Numerical Analysis of Stray Grain Formation during Laser Welding Nickel-based Single-crystal Superalloy Part I: Columnar/Equiaxed Morphology Transition

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Abstract. The thermo-metallurgical modeling of stray grain formation was further developed by couple of heat transfer model, dendrite selection model, multicomponent dendrite growth model, nonequilibrium solidification model and minimum undercooling model during three-dimensional nickel-based single-crystal superalloy weld pool nonequilibrium solidification over a wide range of welding conditions (laser power, welding speed and welding configuration). Welding configuration simultaneously influences distributions of stray grain formation and columnar/equiaxed transition (CET). The stray grain formation and dendrite morphology ahead of solid/liquid interface are symmetrically distributed about the weld pool centerline in the (001)/[100] welding configuration. The stray grain formation and dendrite morphology ahead of solid/liquid interface is asymmetrically distributed in the (001)/[110] welding configuration. Vulnerable [100] dendrite growth region is suppressed in favor of epitaxial [001] dendrite growth region to predominantly facilitate single-crystal dendrite growth with further reduction of heat input. Stray grain formation and solidification cracking are preferentially confined to [100] dendrite growth region. The smaller heat input is used, the less nucleation and growth of stray grain formation with decreasing constitutional undercooling ahead of solid/liquid interface is incurred with mitigation of metallurgical driving forces for solidification cracking and columnar dendrite morphology is increased and vice versa. Symmetrical crystallographic orientation of dendrite growth spontaneously ameliorates microstructure development, and improves resistance to solidification cracking. The mechanism of asymmetrical solidification cracking because of crystallography-dependent stray grain formation and morphology instability is therefore proposed. Optimum low heat input (low laser power and high welding speed) with (001)/[100] welding configuration essentially minimizes both stray grain formation and columnar/equiaxed morphology transition and is beneficial to weldability and weld integrity through morphology control, while undesirable high heat input (high laser power and slow welding speed) with (001)/[110] welding configuration leads to microstructure anomalies and worsens solidification cracking susceptibility. The stray grain formation and morphology transition in the [100] dendrite growth region on the right side of the weld pool are more severe than that in the [010] dendrite growth region on the left side, although the same heat input imposes on both sides of the weld pool in the (001)/[110] welding configuration. The theoretical predictions agree well with the experiment results. Moreover, the promising and reliable model is also applicable to other single-crystal superalloys with similar metallurgical properties for successful crack-free laser welding or laser cladding.
1. Introduction

γ’ and γ’ precipitation-strengthened nickel-based single-crystal superalloys are widely used in the aerospace, energy and automotive industries due to excellent high-temperature mechanical properties, corrosion resistance and microstructure stability. Stray grain formation, columnar/equiaxed transition and solidification cracking are serious weldability issues during laser welding or repair. It is difficult to maintain single-crystal nature of the material for successful defect-free laser welding. Some ongoing research about elimination of stray grain formation and columnar/equiaxed morphology transition during nonequilibrium solidification are briefly introduced as follows. Weiping et al.[1,2] analyzed the effect of melt-pool geometry and substrate orientation on crystallographic orientation of dendrite growth, stray grain formation and microstructure development during three-dimensional melt-pool solidification by laser surface melting nickel-based single-crystal superalloy CMSX-4 through mathematical modeling and experiments. Wang et al.[3,4] analyzed the effect of substrate orientation on columnar/equiaxed transition and stray grain formation by mathematical modeling and experiment during laser repair nickel-based single-crystal superalloy DD6. Anderson et al.[5,6] analyzed the influence of welding parameters, substrate orientation and welding process type on solidification conditions (temperature gradient and dendrite growth velocity) and nucleation and growth of stray grain formation along preferential <100> crystallographic orientations to minimize columnar/equiaxed morphology transition and microstructure anomalies through heat transfer and fluid flow modeling simulation during laser, gas tungsten arc (GTA) and electron beam welding nickel-based single-crystal superalloy CMSX-4. Rappaz et al.[7-10] evaluated the effect of growth crystallography and weld pool shape on microstructure development and solidification behavior on the basis of minimum velocity or minimum undercooling criterion during electron beam welding Fe-15Ni-15Cr ternary single-crystal superalloy along either [100] or [110] welding direction on (001) substrate orientation. Furthermore, the effect of cellular/dendrite microstructure and grain boundary misorientation on solidification cracking susceptibility was analyzed during laser welding nickel-based single-crystal superalloy MC2. Microstructure development modeling during solidification with consideration of the mechanisms of heterogeneous nucleation and dendrite growth (columnar/equiaxed transition, dendrite selection and equiaxed dendrite impingement) was proposed. Vitek et al.[11,12] numerically analyzed the effect of growth crystallography and weld pool shape on microstructure development and solidification behavior on the basis of constitutional undercooling ahead of solid/liquid interface to minimize microstructure degradation during laser welding nickel-based single-crystal superalloy Rene N5. Ojo et al.[13,14] analyzed the effect of minor elements on columnar/equiaxed transition and stray grain formation through modification of primary solidification path during laser welding nickel-based single-crystal superalloys IC6, CMSX-4 and CMSX-486. Gaumann et al., Basak et al. and Ranadip et al.[15-17] optimized laser deposition processing to avoid columnar/equiaxed transition and epitaxially repair nickel-based single-crystal superalloy CMSX-4 on the basis of the processing-microstructure map. Jianwen et al. and Zhaoyang et al.[18,19] numerically analyzed the effect of substrate orientation on dendrite growth and columnar/equiaxed transition to promote epitaxial growth of nickel-based single-crystal superalloy Rene N5 during laser deposition. Vilar et al. [20] analyzed the effect of processing parameters on columnar/equiaxed transition of nickel-based single-crystal superalloy SRR99 during laser cladding. Ramsperger et al.[21] analyzed the effect of processing parameters on stray grain formation and solidification cracking susceptibility during selective electron beam melting nickel-based single-crystal superalloy CMSX-4. Yang et al., Wagner et al. and Grodzki et al. [22-24] analyzed the effect of solute profile and dendrite tip undercooling on columnar/equiaxed morphology transition and stray grain formation during nickel-based single-crystal superalloy directional solidification casting. The goal of this work is therefore to elucidate the effect of welding conditions on stray grain formation and morphology transition to eliminate microstructure anomalies during laser welding.

2. Mathematical model
2.1. Heat transfer model
The three-dimensional weld pool shape of liquidus temperature distribution is acquired by the Rosenthal thick plate solution of moving heat source under steady-state conditions. The weld pool was subdivided into 12 sections of equal length along the X-axis from the maximum weld pool width (where solidification begins) to the end of weld pool centerline (where solidification terminates).

2.2. Dendrite selection model
For FCC nickel, dendrite grows along the six preferential <100> crystallographic orientations. On the basis of minimum growth velocity or minimum undercooling criterion, the relationship between the growth velocity $V_{hkl}$ of dendrite tip along [hkl] crystallographic orientation and welding speed $V_b$ is geometrically derived by

$$V_{hkl} = V_b \frac{\cos \theta}{\cos \psi_{hkl}}$$

where $\theta$ is the angle between solidification interface normal $\hat{n}$ and welding direction. $\psi_{hkl}$ is the misorientation angle between solidification interface normal $\hat{n}$ and the active [hkl] crystallographic orientation. $\phi$ is the angle between the Y-axis and the projection of $\hat{n}$ on the Y-Z plane.

The three components of temperature gradient $G_x$, $G_y$, and $G_z$ along the solid/liquid interface are calculated by derivative of weld pool geometry. The temperature gradient normal to the solid/liquid interface is then calculated by

$$G_n = \sqrt{G_x^2 + G_y^2 + G_z^2}.$$ 

The temperature gradient along the crystallographic orientation of dendrite growth $G_{hkl}$ is subsequently determined by

$$G_{hkl} = \frac{G_n}{\cos \psi_{hkl}}$$

2.3. Columnar/equiaxed transition model
On the basis of constitutional undercooling criterion, the stray grain formation ahead of solidification interface is derived by

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

where $a$ and $n$ are material-dependent constant, $N_0$ is the nuclei density in the liquid and $\phi$ is stray grain fraction ($0.5 \leq \phi \leq 1$ for full equiaxed dendrite growth, $\phi \leq 0.0066$ for full columnar dendrite growth).

2.4. Multicomponent dendrite growth model
The dendrite growth is primarily controlled by the diffusion of Cr and Al in Ni for Ni-Cr-Al ternary single-crystal superalloy. On the basis of marginal stability of planar front criterion, the multicomponent dendrite growth is derived by Kurz-Giovanola-Trivedi (KGT) model under rapid solidification conditions.

$$\frac{4\pi^2 \Gamma}{R^2} + 2 \sum_{i=1}^{2} \frac{P_{ei}m_i C_{0,i} (1-k_i) \zeta_c(P_{ei})}{[1-(1-k_i) I_v(P_{ei})]} + G_{hkl} = 0$$

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, $C_{0,i}$ is the initial concentration for i, $k_i$ is the partition coefficient for i, $\zeta_c(P_{ei})$ is a function of the Peclet number, $I_v(P_{ei})$ is the Ivantsov solution ($i=\text{Cr or Al}$) and $G_{hkl}$ is the average temperature gradient near the dendrite tip.
The more information about dendrite selection, morphology transition, multicomponent dendrite growth, nonequilibrium solidification behavior and dendrite tip undercooling are provided in the literature [6-8,25,26]. 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%). The material properties in the calculation are available in the literature [8,11,27,28].

3. Results and discussion

The effect of welding configuration on the dendrite selection and stray grain formation during three-dimensional single-crystal superalloy weld pool nonequilibrium solidification is shown in Figure 1. For [100] welding direction on (001) substrate orientation, \( \phi \) significantly varies with weld pool shape. There are four [010],[001],[100] and [010] dendrite growth regions with well-defined transition boundaries. Epitaxial [001] dendrite growth region is favored in bottom of the weld pool to facilitate single-crystal dendrite growth. Welding configuration simultaneously influences the dendrite selection and stray grain formation. The distribution of stray grain formation ahead of solid/liquid interface is crystallographically symmetrical about the weld pool centerline. The symmetrical crystallographic orientation leads to symmetrical dendrite growth and morphology development. Columnar/equiaxed transition, equiaxed dendrite morphology and misorientation angle predominantly occur on the top surface center part as consequence of solute enrichment, wider solidification temperature range and
constitutional undercooling ahead of solid/liquid interface at the final stage of solidification. These metallurgical factors weaken the resistance to centerline cracking. It is crystallographically favorable for reduction of overall microstructure anomalies and morphology instability to spontaneously decrease both centerline cracking susceptibility and stray grain formation through modification of growth kinetics of dendrite tip, and improve weld quality. By contrast, for [110] welding direction on (001) substrate orientation, there are three [010],[001] and [100] dendrite growth regions. [010] and [100] equiaxed dendrite growth regions impinge each other for centerline grain boundary formation. The distribution of stray grain formation ahead of solid/liquid interface is crystallographically asymmetrical throughout the weld pool. Asymmetrical crystallographic orientation leads to asymmetrical dendrite growth and morphology development. The discrepancy is essentially attributed to different welding configurations. The stray grain formation in [100] dendrite growth region on the right side of the weld pool (0≤0≤90°,90°≤ρ≤180°) is more than that in [010] dendrite growth region on the left side (0≤0≤90°,0≤ρ≤90°), where is more susceptible to solidification cracking, although the same heat input imposes on both sides. In other words, solidification cracking is primarily confined to [100] dendrite growth region. The size of vulnerable [100] dendrite growth region in the (001)/[110] welding configuration is significantly larger than that of (001)/[100] welding configuration to promote nucleation and growth of stray grain formation with unfavorable solidification conditions (low temperature gradient and slow dendrite growth velocity), and increase solidification cracking susceptibility and microstructure degradation. (001)/[110] welding configuration is detrimental to weldability and weld integrity, while (001)/[100] welding configuration is beneficial to weldability and is kinetically capable of mitigation of stray grain formation. Promising optimization of welding configuration is contributing factor for microstructure morphology amelioration of γ phase. High heat input (high laser power and slow welding speed) is the worst conditions. It is imperative to appropriately optimize welding conditions to reduce stray grain formation. The mechanism of asymmetrical solidification cracking because of crystallography-dependent stray grain formation is therefore proposed.

The effect of increasing welding speed on dendrite selection and stray grain formation during three-dimensional single-crystal superalloy weld pool nonequilibrium solidification is shown in figure 2. For [100] welding direction on (001) substrate orientation, the sizes of dendrite growth region, solute diffusion layer and undercooling region are significantly reduced with increasing welding speed. Epitaxial [001] dendrite growth region is favored at the expense of [100] dendrite growth region to predominantly facilitate single-crystal solidification. Three typical morphologies, columnar dendrite, columnar/equiaxed transition and equiaxed dendrite, coexist. Competition between crystallographic orientations of dendrite growth is clearly elucidated. Morphology development of full equiaxed dendrite is controlled by alloying diffusion in the γ phase, when solidification approaches the weld pool centerline. Complete columnar dendrite occurs near the solid/liquid interface of maximum weld pool width for epitaxial growth. The elliptical weld pool is elongated and θ sufficiently decreases to stabilize [010]/[100] and [010]/[100] dendrite growth transition boundaries near the end of the weld pool. The stray grain formation and dendrite growth are decreased. High welding speed is another alternative contributing factor for prevention of nucleation and growth of stray grain formation, morphology instability and misorientation angle with decreasing dendrite tip undercooling, and improves resistance to centerline cracking with favorable solidification conditions (steep temperature gradient and high dendrite growth velocity), while low welding speed contributes to microstructure degradation and weldability deterioration. By contrast, for [110] welding direction on (001) substrate orientation, the size of vulnerable [100] dendrite growth region is decreased. The higher welding speed is used, the smaller stray grain formation, columnar/equiaxed morphology transition and narrower constitutional undercooling ahead of solid/liquid interface are incurred with mitigation of metallurgical driving forces for solidification cracking and vice versa. Less solute buildup near the dendrite tip, narrower solidification temperature range and finer dendrite trunk spacing and dendrite tip curvature along the solid/liquid interface are simultaneously satisfied. Appropriate low heat input (high laser power and high welding speed) is the favorable one for considerable decrease of stray
grain formation and solidification cracking susceptibility to potentially improve weldability under nonequilibrium solidification conditions, while high heat input (high laser power and slow welding speed) worsens microstructure instability. The nonequilibrium nature of solidification is resistant to solidification cracking. The inappropriate microstructure anomalies are attributed to nonuniform solidification behavior and microstructure development with unfavorable crystallographic orientations. Solidification cracking susceptibility is also crystallographically asymmetrical about the weld pool centerline. Consequently, the typical weld defects, centerline grain boundary formation, stray grain formation and solidification cracking, are mitigated with increasing welding speed. The location of severe stray grain formation and solidification cracking depends on interface morphology, solute redistribution, preferential crystallographic orientation and welding configuration. Further optimization of weld pool geometry is indispensable towards amelioration of dendrite morphology and crystallographic orientation.

The effect of decreasing laser power on dendrite selection and stray grain formation during three-dimensional single-crystal superalloy weld pool nonequilibrium solidification is shown in figure 3. For [100] welding direction on (001) substrate orientation, the sizes of weld pool and different dendrite growth regions are reduced. [001] dendrite growth region is favored. The size of epitaxial [001] dendrite growth region is predominantly larger than that of vulnerable [100] dendrite growth region to essentially promote single-crystal nature of the material that are prevented from reaching top surface. Stray grain formation and columnar/equiaxed morphology transition are decreased with solute
depletion and decrease of alloying partition ahead of the solid/liquid interface. Feasible low laser power is another contributing factor for mitigation of metallurgical driving forces for centerline cracking with favorable solidification conditions (steep temperature gradient and slow dendrite growth velocity) and decreasing dendrite tip undercooling ahead of solid/liquid interface, while high laser power contributes to severe stray grain formation and microstructure degradation and is detrimental to weldability. Moreover, low laser power refines dendrite growth and improves resistance to centerline cracking with preferential crystallographic orientation, and is capable of reduction of irregular morphology. The columnar dendrite morphology is increased in the [001] dendrite growth region and equiaxed dendrite morphology is suppressed in the [100] dendrite growth region at the end of weld pool during terminal stage of solidification. Symmetrical microstructure development crystallographically reduces solidification cracking susceptibility. The desirable dendrite growth and morphology are obtained through proper control of three-dimensional weld pool geometry and heat input.

(a) weld pool geometry, (d) φ distribution, (e) dendrite selection and (b) fraction of stray grain in the (001)/[100] welding configuration. (f) dendrite selection and (c) fraction of stray grain in the (001)/[110] welding configuration  (laser power 2kW, welding speed 2m/min)

Figure 3. The effect of decreasing laser power on dendrite selection and stray grain formation during three-dimensional single-crystal superalloy weld pool nonequilibrium solidification.

By contrast, for [110] welding direction on (001) substrate orientation, the size of centerline grain boundary formation is decreased. Vulnerable [100] dendrite growth region is suppressed in favor of epitaxial [001] dendrite growth region. The smaller laser power is used, the less nucleation and growth of stray grain formation is incurred with narrower constitutional undercooling ahead of solid/liquid interface, and lower susceptibility to solidification cracking is imposed and vice versa. Laser power and welding speed are of significant importance for nonequilibrium solute partition and solute
redistribution ahead of solid/liquid interface. Appropriate low heat input (low laser power and slow welding speed) substantially precludes stray grain formation and grain boundary misorientation under nonequilibrium solidification conditions, and improve weld integrity. Elimination of columnar/equiaxed transition particularly necessitates further optimization of microstructure modification and morphology control with thermo-metallurgical factors consideration. Furthermore, although low laser power is beneficial to morphology stability, sufficient laser power is necessary to melt substrate for epitaxial growth. The reasonable relationship between welding conditions (laser power, welding speed and welding configuration) and stray grain formation is established with controlling mechanism of constitutional undercooling to elucidate which factor plays more important role in spontaneous solid/liquid interface morphology development, and provide prerequisite to optimize the morphology stability and crystallographic orientation to alleviate both severe solidification cracking and crystallography-dependent microstructure anomalies. The thorough numerical analysis facilitates the understanding of anomalous microstructure development and solidification cracking phenomena in the fusion zone for successful defect-free laser welding.

![Diagram](image)

**Figure 4.** The effect of weld pool geometry on dendrite selection and stray grain formation during three-dimensional single-crystal superalloy weld pool nonequilibrium solidification.

The effect of weld pool geometry on dendrite selection and stray grain formation during three-dimensional single-crystal superalloy weld pool nonequilibrium solidification is shown in figure 4. For [100] welding direction on (001) substrate orientation, the size of epitaxial [001] dendrite growth region is predominantly increased at the expense of vulnerable [100] dendrite growth region to facilitate single-crystal dendrite growth. The promising result is quite consistent with foregoing
calculation. The stay grain formation, columnar/equiaxed morphology transition, misorientation angle and interface mobility are decreased to spontaneously contribute to microstructure amelioration and improve resistance to solidification cracking. Full columnar dendrite morphology is increased. Elliptical and shallow weld pool geometry is less susceptible to centerline cracking. It is energetically favorable for less solute enrichment ahead of solid/liquid interface to further decrease dendrite tip undercooling and relieve liquid supersaturation. Nonequilibrium partition or partitionless solidification is kinetically favored with mitigation of metallurgical driving forces for stray grain formation. Crystallography-dependent microstructure development is evaluated over a wide range of welding conditions to minimize the morphology instability and solidification cracking susceptibility. Satisfactory optimization of either heat input or welding configuration provides alternative way to avoid stray grain formation, irregular morphology and microstructure anomalies to stabilize solidification path, and improve weldability. By contrast, for [110] welding direction on (001) substrate orientation, [001] dendrite overgrows and extends almost to the top surface. The size of centerline grain boundary formation with equiaxed dendrite morphology is diminished. The nucleation and growth of stray grain formation are reduced by decreasing constitutional undercooling ahead of solid/liquid interface. The overall stray grain formation and columnar/equiaxed transition in the (001)/[110] welding configuration is more severe than that of (001)/[100] welding configuration regardless of heat input, and results in microstructure degradation. Useful low heat input (low laser power and high welding speed) with symmetrical (001)/[100] welding configuration is the most favorable one for minimizing stray grain formation, microstructure and phase instability under nonequilibrium solidification conditions, while high heat input (high laser power and slow welding speed) with asymmetrical (001)/[110] welding configuration is detrimental to dendrite morphology development and solidification cracking susceptibility. The theoretical predictions of dendrite selection and morphology transition along either [100] or [110] welding direction on (001) substrate orientation agree well with the experiment results[1,2]. Moreover, the asymmetrical solidification cracking susceptibility of (001)/[110] welding configuration is also verified by the experiment results[5,12,29,30]. The reliable numerical analysis provides unprecedent insight into the reduction of nucleation and growth of stray grain formation potential for crack-free weld.

4. Conclusions

The welding configuration, heat input, weld pool geometry, dendrite selection, growth crystallography, stray grain formation and morphology transition are closely correlated. The thorough numerical analysis clearly elucidates where is the solidification cracking and how to eliminate stray grain formation and microstructure anomalies, and is indispensable towards optimization of welding conditions to minimize solidification cracking. This work leads to following conclusions.

- Both stray grain formation and columnar/equiaxed morphology transition strongly depend on welding configuration. The distributions of stray grain formation and columnar/equiaxed transition ahead the solid/liquid interface are crystallographically symmetrical about the weld pool centerline in the (001)/[100] welding configuration.
- The distributions of stray grain formation and columnar/equiaxed transition ahead of the solid/liquid interface are crystallographically asymmetrical about the weld pool centerline in the (001)/[110] welding configuration.
- Epitaxial [001] dendrite growth region is favored at the expense of vulnerable [100] dendrite growth region to spontaneously facilitate single-crystal dendrite growth, and avoid nucleation and growth of stray grain formation and morphology instability through proper control of welding configuration.
- Optimum low heat input (low laser power and high welding speed) with (001)/[100] welding configuration considerably ameliorates morphology development with mitigation metallurgical driving forces for solidification cracking, while high heat input (high laser
power and slow welding speed) with (001)[110] welding configuration worsens the solidification cracking susceptibility and potentially contributes to microstructure degradation.

- The stray grain formation in the [100] dendrite growth region on the right side of weld pool is more severe than that in the [010] dendrite growth region on the left side, although the same heat input imposes on both sides in the (001)/[110] welding configuration.

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