration is less resistant to stray grain formation ahead of the columnar front. This distribution is separated into three parts. First part, large heat input (high laser power and low welding speed) increases stray grain formation potential. This trend is similar with that of distribution in (a) and the theoretical predictions agree well with experiment results [6,10,11]. Second part, stray grain formation initially increases and then decreases with further increase in welding speed, when laser power 2kW is constant. Third part, there is other parabolic shape variation toward high laser power, when welding speed 4m/min is constant, thereby indicating a very sensitive dependence of stray grain formation on heat input. (001) and [100] crystallographic orientation and low heat input are the contributing factors for stray grain formation reduction, and will be favored. In order to improve the defect-free microstructure development, it is therefore imperative to optimize the laser welding conditions.

(a)  (001) and [100] welding configuration
The effect of welding conditions (laser power, welding speed and welding configuration) on the area-weighted average dendrite trunk spacing is shown in figure 2. For (001) and [110] welding configuration in (a), the dendrite trunk spacing is finer (7.6μm < λ1 < 24.7μm). The magnitude of dendrite trunk spacing is smaller in (a) than that in (b). Dendrite trunk spacing monotonically decreases with low heat input. The smaller heat input is used, the finer the dendrite trunk spacing is promoted. This result is particularly promising and controllable. High heat input is prohibited because of severe stray grain formation and coarse dendrite growth. The variation of overall dendrite trunk spacing with heat input is consistent with that of stray grain formation with heat input. Low heat input is more resistant to dendrite growth that is less susceptible to solidification cracking. By contrast, for (001) and [110] welding configuration in (b), the dendrite trunk spacing is coarser (16.28μm < λ1 < 44.46μm) as a result of morphology instability due to misorientation. High heat input detrimentally coarsens dendrite trunk spacing and promotes dendrite growth. To alleviate this, low heat input is used to control dendrite size. Welding configuration plays more important role than heat input in overall dendrite trunk spacing to modify the dendrite growth kinetics and crystallographic orientation. The variation of overall dendrite trunk spacing with heat input is different with that of stray grain formation with heat input. Monotonic dependence of dendrite trunk spacing on heat input is clearly elucidated. Negligible stray grain formation and fine dendrite trunk spacing should be satisfied simultaneously through optimum low heat input. Theoretical predictions are in reasonable agreement with the available experiment results under similar growth conditions [16,17,21]. The variations of dendrite trunk spacing with welding conditions are useful for the following microstructure optimization and weldability evaluation that are the prerequisite of successful crack-free weld.
Figure 3. The effect of laser welding conditions (laser power, welding speed and welding configuration) on the area-weighted average solidification temperature range.
The effect of laser welding conditions (laser power, welding speed and welding configuration) on the area-weighted average solidification temperature range is shown in figure 3. For (001) and [100] welding configuration in (a), the solidification temperature range is of order $6.52 \leq \Delta T \leq 6.66^\circ C$. The variation of solidification temperature range with heat input is clearly discernible. High heat input detrimentally enlarges the solidification temperature range and deteriorates the weldability, while optimum low heat input beneficially suppresses the solidification temperature range and prevent solidification cracking to maintain the single-crystal nature of the material. It is crystallographically favorable for cracking resistance improvement. By contrast, for on (001) and [110] welding configuration in (b), the solidification temperature range is of order $6.86 \leq \Delta T \leq 6.98^\circ C$. Solidification temperature range monotonically increases with high heat input, and high heat input is the worst welding condition for solidification cracking susceptibility. The solidification temperature range is more sensitive to welding configuration than heat input. The overall solidification temperature range in (b) is wider than that in (a). The solidification cracking susceptibility on the right side of the weld is higher enough than that of left side for onset of solidification cracking. Anomalous severe solidification cracking along stray grain boundaries frequently occurs on the right side of weld ([100] dendrite growth region) with centerline grain boundary formation, while no cracking on the left side [11,22,23]. The theoretical predictions agree well with the experimental results with reasonable accuracy and reliability. Proper welding configuration thus provides another promising way for minimizing solidification cracking by alternative solidification behavior. Strict control of the heat input with flexible welding conditions considerably decreases the solidification cracking susceptibility. Low heat input of (001) and [100] welding configuration is feasible for solidification cracking reduction and microstructure control. Therefore, pragmatic heat input and welding configuration are two controlling factors to alleviate the solidification cracking, and the weldability is improved by means of the appropriate combination of low heat input with (001) and [100] welding configuration instead of the combination of high heat input with (001) and [110] welding configuration. Finally, theoretical analysis facilitates the understanding of crystallography-dependent solidification cracking phenomenon during single-crystal weld pool solidification, and thereby provide unprecedent insight into the nonequilibrium solidification behavior and 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 laser welding conditions optimization for successful crack-free weld.

4. Conclusions

The multicomponent microstructure development and nonequilibrium solidification behavior of single-crystal superalloy weld pool during laser welding are numerically analyzed by mathematical modeling for evaluation of solidification cracking susceptibility over a wide range of welding conditions with reasonable accuracy. Some useful conclusions can be drawn from this work.

- For (001) and [100] welding configuration, the stray grain formation, dendrite trunk spacing and solidification temperature range are monotonically minimized by low heat input (low laser power and high welding speed) to ameliorate weldability and avoid weld defects, while high heat input(high laser power and low welding speed) worsen the solidification cracking susceptibility.

- For (001) and [100] welding configuration, the variation of stray grain formation, dendrite trunk spacing and solidification temperature range with heat input are consistent with each other.

- For (001) and [110] welding configuration, optimum low heat input simultaneously mitigates the stray grain formation, dendrite trunk spacing and solidification temperature range, while high heat input deteriorates weldability and weld integrity. Particularly, severe stray grain formation, coarser dendrite size and wider solidification temperature range are highly detrimental than that of (001) and [100] welding configuration to increase the solidification cracking susceptibility.

- The distribution of stray grain formation is significantly parabolic at low laser power or high welding speed for (001) and [110] welding configuration.
• The welding configuration plays an important role in overall stray grain formation, dendrite growth and solidification behavior because of preferential crystallographic orientation. Nonequilibrium solidification suppresses solidification temperature range and refines the dendrite size.

References
[1] Weiping Liu and J N Dupont 2004 Effects of melt-pool geometry on crystal growth and microstructure development in laser surface-melted superalloy single crystals. Mathematical modeling of single-crystal growth in a melt pool (Part I) Acta Mater. 52 4847-33
[2] Weiping Liu and J N Dupont 2005 Effects of substrate crystallographic orientations on crystal growth and microstructure development in laser surface-melted superalloy single crystals. Mathematical modeling of single-crystal growth in a melt pool (Part II) Acta Mater. 53 1545-58
[3] D Dye, O Hunziker and R C Reed 2001 Numerical analysis of the weldability of superalloys Acta Mater. 49 683-697s
[4] O Hunziker, D Dye and R C Reed 2000 On the formation of a centerline grain boundary during fusion welding Acta Mater. 48 4191-4201
[5] T D Anderson, J N Dupont and T Debroy 2010 Origin of stray grain formation in single-crystal superalloy weld pools from heat transfer and fluid flow modeling Acta Mater. 58 1441-54
[6] T D Anderson, J N Dupont and T Debroy 2010 Stray grain formation in welds of single-crystal Ni-based superalloy CMSX-4 Metall. Mater. Trans. A 41 181-193
[7] M Rappaz, S A David, J M Vitek and L A Boatner 1990 Analysis of solidification in Fe-Ni-Cr single-crystal welds Metall. Trans. A 21 1767-82
[8] M Rappaz, S A David, J M Vitek and L A Boatner 1989 Development of microstructures in Fe-15Ni-15Cr single-crystal electron beam welds Metall.Trans. A 20 1125-11
[9] M Rappaz and Ch A Gandin 1993 Probabilistic modeling of microstructure formation in solidification processes Acta Metall.Mater. 41(2) 345-360
[10] J M Vitek 2005 The effect of welding conditions on stray grain formation in single crystal welds-theoretical analysis Acta Mater. 53 53-67
[11] J W Park, S S Babu, J M Vitek, E A Kenik and S A David 2003 Stray grain formation in single crystal Ni-based superalloy welds J. Appl. Phys. 94 (6) 4203-09
[12] S S Babu, M K Miller, J M Vitek and S A David 2001 Characterization of the microstructure evolution in a nickel-based superalloy during continuous cooling conditions Acta Mater.49 4149-60
[13] N Wang, S Mokadem, M Rappaz and W Kurz 2004 Solidification cracking of superalloy single- and bi- crystals Acta Mater. 52 3173-82
[14] R J Moat, A J Pinkerton, L Li, P J Withers and M Preuss 2009 Crystallographic texture and microstructure of pulsed diode laser-deposited Waspaloy Acta Mater. 57 1220-29
[15] M Gaumann, C Bezencon, P Canalis and W Kurz 2001 Single-crystal laser deposition of superalloys: processing-microstructure maps Acta Mater. 49 1051-62
[16] A Wagner, B A Shollock and M Mclean 2004 Grain structure development in directional solidification of nickel-based superalloys Mater. Sci. Eng. A 374 270-279
[17] X L Yang, H B Dong, W Wang and P D Lee 2004 Microscale simulation of stray grain formation in investment cast turbine blades Mater. Sci. Eng. A 386 129-139
[18] A De Bussac and Ch A Gandin 1997 Prediction of a process window for the investment casting of dendrite single crystals Mater. Sci. Eng. A 237 35-42
[19] Edward H Kottcamp 1993 ASM Handbook Volume 3: Alloy phase diagrams (USA: ASM International) pp 49-155
[20] Wu Qiong, Li Shusuo, Ma Yue and Gong Shengkai 2012 First principles calculations of alloying element diffusion coefficient in Ni using the five-frequency model Chin.Phys.B 21(10) 1091021-1-7
[21] Zhang Weigu, Liu Lin, Huang Taiwen and Zhao Xinbo 2009 Influence of directional solidification variables on primary dendrite arm spacing of Ni-based superalloy DZ125
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[22] J M Vitek, S S Babu, J W Park and S A David 2004 Analysis of stray grain formation in single-crystal nickel-based superalloy welds Proceedings of the International Symposium on Superalloys pp 459-465

[23] J M Vitek, S A David and S S Babu 2007 Optimization of weld conditions and alloy composition for welding single-crystal nickel-based superalloys Mater. Sci. Forum 539-543 3082-87