Metallurgical modeling of intergranular HAZ liqutation cracking during laser welding newly developed crystallography-dependent aerospace materials. Part II: Grain boundary alloying segregation of microstructure modification

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Abstract. Metallurgical modeling of the nonequilibrium grain boundary segregation was coupled with a nonequilibrium weld pool solidification to numerically analyze the contributing factors to liqutation cracking resistance. The effect of the welding conditions, material composition, and average grain size on the kinetics of the grain boundary segregation in the Inconel 718-type nickel-based superalloy during laser welding were optimized. The grain boundary segregation of boron near the fusion boundary is of particular interest, and is closely correlated to the intergranular heat-affected zone (HAZ) liqutation cracking. It is indicated that the low heat input, fine-grained material and full penetration contribute to the reversible desegregation of boron and suppress the grain boundary segregation of boron to significantly minimize the segregation-induced grain boundary liqutation and improve the weldability. The subsolidus temperature due to nonequilibrium weld pool solidification is capable of ameliorating the segregation kinetics to reduce the HAZ grain boundary segregation. Interganular HAZ liqutation cracking is evitable with a crack-free weld without using filler wire. The grain boundary segregation decreases and the threshold tensile stress of solid-liquid interfacial decohesion across the intergranular liquid film simultaneously increases in the recrystallized HAZ during the weld shape change from partial penetration to full keyhole penetration. Furthermore, the numerical analysis results are verified indirectly by the experiment results of the total crack length. In addition, this metallurgical modeling is also applicable for the alloying segregation behavior prediction of other nickel-based superalloys with similar metallurgical properties.

1. Introduction

Little information on the grain boundary segregation of the newly developed Inconel 718-type superalloy due to solid-state diffusion during heat treatment and subsequent welding is provided in the literature. Inconel 718-type alloy is a $\gamma'$ precipitation-strengthened nickel-based polycrystalline superalloy, which is widely used in gas turbine engines and power generation turbines due to superior hot corrosion resistance and mechanical properties at high temperature in numerous aerospace and power generation industries. The intragranular and intergranular constitutional liqutation of carbides and the minor alloying grain boundary segregation are the two detrimental metallurgical factors in the
HAZ intergranular liquation cracking during welding. The optimum welding parameters and the base materials-related factors are proposed to preclude the liquation potential and to alleviate severe intergranular liquation cracking. Despite boron is a grain boundary strengthening element, it acts as a melting point depressant and a segregant on heating to facilitate the grain boundary liquation. Also, it extends the solidification temperature range of the liquid film on cooling, decreases the solid-liquid interfacial energy through surface-active wettability, and strongly accelerates the HAZ grain boundary liquation.

In plenitude of ongoing experiments, the boron-assisted intergranular liquation cracking is reduced through the microstructure modification of rejuvenescent heat treatment procedure of either reversible grain boundary segregation or low coincident site lattice (CSL) boundaries of grain boundary engineering. Thompson et al. correlated the intergranular minor alloying of grain boundary segregation of Inconel 718 alloy to the microfissure susceptibility during the heat treatment, and analyzed the migration of the grain boundaries during the weld thermal cycle to alter the chemistry of migration regions [1,2]. Savage et al evaluated the effect of six minor elements S, P, Si, Mn, Ti, and Al on hot cracking susceptibility of Inconel 600 alloy during the gas tungsten arc (GTA) welding. S and P were highly detrimental to the segregation and subsequently reduced the effective solidus and liquidus. Mn, Si, Ti, and Al beneficially increased the liquid-solid interfacial energy and deoxidization to reduce the susceptibility of the hot cracking during the GTA welding [3]. Qian and Lippold evaluated the spontaneous grain refinement through rejuvenation heat treatment, thereby increasing the fraction of twin-generated special grain boundaries and δ phase dissolution, to reduce the HAZ liquation cracking during the welding of wrought Waspaloy and Alloy 718 [4,5]. Ola developed a new pre-weld heat treatment procedure on the basis of microstructure modification through the control of both the boride formation and the intergranular boron segregation to significantly reduce the HAZ intergranular liquation cracking of the 738 LC superalloy and improve the weldability [6]. Chen et al. evaluated strong grain boundary segregation of boron in Inconel 718 during heat treatment and analyzed the mechanisms of segregation and desegregation of boron [7]. Lehockey et al. reduced the intergranular degradation susceptibility of the nickel-based superalloy due to the increasing proportion of the crystallographical special low ΣCSL grain boundaries through heat treatment [8].

Theoretical model on the nonequilibrium grain boundary segregation in boron-austenite system were properly derived and the calculation results were in satisfactory agreement with experiment measurement on an atomic scale. Williams et al. proposed a model of nonequilibrium grain boundary segregation of boron in 316 stainless steel during the solution heat treatment on the basis of the existence of mobile vacancy-boron complexes [9]. Xu and Song proposed a new kinetic model of nonequilibrium grain boundary segregation and desegregation of boron with a phenomenological theory during heat treatment, and developed a method to experimentally determine the critical time and critical cooling rate of the nonequilibrium grain boundary segregation of boron in Fe-30% Ni austenitic alloy [10-12]. Faulkner developed a kinetic model of nonequilibrium grain boundary segregation and desegregation of boron in 316 stainless steel during the solution heat treatment [13]. Karlsson and Norden experimentally evaluated the nonequilibrium grain boundary segregation of boron in 316L stainless steel during the heat treatment and no segregation was detected at coherent twin boundaries [14].

Segregation-induced grain boundary liquation is indispensable in the development of an optimum weld thermal cycle through grain boundary chemistry modification to eliminate HAZ intergranular liquation cracking. The objective of the present work is to propose an effective method through various combinations of welding conditions and base material-related factors to reduce the HAZ grain boundary segregation of boron during the weld thermal cycle by means of grain boundary engineering. Furthermore, an alternative mechanism of direction and extent of the grain boundary segregation and suppression through grain refinement is elucidated.

2. Experiment procedure
The chemical composition of the wrought 718-type derivative superalloy suffices the following upper
limit 54.43Ni-17.9Cr-17.8Fe-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 80x15x6mm were subjected to a solution heat treatment at 1323K for one hour and then air cooled. Bead-on-plate weld was carried out by using the fiber laser welding. Laser beam size was 0.5mm. The shielding gas flow rate was 20 L/min. The laser power ranged from 2kW to 5kW and the weld speed ranged from 1m/min to 4m/min. Ten transverse sections of a sample per each welding condition were polished and electrolytically etched by oxalic solution. The total crack length (TCL) of the sections was a unique characteristic of cracking response to weld thermal cycle and was measured by the microanalysis using the scanning electron microscope (SEM).

3. Results and discussion

3.1. Effect of welding conditions on boron-assisted intergranular liquation cracking within grain coarsened HAZ

The dependence of the grain boundary segregation of boron and the effective segregation time on the isothermal in HAZ crack vulnerable region are shown in figure 1. In figure 1(a), longer effective time at fusion boundary is more prone to boron segregation than others, and the intergranular segregation of boron heterogeneously promotes the grain boundary liquation [15]. On the other hand, a longer effective time increases the nucleation rate of boride by virtue of binding the boron atoms at the grain boundaries and interphase interfaces. Nano-size boride phase is induced by the intergranular desegregation of boron [16] and intergranular segregation of boron leads to borides [17]. The optimization of the weld thermal cycle to ameliorate the material weldability by minimizing boron segregation is discussed below. In figure 1(b), on the one hand, the grain boundary segregation of boron significantly reduces with the increasing distance from the fusion boundary and there is a concentration gradient. The closer the distance to the fusion boundary, the greater the accumulation of the boron atoms segregation. The presence of boron segregation on the internal surfaces of the arterial crack network in the subsolidus portion of HAZ improves the low-melting terminal eutectic reaction of boride in the backfill along the crack path and results in the formation of an incoherent interface.

![Figure 1](image_url)

**Figure 1.** Role of temperature distributions near fusion boundary of HAZ in (a) effective segregation time and (b) grain boundary segregation of boron.

Focus position is an effective factor to determine the heat input and weld profile during the laser welding. The interaction between the focus position and the material surface, which is above or below
the material surface, modifies the heat transfer mode and grain boundary chemistry. The power intensity of focus position is much higher than that of defocus one. The role of focus position in grain boundary chemistry and weldability is shown in figure 2. Figure 2(a) shows that the grain boundary segregation is suppressed by the defocus positions. There is an enrichment of boron at the grain boundary by virtue of the focus position to significantly deteriorate liquation cracking susceptibility. In figure 2(b), the experimental results elucidate the effect of focus position on the microcrack length, and the total crack length increases at the focus position while maintaining other welding conditions. The theoretical predictions are in good agreement with the experiment results, and the detrimental effect of the minor boron on HAZ cracking susceptibility is correlated with the weldability. The development of increasing twin grain boundaries to reduce the boron segregation through grain boundary engineering during laser welding is underway.

![Figure 2](image)

**Figure 2.** Role of laser beam focus position in (a) grain boundary segregation of boron and (b) total crack length.

The role of laser welding conditions in grain boundary segregation and weldability is shown in figure 3. In figure 3(a), the theoretical predictions of the extent and direction of grain boundary segregation of boron under nonequilibrium solidification conditions of weld pool are compared. The point at 1.5m/min and 1.5kW is a turning point. Below it, desegregation dominates, while above it, the segregation prevails. It is clear that the decreasing laser power causes a parabolic distribution of the boron concentration. Meanwhile, the peak magnitude of the boron concentration decreases with low laser power. The grain boundary segregation of boron within quite narrow range of weld thermal cycle is differed and detrimentally determines the potential cracking location. In other words, the parabolic profile of grain boundary segregation is established under the restriction of low heat input (low laser power and slow welding speed). Beyond the foregoing conditions, such a phenomenon failed to occur. A nonlinear boron profile is distinguished under the small heat input of laser welding conditions; boron profile is monotonically distributed under the high heat input of the laser welding conditions. In figure 3(b), the experiment results of the microcrack length within the coarsened HAZ with the welding conditions is shown. Initially, the response of boron concentration to rapid weld thermal cycle exerts a powerful effect on the HAZ intergranular liquation cracking, and the as-segregated grain boundary is closely correlated to the HAZ microcrack. The risk of microcrack deterioration is
imminent at the location where the maximum amount of boron segregation occurs. Secondly, the anomalous effect of the welding speed on HAZ crack length with various laser powers is proposed [18], and a parabolic distribution is consistently extrapolated. The small heat input is consistently favored with sound weld pool geometry. It is feasible to modify the boron concentration by variety of welding conditions. The theoretical predictions are in satisfactory agreement with the microanalysis indirectly. Therefore, it is an important step towards a reasonable understanding the HAZ liquidation cracking behavior of nickel-based superalloys.

The dependence of critical time and critical time constant on weld thermal cycle through grain refinement is shown in figure 4. In figure 4(a), the distribution of the critical time and critical time constant of grain boundary segregation of boron are theoretically developed. It is indicated that the critical time of refined grain is lesser than that of the coarse ones. Sufficient time is not available for grain boundary saturation of boron under this welding condition. Only if the cooling time exceeds the critical time, a further reduction of critical time of segregation through grain refinement significantly facilitates the presence of grain boundary desegregation to deplete the boron concentration, otherwise the grain boundary segregation is intrinsically exacerbated. It is therefore implied that there is an inevitable critical grain size, below which the desegregation dominates, while above which the segregation prevails. In figure 4(b), the critical time constant of this superalloy is of the order of $10^2$ and controls the superalloy propensity of grain boundary segregation during laser welding. The critical time constant of refined grain is large than that of coarse ones, and initially increases at the depressed solidus temperature and then decreases. Furthermore, it monotonously reduces with subsequent cooling. In other words, the increasing critical time constant takes place at the onset of the cooling, when the mobility of species and the grain growth are highly activated. In figure 4(c), the HAZ grain size extensively coarsens in the presence of dissolving niobium carbide. An average grain size is 94μm after a preweld solution heat treatment, the actual HAZ recrystallized grain size is experimentally evaluated to about 160μm and the theoretical predictions are verified. Grain size refinement retards the grain growth while undergoing the weld thermal cycle. Besides the grain size strongly influences the segregation kinetics as shown in figure 4(a), the intergranular liquid film is more prone to spread along

![Figure 3. Role of laser welding parameters in (a) grain boundary segregation of boron and (b) total crack length.](attachment:image)
increasing grain boundary surface area and the thickness of liquid film is effectively relieved by a substantial liquid film migration through grain refinement. Therefore, grain refinement has powerful advantages to completely annihilate the HAZ intergranular liquation cracking and consistently conforms to the metallographic observation of crack-free weld through grain refinement, because nonequilibrium weld pool solidification reduces the solidification temperature range and ameliorates liquation cracking susceptibility. An attractive grain size refinement increases the grain boundary surface area [19,20] and minimizes the grain boundary segregation of boron [21] to effectively reduce the thickness of the intergranular liquid film and prevent the HAZ liquation cracking. A further reduction in HAZ liquation cracking through grain refinement after the welding conditions optimization is available. The weld thermal cycle, critical grain size and grain boundary segregation are closely interrelated, and refined grain size fairly attributes to stabilize the grain boundary desegregation during the weld thermal cycle. In figure 4(d), the solidus temperature, $T_s$, liquidus temperature, $T_L$, and depressed solidus temperature, $T_E$, are clearly indicated in the weld thermal cycle, and the grain boundary segregation of boron is insensitive after cooling down to $0.5T_m$.

![Figure 4](image-url)

**Figure 4.** Role of laser welding condition in (a) critical time, (b) critical time constant, (c) HAZ grain size and (d) weld thermal cycle through grain refinement.

### 3.2. Effect of boron-containing intergranular liquid film on the development of threshold tensile stress of solid-liquid interfacial decohesion within grain coarsened HAZ

In order to better understand the HAZ intergranular liquation cracking phenomenon, the theoretical predictions of threshold tensile stress development with partial and complete weld penetrations and experiment microcrack length are shown in figure 5. In figures 5(a) and 5(b), the effect of laser welding conditions on grain boundary segregation of boron is of particular concern. Grain boundary segregation of boron monotonically decreases with increasing welding speed, and monotonically increases with high laser power and vice versa, indicating that the optimum low heat input (high welding speed and low laser power) reduces the grain boundary segregation of boron to suppress the grain boundary liquation and therefore possesses the desirable advantages of the laser welding. In
figure 5(c), initially, the threshold tensile stress under full penetration is larger than that of the partial penetration within the retention stage of the high-temperature liquid film. A high heat input reduces the threshold tensile stress for full penetration conditions and sensitively affects the formation of potential crack nucleation sites. Tensile stress significantly decreases and imposes reliable order of magnitude just below the liquidus temperature. Secondly, full penetration produces a satisfactory weld geometry, improves the weldability, and is of significant importance. Heat input and material thickness are the two factors that control the weld shape, heat transfer and penetration. Weld with internal keyhole and backside complete penetration inevitably loses the transferable energy to the material and varies the mode of heat flow, while weld with a partial penetration adequately consumes the available heat input. A complete penetration is therefore energetically favorable to overall reduce the grain boundary segregation and the thickness of the intergranular liquid film, and directly increases the threshold tensile stress of solid-liquid interface decohesion, as compared with that of incomplete penetration. In figure 5(d), the experiment results of microanalysis measurement are compared. The conclusion is further corroborated by the experiment results in an indirect way. Full penetration is convincing for a high resistance to HAZ cracking, while partial penetration deteriorates the weldability instead of reducing the cracking.

The threshold tensile stress scales with the heat input, and the theoretical predictions of the thermal and mechanical responses of intergranular liquid film to various heat inputs for interfacial decohesion is shown in figure 6. In figure 6(a), initially, increasing heat input mitigates the threshold tensile stress to facilitate intergranular liqutation cracking. It further confirms the foregoing conclusion that the high heat input condition is detrimental to the weldability of this superalloy. Secondly, high heat input, on the one hand, favors the propensity of efficient diffusivity and solubility of boron in intergranular liquid film to significantly reduce the grain boundary energy and the solid-liquid interfacial energy and thicken intergranular liquid film. On the other hand, it predominantly facilitates the cracking at the
liquid film stage because local tensile stress component exceeds the strength of the solid-liquid interface, and degrades the capability of the superalloy to accommodate the thermal stress. Heat input is neither excessive high to induce the severe HAZ intergranular liquidation cracking nor is extreme low to fail in desirable weld geometry. Finally, HAZ intergranular liquidation cracking beneath the surface is effectively forestalled or lessened through careful control of laser welding heat input, instead of relying solely on suppression of boron segregation by the preweld heat treatment. Figure 6(b) shows that the grain boundary liquation and then solidification occur in a typical order of 0.1 s within the retention time on heating and cooling stages. An instantaneous weld thermal cycle is accurate. High heat input rapidly reaches the liquidus temperature during heating period near fusion boundary in HAZ. High laser power accelerates the grain boundary liquidation due to boron segregation to weaken the grain boundary. Low laser power tolerates the threshold tensile stress and increases the critical value to a certain extent. The relationship between the laser welding conditions, weld shape, material composition, grain boundary segregation of boron, constitutional liquation of carbide, HAZ grain size, liquation film and threshold tensile stress is established.

Figure 6. Role of heat input in (a) development of threshold tensile stress of solid-liquid interfacial decohesion and (b) weld thermal cycle.

4. Conclusions

- The distributions of segregation profiles in the coarsened HAZ are established under the restriction of heat input. The response of boron concentration to rapid weld thermal cycle exerts a powerful effect on HAZ intergranular liquation cracking.
- Weld profile plays a significant role in the grain boundary segregation. Full penetration is energetically favorable for the high resistance to HAZ intergranular liquidation cracking, whereas partial penetration deteriorates the weldability instead of reducing the cracking.
- Grain boundary segregation of boron is reduced with increasing welding speed and elucidates a parabolic-shape curve under a low laser power, while monotonously decreases under high laser power in this superalloy.
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