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Prediction of Dendrite Orientation and Stray Grain Distribution in Laser Surface-melted Single Crystal Superalloy

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A vectorization analysis technique for crystal growth and microstructure development in single-crystal weld was developed in our previous work. Based on the vectorization method, crystal growth and stray grain distribution in laser surface remelting of single crystal superalloy CMSX-4 were investigated in combination of simulations with experimental observations. The energy distribution of laser was taken into consideration in this research. The experimental results demonstrate that the simulation model applies well in the prediction of dendrite growth direction. Moreover, the prediction of stray grain distribution works well except for the region of dendrites growing along the [100] direction.

1. Introduction

Single crystal (SX) superalloys have been widely used in turbine blades for their prominent temperature capability. In order to extend the life cycle of SX components, SX laser deposition of superalloy was proposed. The laser surface-melted process can be treated as the laser deposition with a powder feed rate equal to zero. Consequently, research of laser surface-melted process will contribute to a better understanding of the SX laser deposition.

In the laser surface-melted process, the weld pool shape and thermal conditions play significant roles. The Rosenthal solution[1] was employed to define weld pool shape and thermal conditions by Vitek[2], and the modified Rosenthal approach was used to calculate the temperature field in the SX laser deposition[3]. In the work of Anderson et al.[4], the simulations were carried out by using the heat transfer and fluid flow code developed by Mundra et al.[5] and De and DebRoy[6]. These works are helpful to understand the thermal conditions. However, calculation details of some works are untraceable. Besides the simulation code, commercial FEM software is another choice[7–9]. But it is far from easy to generate a mesh on the solid–liquid interface and to get thermal conditions on these mesh grids by FEM.

Based on the prediction of melt–pool shape and thermal conditions, the dendrite growth direction, dendrite growth velocity (V_d) and thermal gradient along dendrite (G_d) growth direction can be calculated[10,11] by utilizing the geometry model derived by Rappaz et al.[12–14]. Liu and DuPont[15,16] studied the effects of variations in the geometrical parameters (measured parameters rather than simulation results) on the microstructure development in the weld pool. Recently, a vectorization method has been developed in our previous article[17], which handles various orientations very well. In addition, the computing codes of the method are easy to be written.

In the surface-melted process, research of stray grain (SG) is significant. Owing to Hunt[18], prediction of SG distribution can be realized. Hunt firstly developed the model to describe columnar to equiaxed transition (CET) under steady state conditions. Gaumann et al.[19] extended Hunt's model to a wider range of solidification conditions and applied it to laser fabrication of SX superalloy[3]. In later research, effects of welding conditions on the SG formation were studied in the works such as SG formation in weld[4,20–22], effects of substrate orientations on the CET transition[10,11], and coupled model (thermal and fluid flow) for laser processing[7,8]. However, the difference between predicted SG distribution and experimental result has not been discussed.

Although SX laser deposition was researched by Refs. [23–26], it is hard to select suitable processing parameters through simulation until now. Therefore, we attempt to get the parameters through simulation in this study. During this simulation, the processing

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parameters of laser beam diameter, power distribution and the laser absorptivity were taken into consideration. The thermal conditions were calculated and the distribution of SG was predicted based on the CET model[3,19]. Comparisons of SG distribution between experimental and calculated results were carried out. The results indicate that the CET model cannot predict the SG accurately in all regions of the weld, and the imperfection of the CET model was discussed. Furthermore, a rough model was given out to guide laser deposition parameters through simulation.

2. Procedure

2.1. Calculation of the weld pool shape and thermal conditions

Table 1 shows the list of symbols. In order to get the weld pool shape and thermal conditions, the width and depth were calculated firstly. Then the uniform grid points were generated in the cross section (Y–Z plane) of the pool. Thirdly, the X-coordinates were defined for these grids. In the calculation process, a specific finite element mesh was used to define the laser power distribution, which can refine the mesh around the solid–liquid interface.

A solution for the temperature field in the metal for a moving point heat source was proposed by Rosenthal[1]. By integrating this point source solution over an area, the heating from line sources, disc sources or any other definable distribution can be calculated. According to Dowden's book[27], the solution of steady state temperature field for the specified incident intensity distribution is:

$$T(x,y,z)=T_0+\frac{1}{2\pi k}\int_{x_1=-\infty}^{\infty}\int_{y_1=-\infty}^{\infty} I_a(x_1,y_1)\times\frac{\exp\left\{\frac{-V_b}{2\alpha}\left(\sqrt{(x-x_1)^2+(y-y_1)^2+z^2}-(x-x_1)\right)\right\}}{\sqrt{(x-x_1)^2+(y-y_1)^2+z^2}}\,dy_1dx_1 \tag{1}$$

where $I_a(x_1,y_1)$ is the absorbed intensity distribution of laser power falling on the surface of the work piece. Material properties were all based on CMSX-4 superalloy from Ref. [3]. $T = 1660$ K, $k = 22$ W m^{-1} K^{-1}, $\alpha = 3.66\times10^{-6}$ m^2 s^{-1}. The following simplifications are made for Eq. (1):

(1) The work piece material is assumed to be homogeneous and isotropic. An average value of the physical coefficients for the material such as thermal conductivity is used to provide a reasonable approximation.
(2) Compared with the external heat sources in the laser process, the latent heat of fusion is smaller and neglected.
(3) The equation applies only to conduction mode welds[28–30] in which the velocity of fluid flow is slow and neglected. And the absorption efficiency used in calculation is the real absorption efficiency deducting the loss of thermal radiation and heat transfer caused by carrier and shielding gas etc.
(4) The equation applies to the laser processing approximately except beginning and end location.
(5) The size of substrate is large enough, and hence the rise of substrate temperature is negligible for subsequent calculations.

The intensity profile for laser with a near top hat mode (TEM$_{01}$)[29] can be well described by Eq. (2).

$$I(x_1,y_1)=\frac{4P(x_1^2+y_1^2)}{\pi w^4}\times\exp\left[\frac{-2(x_1^2+y_1^2)}{w^2}\right]. \tag{2}$$

In Eq. (2), P is laser power; w is the beam radius. The CO$_2$ laser used for all experiments is TEM$_{01}$ mode in this work. Eq. (2) is transformed into Eq. (3) for the finite element calculation. As seen in Fig. 1, (x_1,y_1) is coordinate of triangular center, and ΔS is the area of triangle used in finite clement calculation. η is the absorption efficiency of the laser.

$$\Delta I_a(x_1,y_1)=\frac{4P(x_1^2+y_1^2)\eta}{\pi w^4}\times\exp\left[\frac{-2(x_1^2+y_1^2)}{w^2}\right]\Delta S,\quad \left((x_1^2+y_1^2)^{0.5}\le 1.5w\right). \tag{3}$$

It can be calculated that 94% of the laser power is concentrated in the area of $(x_1^2+y_1^2)^{0.5}\le 1.5w$; the power out of the area was discarded in this work. The absorption efficiency was defined with calculating and experimental results. The grid size of mesh can be properly large under the precondition of ensuring calculating precision. Fig. 1 is a schematic diagram for better visibility, and the mesh used in calculation is much denser than it.

Combined with Eq. (3), Eq. (1) is transformed into,

$$T(x,y,z)=T_0+\frac{1}{2\pi k}\sum\Delta I_a(x_1,y_1)\times\frac{\exp\left\{\frac{-V_b}{2\alpha}\left(\sqrt{(x-x_1)^2+(y-y_1)^2+z^2}-(x-x_1)\right)\right\}}{\sqrt{(x-x_1)^2+(y-y_1)^2+z^2}},\quad \left((x_1^2+y_1^2)^{0.5}\le 1.5w\right). \tag{4}$$

If the laser beam $((x_1^2+y_1^2)^{0.5}\le 1.5w)$ is fully located in the weld pool, the finite element mesh is generated as Fig. 1(a) and the thermal conditions can be calculated directly based on Eq. (4).

Table 1
List of symbols

T	Solidification temperature
T_0	Substrate temperature
P	Laser power
V_b	Velocity of laser beam
k	Thermal conductivity
α	Thermal diffusivity
G_{sl}	Thermal gradient on solidification front
G_x, G_y, G_z	Component of thermal gradient along x, y, z axes
G_d	Component of thermal gradient along dendrite growth direction
V_{sl}	Growth velocity of solid–liquid interface
V_d	Dendrite growth velocity along preferred orientation
Φ	Areal fraction of stray grains of each point in the solidification front
I	Intensity distribution of laser
I_a	Absorbed intensity distribution of laser
η	Laser absorptivity
w	Laser beam radius

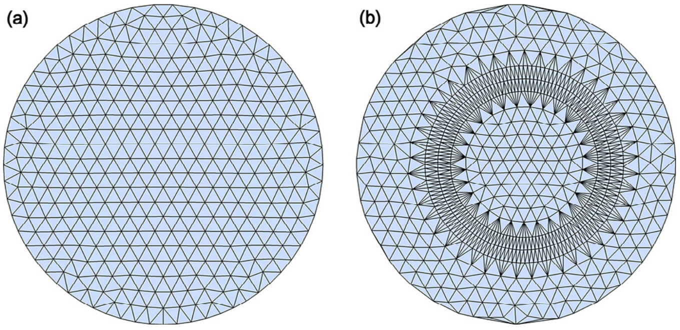

Fig. 1. Schematic illustration of generating finite element mesh: (a) laser beam is fully located in the weld pool; (b) part of laser beam out of weld pool.

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