Metallurgical modeling of intergranular HAZ liquation cracking during laser welding newly developed crystallography-dependent aerospace materials. Part I: Spontaneous microcrack repair of microstructure development

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Abstract. Metallurgical modeling of microcrack self-repair during laser welding of nickel-based superalloys has been properly established. Metallurgical mechanism of crystallographic control self-repair intergranular liquidation cracking of heat-affected zone (HAZ) through spontaneous feed of interdendritic liquid beneath the surface is proposed. Self-repair of arterial crack network with dendrite substructure of backfill enables crack resistance amelioration and is dependent on alloying element and heat input. Microstructure development and solidification behavior are controlled to minimize the severe liquation cracking near the fusion boundary by optimization of laser welding conditions through numerical analysis. Liquid healing of incipient cracking in the HAZ through available feeding fluid flow due to accessible to weld pool are sensitive to grain size and weld pool geometry to metallurgically suppress liquation crack, stabilize the primary solidification path and improve the weld integrity, simultaneously. It is revealed that optimum low heat input is favored to reduce liquation cracking. Theoretical predictions are in satisfactory agreement with microanalysis of measurement result indirectly. In addition, this metallurgical modeling is also applicable to other nickel-based superalloys with similar metallurgical properties.

1. Introduction

As being ubiquitously used as aerospace material for gas turbine engine and various accessories, intermetallic gamma prime (γ’) and gamma double prime (γ’’) precipitation-strengthened nickel-based superalloys and their derivatives are highly prone to either by interdendritic solidification cracking of fusion zone or intergranular liquation cracking of HAZ (also called microfissuring or hot cracking). Despite of the considerable difference in chemistry, complete and partial healing of interior crack in fusion zone and HAZ by weld pool backfill is considered to be the primary reason for the weldability improvement of newly developed nickel-based superalloys. A series of ongoing experiment research recently involves the essential of cracking phenomena during welding. Some minor alloying elements serve as segregant, depressant and surfactant, and closely relate to HAZ intergranular liquation cracking. Knorovsky et al established pseudobinary solidification constitution diagram with Nb of Inconel 718. Solidification sequence and fraction eutectic were analyzed during Gas Tungsten Arc (GTA) welding [1]. Dupont et al developed γ-Nb-C pseudoternary solidification diagrams of Ni-based
alloys and eutectic-type solidification sequences of microstructure development during GTA welding. Weld pool solidification behavior of Nb-bearing nickel alloy controls segregation of alloying elements, terminal eutectic-type phase formation, size and morphology of microstructure, and solidification temperature range [2,3].

Theoretical analysis on the forefront of reducing or eliminating internal crack is rarely introduced and greatly expected because of the demanding aspect of quantitative description of welding metallurgy. Dye et al developed a general model of numerical analysis to predict weld defects, such as centerline grain boundary, interdendrite microporosity, constitutional liquation and solidification cracking during Tungsten Inert Gas (TIG) welding of nickel-based superalloy IN 718 [4]. Radhakrishnan and Thompson analyzed microstructure development model of HAZ grain boundary liquid film formation of constitutional liquation to predict liquation cracking susceptibility during welding IN 718 alloy [5]. Trivedi and Kurz proposed a more general planar interface stability criterion of constitutional supercooling on the basis of linear perturbation theory of Mullins and Sekerka for stability of a planar interface, and developed the eutectic microstructures model of rapid solidification [6,7]. Wang et al developed a sharp interface model of multicomponent alloys with rapid solidification conditions on the basis of the thermodynamic extremal principle and irreversible thermodynamics [8]. Galenko et al analyzed the kinetics of dendrite rapid solidification in the ternary Ni-Zr-Al through experiments and modeling within undercooling range [9]. The objective of this work arises from the scarcity of pertinent mathematical modeling on cracking amelioration and the existing methods are further extended to predict the liquation cracking susceptibility and self-repair in more quantitative senses. As long as the rule of strategic priority is taken into account, the weldability is significantly improved during laser welding rather than traditional aftermath overhaul.

2. Mathematical description of incipient crack self-repair

In order to establish reasonable mathematical modeling, several necessary assumptions are made in this work unless otherwise stated: (I) under the consideration of present growth velocity, the solubility limit extension is neglected and the matrix composition is uniform without composition fluctuation; (II) dissolution of niobium carbide particle in the subsolidus portion of HAZ commences just above the dissolution temperature and continues until niobium carbide reproprecipitates during solidification; (III) the diffusivity of niobium in the molten weld pool increases due to local overheating in excess of liquidus temperature; (IV) thermodynamic equilibrium is maintained at the solid-liquid interface of carbide-matrix, and the instantaneous carbon concentration at the interface is constant; (V) the grain boundary segregation and desegregation of boron are supposed to be kinetically insensitive after cooling down to 0.5Tm; (VI) the effect of entropy and geometric terms on the formation of vacancies and vacancy-boron complexes is not considered, and the atomic misfit in crystal lattice is energetically favorable for boron to segregate at high energy sites; (VII) the modification of boron segregation behavior by interaction of co-segregation and selective segregation in multicomponent alloy systems is neglected.

2.1. Nonequilibrium solidification behavior of weld pool

2.1.1. Dendrite growth velocity and temperature gradient. Specific information about temperature-time relationship is an important first step towards the deep understanding of weld pool solidification. Rosenthal thick plate solution characterizes the three-dimensional temperature distribution at pseudo-steady state as follows:

\[ T - T_0 = \frac{q\eta}{2\pi\lambda} \left( \frac{1}{R} \right) \exp \left[ - \frac{v}{2a} (R + x) \right] \]  

(1)

where \( R = \sqrt{x^2 + y^2 + z^2} \); \( T_0 \) is the ambient temperature; \( \lambda \) is the thermal conductivity; \( q \) is the laser power; \( \eta \) is efficiency factor owing to heat losses by convection and radiation; \( v \) is the welding speed in \( x \) direction; \( a \) is the thermal diffusivity.
Because the shape of the weld pool remains constant under steady-state conditions, the velocity of the solidification interface is geometrically related to welding speed. In the $x$-$y$ plane, where $\phi = 0$ and $0 \leq \theta \leq 90^\circ$, the solidification interface velocity $v_s$ is given by:

$$v_s = v \cos \theta = \frac{G_x}{|\vec{G}|}$$

(2)

In the $y$-$z$ plane, where $\theta \approx 90^\circ$, $\cos \phi$ is calculated by the following:

$$\cos \phi = \frac{G_y}{|\vec{G}|}$$

(3)

where $G_x$, $G_y$, $G_z$ are the temperature gradient components that is derived from geometry model of weld pool in the $x$, $y$ and $z$ direction, separately, and $|\vec{G}| = \sqrt{G_x^2 + G_y^2 + G_z^2}$.

The dendrite growth velocity and temperature gradient are given by:

$$v_d = \frac{v_s}{\cos \psi} = \frac{v \cos \theta \cos \psi}{\cos \psi}$$

(4)

$$G_d = |\vec{G}| \cos \psi$$

(5)

$$\cos \psi = \frac{\vec{u}}{\vec{n}}$$

(6)

where $\psi$ is the misalignment angle between the solidification front normal and dendrite growth direction; $\vec{u}$ is the dendrite growth velocity vector along the [hkl] direction.

2.1.2. Stability of the advancing solidification interface. Traditional theories of rapid solidification are extrapolated to laser welding and are advanced, and solidification conditions correlate with weld microstructure development and hot cracking [10]. On the basis of stability of planar interface shape during solidification of dilute binary alloy, stability criterion of dendrite growth and general framework of tip radius, interface undercooling and primary arm spacing were proposed [11-13].

KGT model of microstructure development during rapid solidification is theoretically given by Kurz, Giovanola and Trivedi as follows [14].

$$\frac{4\pi^2 \Gamma}{r_d^2} + \frac{2PmC_0(1-k)}{[1-(1-k)\nu(P)r_d]} + G = 0$$

(7)

where $C_0$ is the initial liquid concentration; $\nu(P)$ is the Ivantsov’s solution; $\Gamma$ is the Gibbs-Thomson coefficient; $m$ is the liquidus slope; $G$ is the mean temperature gradient at the interface; $k$ is the partition coefficient; $P$ is the solutal Peclet number.

$$\xi_c = 1 - \frac{2k}{\left[1 + \left(\frac{2a_0v_s}{P}\right)^2\right]^2} - 1 + 2k$$

(8)

Partition coefficient is dependent on interface velocity and temperature as follows:

$$k = \frac{k_0 + \left(a_0v_s\right)}{1 + \left(a_0v_s\right)}$$

(9)

where $k_0$ is the equilibrium partition coefficient; $a_0$ is related to the interatomic distance; $D_L$ is the diffusivity in liquid.
2.1.3. Morphology of solidification microstructure. The dendrite trunk spacing in the vicinity of mushy zone is given by:

\[ \lambda_1 = \left(\frac{3\Delta T^* r_d}{G}\right)^{1/2} \]  

(10)

where \( \Delta T^* \) is difference between tip temperature and nonequilibrium solidus temperature.

For secondary dendrite arm spacing, continuous ripening process takes place as the consequence of the disparity in interfacial energy between branches with different curvature as analogous to the Ostwald ripening of precipitate. The development of the secondary dendrite arm spacing during weld pool solidification is given by:

\[ \lambda_2 = 5.5(Mt_0)^{1/3} \]  

(11)

where \( t_0 \) is the local solidification time and \( M \) is a mobility term in regards to the phase diagram, separately.

\[ T_0 = \frac{g}{v_s} = \frac{\Delta T^*}{Gv_s} \]  

(12)

\[ M \approx \frac{\Gamma D_L \ln\left(\frac{C_E}{C_0}\right)}{m_E (1 - k)(C_0 - C_E)} \]  

(13)

where \( C_E \) is the eutectic concentration and \( m_E \) is the slope of the liquidus curve under the nonequilibrium solidification conditions.

\[ M_E = \frac{T(C_l^*) - T_E}{C_l^* - C_E} \]  

(14)

where \( T(C_l^*) \) and \( C_l^* \) are temperature and liquid concentration at the interface; \( T_E \) and \( C_E \) are the eutectic temperature and concentration, separately.

2.1.4. Solute redistribution at dendrite tip. For Ivantsov’s solution around parabolic interface, the supersaturation of the liquid at the solid-liquid interface is given by:

\[ \Omega = \frac{C_l^* - C_0}{C_l^* - C_s} = \frac{C_l^* - C_0}{C_l^*(1 - k)} = Iv(P) \]  

(15)

where \( C_s \) is the solid concentration at the interface.

The tip temperature \( T_t \) is given by:

\[ T_t = T(C_l^*) - \Delta T \]  

(16)

Where \( \Delta T \) is the undercooling.

For the sake of simplicity, liquidus curve is straight line and \( T(C_l^*) \) is given by:

\[ T(C_l^*) = T_m + mC_l^* \]  

(17)

where \( T_m \) is the melting point of the pure component.

Because nucleation requires an additional undercooling, the minimum undercooling criterion at the dendrite tip is given by Burden and Hunt [15]:

\[ \Delta T = \Delta T_C + \Delta T_R = \left[ -\frac{8m\Gamma}{D_L v_s C_0 (1 - k)} \right]^{1/2} + \frac{D_L G}{v_s} \]  

(18)

where \( \Delta T_C \) is the constitutional undercooling; \( \Delta T_R \) is the capillarity undercooling.
The nonequilibrium eutectic temperature at the terminal stage of solidification widens solidification temperature range and is given by:

\[ T_E = C_l^* - \frac{C_l^0}{k} + \frac{C_l^0 T_m - T(C_l^0)}{T_m - T(C_l^0)} \]

where \( C_{s}^{\text{max}} \) is the maximum solid solubility and \( C^0 \) is the solid solubility at ambient temperature; \( T_E \) is the eutectic temperature during equilibrium condition.

The amount of eutectic-type constitute \( f_E \) is given by Sarreal and Abbaschian [16]:

\[ f_E = (1 - \Omega) \left( \frac{C_{s}^{\text{max}}}{kC_l^*} - \frac{\Omega k}{a_E k^{k-1}} \right) \]

where \( \alpha_E = \frac{D_L}{m_k v_k C_0} \)

### 2.2. Dissolution of niobium carbide particle in the subsolidus portion of HAZ

Intergranular liquation cracking is sensitive to the amount, size and distribution of niobium carbide (NbC) particles. The constitutional liquation of NbC in terms of a diffusion couple between NbC and \( \gamma \) matrix in a \( \gamma \)-NbC-Laves pseudoternary solidification diagram is proposed by Radhakrishana and Thompson [17]. Weld thermal cycle in the subsolidus portion of HAZ enables the partial or complete dissolution of fine dispersed niobium carbide particles along the grain boundaries due to the diffusion couple development between NbC and \( \gamma \) matrix, and the general case time-dependent model for the precipitate dissolution kinetics is given by Whelan [18]:

\[ \frac{f}{f_0} = f_0 \left( 1 - \frac{2}{r_0} \int_{t_1}^{t_2} \alpha D_L \, dt \right)^{\frac{3}{2}} \]

where \( \alpha \) is the dimensionless supersaturation; \( t_1 \) and \( t_2 \) are the total time spent on dissolution of niobium carbide particle; \( f_0 \) is the initial particle volume fraction; \( r_0 \) is the initial particle radius.

Because the dissolution rate of niobium carbide particle is controlled by the diffusion of niobium in \( \gamma \), \( \alpha \) becomes the following through the simple stoichiometry:

\[ \alpha = \frac{C_i - C_m}{C_p - C_i} \]

where \( C_i \) is the niobium concentration at the NbC-matrix interface; \( C_p \) is the niobium concentration in the NbC; \( C_m \) is the concentration in the matrix.

The equilibrium concentration of niobium at the interface is obtained through the solubility product as follows:

\[ C_i = \frac{\exp(\Delta S^*/R)}{C_c} \exp \left( \frac{\Delta H^*}{RT} \right) \]

where \( R \) is the universal gas constant; \( C_c \) is the carbon concentration; \( \Delta S^* \) is the standard entropy of reaction; \( \Delta H^* \) is the standard enthalpy of reaction.

The niobium concentration in the NbC is given by:

\[ C_p = \frac{M_{Nb}}{M_{Nb} + M_c} \]

where \( M_{Nb} \) and \( M_c \) are the atomic weights of niobium and carbon, separately.
2.3. HAZ grain grow in the present of dissolving particle

Grain size development depends on the interaction between grain and grain boundary liquid in the HAZ. HAZ grain either immediately coarsens until it is stable up to a limiting grain size by unpinning of grain boundaries or is refined because of the occurrence of substantial liquid film migration \[19,20\].

The dependence of the average grain size on time and temperature with the grain boundary pinning particles is given in a more general form as follows:

\[
\frac{d\bar{D}}{dt} = M_0^*\exp\left(-\frac{Q_{\text{app}}}{RT}\right)\left[1 - \frac{1}{k_z r}\right]^{-1-n}\]

where \(k_z\) is the Zener coefficient; \(M_0^*\) is the modified kinetic constant; \(Q_{\text{app}}\) is the apparent activation energy for grain growth.

Kinetically, there is a competition between particle dissolution and grain growth during weld thermal cycle about the thermal instability of the particle and the resulting average grain size with particle dissolution is given by:

\[
\bar{D} = \frac{(\bar{D}_0)^3}{(\bar{D}_0)^2 - \left(\frac{k_z}{f_0}\right)^2 \left(2 \int_0^{t_1} d\bar{D}_L dt\right)}
\]

and

\[
\bar{D}_0 = k_z r_0 f_0
\]

2.4. Development of intergranular liquid film in the subsolidus portion of HAZ

With the assumption that the NbC-matrix interface is flat and metastable liquid continuously distributes along the grain boundaries, the cumulative thickness of intergranular liquid film is correlated to the grain size \[5\]:

\[
L = \frac{(\bar{D}/2)(f_{\text{NBC}}/\rho_{\text{NBC}})}{f_{\text{NBC}}/\rho_{\text{NBC}} + f_\gamma/\rho_\gamma}
\]

where \(\rho_{\text{NBC}}\) and \(\rho_\gamma\) are the densities of NbC and \(\gamma\); \(f_{\text{NBC}}\) and \(f_\gamma\) are the weight fractions of NbC and \(\gamma\).

2.5. Sensitive time interval of cracking

Two cracking behaviors near the fusion boundary, either acting alone or simultaneously, are considered together in this case. In the HAZ, the time range between beginning of constitutional liquation of niobium carbide and reprecipitation of intergranular liquid film is mainly responsible for intergranular liquation cracking. In the fusion zone, the solidification time range between the beginning temperature of proeutectic \(\gamma\) and the terminal solidus temperature owing to \(L \rightarrow \gamma +\text{Laves}\) reaction is highly susceptible to interdendritic solidification cracking. In view of above two factors, the time duration from the onset of niobium carbide dissolution to the liquidus temperature of the molten weld pool and then down to actual solidus temperature is defined as a criterion to evaluate the material resistance or susceptibility to cracking as follows:

\[
\Delta t_s = t_E - t_D
\]

where \(t_E\) is the time of depressed eutectic temperature during nonequilibrium solidification; \(t_D\) is the time of incipient dissolution of niobium carbide particle during on-heating part of weld thermal cycle.

2.6. Boron induced solid-liquid interfacial decohesion of intergranular liquid film

Boron-doped superalloys are highly susceptible to HAZ intergranular liquation cracking, because boron in the intergranular liquid serves as a strong surfactant and depressant, facilitates an extensive
increment of the thickness of intergranular liquid film, and deteriorates the superalloys weldability. Although back-diffusion of boron across the solid-liquid interface, the grain boundary segregation of boron during weld thermal cycle increases boron concentration to lower solid-liquid interfacial energy and grain boundary energy, and substantially promotes wettability of the metastable liquid along grain boundary. The grain boundary wettability is proposed in a more general form:

\[ \gamma_{gb} \leq 2\gamma_{SL} \]  \hspace{1cm} (30)

where \( \gamma_{gb} \) is the grain boundary energy, and \( \gamma_{SL} \) is the solid-liquid interfacial energy. Both are boron-sensitive and temperature-dependent.

Random high-angle grain boundaries are inherence of higher energy than the special grain boundaries, such as twin-generated grain boundaries; the latter effectively improves resistance to HAZ intergranular liquation cracking. Constitutional liquation rather than segregation-induced grain boundary melting is the prime source of intergranular liquid, and the coupling effect of the dissolution of niobium carbon particle and boron segregation on intergranular liquid film stability is developed. The threshold tensile stress to overcome surface tension of intergranular liquid film with boron at a specific temperature is given by the empirical equation, and the aptness is rather satisfactory.

\[ \delta = \frac{2\gamma_{SL}}{L} \]  \hspace{1cm} (31)

where \( L \) denotes the cumulative thickness of intergranular liquid film. It is indicated that thick intergranular liquid film reciprocally lowers the magnitude of threshold stress to incur decohesion of solid-liquid interface. The boron, despite in small quantities, has quite considerable effect on the diminution of grain boundary energy with the temperature increase.

This current calculation mathematically extrapolates the traditional theories of solidification and welding metallurgy, and combines with the recent headways in the theories of nonequilibrium solidification and nonequilibrium grain boundary segregation. In summary, the general procedure for the analysis is outlined as follows:

- Calculate the three-dimensional weld pool geometry at a certain welding condition, and compare the weld pool geometry, such as weld pool width and penetration, with the experiment results;
- Determine geometrically the dendrite growth velocity along preferential crystallographic orientation and corresponding temperature gradient along the solid-liquid interface of maximum transverse and longitudinal cross-sections of weld pool;
- Calculate the dendrite tip radius, dendrite trunk spacing and subdendrite arm spacing with consideration of various niobium concentrations, crystallographic orientations and locations on the base of minimum velocity criterion, separately;
- Calculate the undercooling, eutectic temperature and eutectic amounts through the criterion of minimum undercooling and solidification phase diagrams according to equations (18), (19) and (20), separately;
- The effect of dissolution of niobium carbide particle on the resulting HAZ grain growth in the course of weld thermal cycle is determined and the thickness development of intergranular liquid film among the grain boundaries is calculated by using equations (21), (26) and (28);
- The sensitive time interval of cracking during welding is calculated according to equation (29) with the combination contributions of solidification-induced and liquation-induced cracking behaviors under nonequilibrium solidification of weld pool;
- The effect of nonequilibrium solidification of weld pool on nonequilibrium grain boundary segregation of boron and solid-liquid interfacial decohesion within grain-coarsened HAZ are calculated by using equations (28), (30) and (31).

The influence of the welding conditions on the weld pool geometry, dendrite morphology, nonequilibrium solidification behavior, thermal stability of niobium carbide particle, HAZ grain growth, development of intergranular liquid film, sensitive time interval of cracking and grain boundary
segregation of boron are routinely determined again according to the step (1) to (7) by updating a new set of welding conditions. Exact solutions were calculated by iterative solving equations with available computer capacity.

3. Experiment procedure

The chemical composition of the wrought 718-type derivative superalloy suffices the following upper limit, 54.43Ni-17.9Cr-17.8Fe-5.4Nb-2.9Mo-0.9Ti-0.5Al-0.05Si-0.05Mn-0.04B-0.025C-0.004P-0.001 Mg (wt%). Before laser welding, the materials with dimensions of 80×15×6mm were undergone solution heat treatment at 1323K throughout one hour and then followed air cooling. Ten transverse sections of a sample per each welding condition were polished and electrolytically etched by oxalic solution; total crack length of them as a unique value is characteristic of cracking response to weld thermal cycle and measured by the microanalysis of scanning electron microscope (SEM). The relevant data applicable to the calculation from the miscellaneous sources are listed in table 1.

| Properties | Unit | Value | Reference |
|------------|------|-------|-----------|
| α | Thermal diffusivity | mm²/s | 3.38 | [21] |
| a₀ | Length scale | nm | 5 | [14] |
| λ | Thermal conductivity | W/mmK | 0.0176 | [21] |
| ρ_c | Volume heat capacity | J/mm³K | 0.00356 | [21] |
| T_L | Liquidus temperature | K | 1609 | [21] |
| Γ_{Nbc} | Gibbs-Thomson coefficient | K mm | 0.0000958 | [22] |
| Γ_{Laves} | Gibbs-Thomson coefficient | K mm | 0.0002 | [23] |
| Γ_{Boride} | Gibbs-Thomson coefficient | K mm | 1.16×10⁻⁷ | |
| D_L | Diffusion of niobium in nickel | mm²/s | 1.04exp(−202590/RT) | [24] |
| D_C | Diffusivity of recombined complex in γ | mm²/s | 2exp(−1.15/kT) | [25] |
| D_b | Diffusivity of boron in γ | mm²/s | 0.2exp(−1.15/kT) | [25] |
| m_{Nbc} | Slope of the liquidus curve | K per wt% | 11 | [17] |
| m_{Laves} | Slope of the liquidus curve | K per wt% | 11.85 | [1] |
| m_{Boride} | Slope of the liquidus curve | K per wt% | 93.75 | [26] |
| M_{Nb} | Atomic weight of niobium | g /mol | 92.9 | [27] |
| M_c | Atomic weight of carbon | g /mol | 12 | [27] |
| ρ_{Nbc} | Density of niobium carbide | kg/m³ | 6500 | [27] |
| ρ_y | Density of matrix | kg/m³ | 8190 | [21] |
| ΔS° | Standard entropy of reaction | JK/mol | 43.26 | [27] |
| ΔH° | Standard enthalpy of reaction | J/mol | 129578 | [27] |
| C^b_{max} | Maximum solid solubility of niobium | wt% | 9.3 | [1] |
| C^b_{max} | Maximum solid solubility of boron | wt% | 0.016 | [26] |
| M_{o} | Modified kinetic constant | μm²/s | 37×10⁹ | [27] |
| D_0 | Initial grain size | μm | 98.8 | |
| η | Efficiency factor | 0.36 | |
| k_{0Nb} | Equilibrium partition coefficient of Nb | 0.47 | [1] |
| k_{0B} | Equilibrium partition coefficient of B | 0.004113 | [28] |

4. Results and discussion

4.1. Effect of welding conditions on the weld pool geometry

The dependence of isothermal fusion boundary on the welding conditions are shown in figure 1. In figure 1(a), first of all, heat input plays a very significant role in determining the penetration of weld pool, and the penetration rapidly shrinks and becomes narrow with low heat input (low laser power or high welding speed). Secondly, the range of the penetration is lower than that of experimental one due to the uncertainty of the absorptivity of laser beam with process instability to loss the transferable
energy. In figure 1(b), initially, the weld pool length is nearly independent of the welding speed during steady-state condition. The extent of the weld pool elongation and the maximum width of the weld pool are substantially proportional to the laser power, and inversely proportional to the welding speed. Secondly, the elliptical temperature profiles are expanded behind the laser beam and widely compressed ahead of the molten weld pool owing to the advance of the solid-liquid interface during increment of laser power. Finally, the range of the maximum width of the weld pool is 1.193 to 2.363 mm, which is reasonably close to the range of experimental results of 1.122 to 2.428 mm. In both cases, comparable agreement between the calculation results and measurement results is reached.

![Figure 1](image)

**Figure 1.** The role of welding conditions in (a) transverse cross-section weld pool shape and (b) top surface of weld pool shape, separately.

4.2. Effect of grain boundary carbon alloying and welding conditions on the development of intergranular liquid film

Metallurgically, the dependencies of thermal stability of niobium carbide particle and grain size near the fusion boundary on carbon concentration at grain boundary are shown in figure 2. In figure 2(a), the grain size depends on the unpinning efficiency of precipitates. Grain growth in HAZ region is thermodynamically driven by dissolving niobium carbide particle during weld thermal cycle and the low carbon alloying gradually exacerbates grain growth as long as the precipitates are thermally unstable at high temperature. In figure 2(b), the dissolution rate of niobium carbide particle is strongly dependent upon the thermal path and grain boundary carbon alloying. Niobium carbide particle around low-carbon grain boundary is more susceptible to dissolution that facilitates an extensive increment of the thickness of intergranular liquid film. However, niobium carbide particle around high-carbon grain boundary is more thermal stable to partially dissolve the particle due to lack of sufficient energy; the enrichment of carbon concentration at grain boundary retards the dissolution of niobium carbide particle. Moreover, high carbon and low niobium concentrations extensively adjust the primary solidification path near the fusion boundary towards the eutectic-type reaction \( L \rightarrow \gamma + \text{NbC} \) at high temperature instead of \( L \rightarrow \gamma + \text{Laves} \) at the terminal stage of solidification, and thus decrease the solidification temperature range [2]. Carbon-rich fusion boundary and grain boundary consistently
improve the liqution cracking resistance to ameliorate the weldability.

Figure 2. The role of grain boundary carbon alloying in (a) HAZ grain growth and (b) cumulative thickness of intergranular liquid film, separately.

Figure 3. The dependency of niobium carbide particle dissolution on (a) grain boundary carbon alloying and (b) particle size during rapid on-heating part of weld thermal cycle, separately.

The dependency of particle dissolution on grain boundary carbon alloying and particle size during
rapid on-heating part of weld thermal cycle is shown in figure 3. Niobium carbon particles situate in the three locations of molten weld pool, mushy zone and HAZ. In figure 3(a), the niobium carbon particles completely dissolve in the molten weld pool regardless of the carbon concentration and particle size, and become small in the mushy zone and HAZ due to insufficient time and temperature. High-carbon grain boundary induces partial particle dissolution. In figure 3(b), as the temperature further increases, submicron size particles readily dissolve in the mushy zone and HAZ and directly contribute to intergranular liquid film. Fine particle induces the appreciable dissolution during up to the peak temperature, while coarse one is refractory. There is still abundance of partial dissolution particles that preclude the grain growth.

The roles of laser power in the cumulative thickness of intergranular liquid film are shown in figure 4. Indigenous niobium carbide dissolution instantaneously occurs and the process continues until the metastable reprecipitates from intergranular liquid during cooling due to the high diffusivity of atomic carbon and niobium. The development profile of the thickness of intergranular liquid film is parabolic and time-dependent, and the high heat input produces thick intergranular liquid film for a long period and incurs more liquid with threshold tensile stress reduction, and the interfacial wetting conditions are significantly improved.

![Figure 4](image)

**Figure 4.** The role of laser power in the cumulative thickness of intergranular liquid film.

The roles of welding speed in the cumulative thickness of intergranular liquid film are shown in figure 5. Compared to that of laser power in the figure 4, average grain size increases with decreasing welding speed, and widens the liquid film duration. The thickness of continuous liquid film induces parabolic-shape distribution on rapid heating and cooling parts over wide temperature range during weld thermal cycle. Average grain size initially increases and then stabilizes, and the grain size coarsens because of the sufficient time available for dissolving carbide particle under high heat input than that of low heat input. The extensive grain growth further alters the kinetics of the subsequent solid-state grain boundary segregation. It is necessary to decrease the grain size through optimum heat input to pin grain boundary by carbide particles. Fine grains possesses substantial grain boundary curvatures and increase grain boundary surface area that enhance the solidification of grain boundary liquid film by liquid film migration to reduce the liquation cracking susceptibility. The cumulative intergranular liquid builds up with increasing time and temperature. Thick intergranular film and
coarse grain size are detrimental to the weldability. Optimum low heat input (high welding speed and low laser power) is advantageous to limit grain growth and reduces the thickness of metastable intergranular liquid film to slow down grain boundary liqutation migration and prevent grain boundary degradation and thermal instability, which suppress severe intergranular liqutation cracking in subsolidus HAZ. As a consequence, it is of significant importance to use feasible laser welding for weldability improvement.

Figure 5. The role of welding speed in the cumulative thickness of intergranular liquid film.

4.3. Effect of niobium alloying and welding conditions on self-repair of arterial crack network in HAZ

The solidification cracking susceptibility is high for the niobium-rich alloys than that of the niobium-free alloys [29], while the interdendrite solidification cracking in the niobium alloying nickel-based superalloys is effectively immunized by virtue of arterial crack network repair. The dependency the dendrite trunk spacing, the amount of eutectic-type constituents, γ/NbC and γ/Laves, and depressed eutectic temperature on niobium alloying near the fusion boundary is shown in figure 6. In figure 6(a), the dendrite trunk spacing is strongly dependent on the shape of weld pool and niobium alloying. Niobium-rich addition sensitively favors fine-scale dendrite trunk spacing, and beneficially decreases the dendrite trunk gradient. The dendrite trunk spacing detrimentally coarsens at the upside region to develop high-constraint microstructure, and closely relate to stray grain formation, metallurgical discontinuity and potential interdendrite solidification cracking to deteriorate the weld integrity and mechanical properties.

In figure 6(b), first of all, the effect of niobium-rich addition on promoting the formation of major phases, γ/NbC and γ/Laves, is rather apparent; the maximum amount of eutectic-type constituents exists near the upside of the weld pool. Secondly, the backfill of interdendrite liquid throughout the arterial crack network actively self-repairs the severe crack, however, it also facilitates heterogeneous eutectics, misalignment and reorientation of dendrite substructure to induce incoherent interface because of enrichment of low-melting eutectic liquid. Finally, the amount of the eutectic-type constituents is correlated with the crack self-repair due to the accessibility to molten weld pool to supply feeding channel of available backfill of interdendrite liquid. The less addition of niobium, the less eutectic-type constituents will be produced to minimize the cracking through alloy-dependent self-
healing.

![Graph](image_url)

**Figure 6.** The role of niobium alloying in nonequilibrium solidification behavior of weld pool.

In figure 6(c), a small variation of niobium alloying differs the solidus temperature to a point where the $\gamma$/Laves eutectic-type constituent occurs. First of all, the depressed eutectic temperature maximizes near the bottom of the weld pool and results in a steep temperature gradient. High-niobium concentration stabilizes the primary solidification path of $L \rightarrow \gamma + \text{Laves}$ reaction, increases the solidification temperature of terminal stage, narrows the effective solidification temperature range, refines microstructure, decreases weld pool geometry, and thus significantly improve cracking resistance. Secondly, it also decreases the available time and amount of terminal liquid for self-repair by backfill of interdendrite liquid to bridge the cracks. Moreover, since the high-niobium concentration thermodynamically increases the actual solidus temperature under nonequilibrium solidification of weld pool, it further promotes the solid-state non-equilibrium grain boundary segregation. Finally, the major impetus to repair incipient cracking by spontaneous merging portion of arterial crack network through influx of interdenrite liquid without using filler wire leads to control solidification behavior. Internal intergranular liquidation cracking is confined around the periphery of the fusion boundary. Arterial crack network intersects the mushy zone of the molten weld pool, which intragranularly deflects or intergranularly propagates at high-angle grain boundaries, and suffices liquid to thermocapillarily flow into the crack space; therefore, portion of cracks within HAZ are predominantly immune from cracking with merging through considerable weld pool influx. The inside liquid of crack dendritically solidifies to develop fine-scale dendrite substructure.

The dependency of major contributing factors to self-repair of arterial crack network in HAZ on welding conditions and alloying element near the fusion boundary is shown in figure 7. In figure 7 (a), the role of welding conditions in the cumulative thickness of intergranular liquid film within coarsened HAZ is shown. First of all, high heat input produces thick intergranular liquid film, while low heat input incurs less intergranular liquid. Secondly, continuous and thicker intergranular liquid film is more prone to engender boundaries detachment due to incapable accommodation of the local tensile...
components, and therefore is fairly susceptible to intergranular liqutation cracking. While thinner one is chemically eliminated by subgrain coalescence and liquid film migration owing to release of coherency strain energy before the onset of liqutation cracking, either acting along or simultaneously. The scale of liquid film thickness on HAZ grain boundaries is typical order of few microns and was experimentally measured within 2-8μm [30,31]; the theoretical predictions are validated by experiment results. Finally, the evidence of coexistence of the severe HAZ intergranular liqutation cracking and the sparse liquid film migration within the region of grain coarsened HAZ indicates that liquid film migration is incapable of preventing liqutation cracking. This is mainly attributed to the following two factors: the formation of thick intergranular liquid film and lack of external source of backfill from weld pool.

In figure 7(b), the role of welding conditions in the grain boundary liqutation in terms of sensitive time interval of cracking is shown. First of all, high heat input significantly widens the sensitive time duration, and induces complete particle dissolution to deteriorate grain boundary liqutation, while low heat input delays grain boundary liqutation. The longer the sensitive time interval of cracking, the greater is susceptible to cracking. Secondly, sensitive time duration of cracking serves as one of cracking susceptibility criteria. The critical range of weld thermal cycle near the fusion boundary of weld pool is of typical order of 0.1s during laser deep penetration welding [32,33], and therefore the theoretical predictions by this criterion are acceptable. Finally, it is also controversial that high heat input provides longer time for backfill of interdendrite liquid to self-repair arterial crack network, but this contribution is inferior to that of crack degradation and need the application of the extra filler wire to supply additional source to completely heal the arterial crack network.
In figure 7(c), the role of welding conditions in the subdendrite arm spacing near the backfill of fusion boundary is shown. Dendrite substructure occurs during influx solidification in crack internal, if the thermal conditions are favorable and possible interface protuberances are stabilized to lead to microstructure refinement, strongly promotes spontaneous self-mergence. The size and morphology of crystallographic substructure of backfill inside narrow crack network are dependent on heat input. High heat input produces coarser substructure, while low heat input incurs small subdendrite to facilitate substructure integrity and microstructure control. The theoretical predictions of subdendrite arm spacing of backfill near the fusion boundary are the order of 0.1-1 μm and comparable with the measurement results.
In figure 7(d), the major eutectic-type constituents of γ/NbC and γ/Laves enrich niobium, and heterogeneously mix in the arterial crack network to give rise to incoherent interface and weaken the HAZ integrity[34]. First of all, high heat input produces large amount of eutectic-type constituents, however, the mere pursuit of sufficient amount of liquid to initiate the influx of backfill through the mushy zone to heal incipient cracking by further increasing heat input is incapable of acting as a preference because high heat input simultaneously induces other detrimental consequences. Niobium-rich concentration promotes eutectic-type reactions and stabilizes primary solidification path in the backfill. Secondly, the heat input should not only withstand excessive niobium segregation and optimize weld pool dynamics with turbulent multiphase flow to expel the interdendrite liquid into crack network, but also prevent the oscillation disturbance and instabilities of weld pool and suffice the adequate time of interdendrite liquid influx to completely heal the incipient crack morphology within the duration of trailing edge solidification of the weld pool.

In figure 7(e), the effect of the boron-rich eutectic on weldability of this nickel-based superalloy is of particular concern, and the dependence of eutectic-type γ/boride fraction on welding conditions and boron alloying is shown. The theoretical fraction of γ/boride is considerably small owing to stringent limitation of boron composition in the material. High heat input contributes the more nucleation of eutectic-type γ/boride, whereas low heat input results in less amount of eutectic. Boron-rich composition further promotes the low-melting terminal eutectic-type reaction and thereby facilitates the formation of more amount of boride. The weldability deterioration with the formation of boride in the residual liquid of backfill is imminent, thus leading to introduce ideas of optimization of boron segregation profile by virtue of preweld heat treatment and weld thermal cycle to reduce the segregation of boron and the boride formation. Simultaneously, niobium partitions into backfill and subsequently promotes proeutectic γ, eutectic γ/NbC and γ/Laves; the heterogeneous mixture of eutectics decorate dendritic substructure within crack network to deteriorate the weldability as well.

In figure 7(f), boron concentration is lessened by the decrease in actual solidus temperature because solidus boundary extends into the material during laser welding. Segregation proceeds along, without the occurrence of the grain boundary desegregation. The strong dependence of grain boundary segregation of boron on different welding conditions is shown. It is elucidated that high heat input significantly prompts the grain boundary segregation of boron, while low heat input leads to the mitigation of grain boundary segregation, thereby suggesting that as-segregated boron monotonously reduces with low heat input and implies the necessity of heat input restriction. Boron segregation behavior is consistently interrelated with the weld pool solidification, constitutional liquation of particles, HAZ recrystallization, and eutectic-type reactions throughout this work that is an indispensable factor to equally contribute to the susceptibility of HAZ intergranular liquation cracking.

In figure 7(g), the effect of welding conditions on experiment results of microcrack length within coarsened HAZ is shown. Microcrack length beneath the surface widely varies with different welding conditions, and total crack length monotonically increases with high heat input [35,36]. Magnitude of total crack length is of the typical order of millimeter and characteristically ascertains the necessity of other ways to annihilate HAZ intergranular liquation cracking in order to produce crack-free weld. The theoretical predictions of cracking susceptibility in the foregoing discussions are in satisfactory agreement with the experiment results indirectly. Thus, the metallurgical modeling correctly serves as phenomenological explanations as well as predictions.

Comparing with figures 7(a)-7(g), theoretical predictions are consistent with each other, and further confirm that high heat input is rather detrimental to weldability and should be strictly forestalled. However, the low heat input mitigates the HAZ intergranular liquation cracking at the expense of weld penetration.

5. Conclusions
Metallurgical modeling of microcrack self-repair has been established and the integrity, accuracy and
reliability of mathematical models succeed in guiding the laser welding application to meet the ever-increasing challenges for welding high-temperature aerospace materials. Several expedient ways to efficaciously improve cracking resistance is proposed in this work, and some conclusions are briefly drawn as follows.

- Niobium-rich alloying beneficially refines weld microstructure, stabilizes the primary solidification path, increases the terminal solidification temperature and concomitantly decreases the weld pool geometry. However, it also decreases the available time and the amounts of terminal liquid for self-repair liquation crackling. The niobium concentration should rigorously balance the multivariable and multitarget strategies to produce crack-free weld.
- Niobium carbide particle around low-carbon grain boundary is more susceptible to complete dissolution to induce thick intergranular liquid film, while niobium carbide particle around high-carbon grain boundary is more thermal stable to less contribute to the intergranular liquid film.
- High heat input is detrimental to this superalloy weldability. High heat input produces thick intergranular liquid film and large amount of eutectic-type constitutes,\(\gamma/\text{NbC}\) and \(\gamma/\text{Laves}\), lessens the threshold tensile stress of solid-liquid interfacial decohesion, prompts the low-melting terminal eutectic-type reaction of boride, and promotes grain boundary segregation of boron.

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