Effects of melt-pool geometry on crystal growth and microstructure development in laser surface-melted superalloy single crystals. Mathematical modeling of single-crystal growth in a melt pool (part I)

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Abstract

The effects of melt-pool geometrical parameters on crystal growth and microstructure development during laser surface melting of single-crystal alloys were studied by means of mathematical modeling and experiments. A mathematical model was developed for the three-dimensional (3-D) melt-pool geometry and single-crystalline melt-pool solidification in laser surface melting. The 3-D melt-pool geometry corresponding to the solidification interface is described by four geometrical parameters ($w$, $l$, $h$, $a$). The model was used to study the effects of variations in the geometrical parameters on crystal growth and microstructure development in the melt pool. Laser surface melting experiments with single-crystal nickel-base superalloys were conducted to verify the computational results of microstructure development in the melt pool. Results indicate that the melt-pool geometrical parameters have profound influences on the dendrite growth velocity and growth pattern in the melt pool. For the (001)/[100] substrate orientation, variations in $l/w$ and $a$ can influence both the number and the relative sizes of growth regions while the variation in $h/w$ can only influence the relative sizes of the growth regions. Unidirectional dendrite growth along the [001] crystallographic direction can be achieved for an $a$ value of 45° or below. The maximum ratio of dendrite-growth velocity to the beam velocity in the melt pool is related to $a$ and $l/w$. Experimental microstructure observations agreed well with the computational results. These findings show that the desired dendrite growth velocity and microstructure can be obtained through proper control of the 3-D melt-pool geometry.

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1. Introduction

Nickel-base superalloys are critical high-temperature materials to the aerospace and energy industries due to a combination of superior strength, ductility, and crack resistance at elevated temperatures. Directionally solidified single-crystal nickel-base superalloys have been used in high-temperature gas turbines as blades and vanes in order to increase the operating temperature and, in turn, to improve the overall efficiency of the gas turbines [1,2]. There are two distinct advantages in the use of single-crystal superalloy components. First, both the creep resistance and thermomechanical fatigue behavior are enhanced due to the absence of grain boundaries. Secondly, the minor elements required for grain boundary strengthening in the polycrystalline superalloys, such as carbon, boron and zirconium, can be removed, which increases the incipient melting temperatures of the SX superalloys.
Although modern gas turbines are extremely reliable, wear and other types of damage (e.g., blade tip erosion, and thermal fatigue cracks) to components, especially those under severe thermo-mechanical and corrosive conditions are unavoidable. The high replacement costs of gas turbine engine components necessitate the repair of worn or damaged components. The economic benefit is even more tremendous for the repair and reshaping of damaged single-crystal gas turbine blades and vanes. In addition, there is also a serious need to repair the single-crystal components for salvaging the defects (such as surface pores) in as-cast parts. A successful single-crystal repair should ensure the preservation of the single-crystal nature, i.e., a single-crystal weld or deposit needs to be produced which is epitactic with the substrate, since the single-crystal superalloys do not contain grain boundary strengtheners [3]. Fusion welding processes are widely used for general repair applications. However, recent studies on electron beam and pulsed laser beam welds of single-crystal nickel-base superalloys by David et al. [4,5] showed that it was difficult to maintain the single-crystal nature of the nickel-base superalloys during welding due to stray grain formation. Moreover, single-crystal nickel-base superalloys were found to be very prone to cracking during welding. In contrast to nickel-base superalloys, Rappaz et al. [6,7] and David et al. [8] observed nearly complete absence of stray grains and nearly perfect retention of the single-crystal nature in electron beam welds of an austenitic stainless steel single-crystal alloy Fe–15Cr–15Ni (in wt%).

Laser engineered net shaping (LENS) is a solid freeform fabrication (SFF) process based on laser cladding, which involves laser processing fine metal powders into fully dense three-dimensional shapes directly from a computer-aided design (CAD) model. The LENS process was first developed at the Sandia National Laboratories and subsequently commercialized by the Optomec Design Company in Albuquerque, New Mexico. This novel process is able to fabricate complex prototypes in near-net shape, leading to significant time and machining cost savings. A variety of alloys and composites have been deposited by LENS processing such as H13 tool steel, stainless steels, nickel-base superalloys, titanium alloys, and cermets [9–13]. It also has potential for precision repair, fast tooling, and small lot production [12]. As a process for repair applications, the LENS process has several potential advantages over the conventional processes. It exposes the part to far less heat than conventional welding techniques, and the heat-affected zone (HAZ) is much smaller, thus significantly reducing any structural and mechanical degradation to the part while repairing a specific area. The LENS process can also offer exceptional material properties and interface characteristics to the repaired part for property enhancements. For example, refined microstructures in the repaired area can be produced due to the rapid solidification conditions associated with the laser processing. Functionally graded materials and coatings can be fabricated to improve the interface characteristics and/or the surface properties of the repaired part [13].

The melt-pool solidification conditions during LENS processing, as in the case of laser cladding or laser surface melting, generally result in a dendritic microstructure with columnar or equiaxed growth morphology [10]. Recent studies by Gaumann et al. [14,15] using a laser metal forming (LMF) technique indicated single-crystalline solidification could be achieved in the melt pool of nickel-base superalloy by a careful selection of the processing parameters, to allow only the epitaxial growth of columnar dendrites from the substrate and to avoid the columnar-to-equiaxed transition (CET) when a single-crystal substrate was used. Our most recent work on LENS processing of single crystal superalloys showed that the LENS process could be used as a potential method to repair single-crystal components.

The laser surface melting process can be treated as a laser cladding process without any powder feeding. This process can be used for removal of casting defects (such as surface porosity, surface secondary grains) in single-crystal components for repair applications. The laser surface melting process has been also widely used as a rapid solidification technique for surface modification of materials [16,17]. Recently, research was conducted on microstructure developments in the melt pool of single-crystal alloys produced by laser surface melting [15,18,19] and electron beam welding [6–8]. Narasimhan et al. [18] were among the first to investigate the microstructure of a laser surface-melted single crystal nickel-base superalloy (Udimet 700). Rappaz et al. [6,7] and David et al. [8] conducted extensive studies on the microstructure formation in single-crystal welds of stainless steel Fe–15Ni–15Cr alloy and nickel-base superalloys, respectively. Rappaz et al. [6] also established a relationship between the growth velocity of selected dendrite variants and the welding velocity. Yang et al. [19] experimentally investigated the microstructure evolution in the laser surface-melted pool of a single-crystal superalloy by changing the processing conditions. Gaumann et al. [15] conducted a theoretical modeling study on processing/microstructure-selection relationship in laser surface remelting of single-crystal superalloys. A microstructure criterion to avoid the CET was developed.

The main objective of this work is to study systematically the effects of the melt-pool geometry (geometrical parameters) and substrate crystallographic orientation on the crystal growth (direction and velocity) and microstructure evolution in laser surface melting of single-crystal alloys. For this purpose, the solid/liquid interface of the melt pool formed during laser surface melting was first represented in 3-D as a segment of an ellipsoid using four geometrical parameters. The melt-pool model
was then used in combination with the dendrite growth concepts to predict the dendrite growth directions and velocities as a function of the melt-pool geometrical parameters and substrate crystallographic orientations. This paper addresses the effects of melt pool geometry on crystal growth directions and velocities in laser surface melting of single-crystal alloys. In another companion paper, the effects of the substrate crystal orientation during laser surface melting of single-crystal alloys will be discussed. Laser surface melting experiments were conducted on single-crystal nickel-base superalloys using a Nd:YAG laser in the LENS system to verify the computation results. It is expected that future work could combine the modeling results presented here with a heat and fluid flow model (to predict the geometrical parameters of the melt pool) and the analytical CET model to develop a complete model for predicting the desired processing conditions needed to maintain the single-crystal nature.

2. Mathematical model and analysis

2.1. 3-D melt-pool shape and geometrical parameters

The interaction of a laser beam with the irradiated material is a complex physical phenomenon. Considerable theoretical and experimental research conducted so far in the area of partial-penetration arc welding and laser surface melting suggests the melt-pool shape generally acquires the form of an ellipsoid (but asymmetric in the traveling direction of the heat source) [18–26]. The theoretical analysis by Christensen et al. [20,24] based on the Rosenthal thick plate solution [21] derived an elliptical (in the traveling direction of the heat source) melt-pool shape with a transverse semi-circular contour (the maximum pool depth equal to half of the maximum pool width). To overcome the problem with the transverse semi-circular contour that differs from the experimental observations, Goldak et al. [26] in their research assumed a double-ellipsoid weld pool shape that consisted of the front and rear ellipsoid quadrants. In all of these melt-pool models, the angle between the workpiece surface and the tangent of the melted trace in the transverse cross-section. It is worth noting that $h \equiv w$ and $x \equiv 90^\circ$ for the melt-pool shape obtained from the Rosenthal analytic solution to the temperature field induced by a moving point heat source along the surface of a semi-infinite solid [21,23,24]. The melt-pool geometrical parameters are directly related to the heat and fluid flow conditions during processing (i.e., the laser surface processing conditions). They can be determined either computationally from a 3-D melt pool heat and fluid flow simulation [27,28] or experimentally by directly measuring these parameters in-situ or after processing. The melt-pool shape corresponding to the solidification front is given by the following function (see Appendix A for details):

$$x = f(y, z) = -A \left[ 1 - \frac{y^2}{B^2} - \left( \frac{z - D}{(h + D)^2} \right)^2 \right]^{0.5},$$

where

$$D = \frac{h^2}{w \tan x - 2h},$$

$$A = \frac{l(h + D)}{(2hD + h^2)^{0.5}},$$

Fig. 1. Schematic representation of (a) 3-D melt-pool shape and (b) geometrical parameters used.
\[ B = \frac{w(h + D)}{(2hD + h^2)^{0.5}}, \]  
(4)

and \( A, B, D \) are all positive real numbers. The unit vector of the normal to this surface can be represented by the following components:

\[ \vec{n} = \frac{1}{\left[1 + (\partial f/\partial y)^2 + (\partial f/\partial z)^2\right]^{0.5}}(1 - \partial f/\partial y - \partial f/\partial z). \]  
(5)

It should be pointed out that the above melt-pool model is developed for laser surface processing and obviously cannot be used for full-penetration welding or other processes where the melt-pool shape deviates significantly from a segment of an ellipsoid.

2.2. Dendrite growth velocity and direction

In the present analysis, it is assumed that the growth of dendrites is epitaxial from the substrate and the single-crystal nature of the substrate is thus maintained after the laser surface melting processing. Under welding and laser solidification processing conditions, the velocity of the solid–liquid interface \( (V_n, \text{i.e., the normal velocity of the melt-pool interface}) \) is linked geometrically to the heat source travel speed \( (V_b) \) by the angle \( (\theta) \) between the normal to the melt-pool interface and the travel direction of the heat source, as given by the following equation [29]:

\[ |\vec{V}_n| = |\vec{V}_b| \cdot \cos \theta. \]  
(6)

In Rosenthal’s analytical solution [21,23,24] where \( z = 90^\circ \), \( V_n \) increases from zero at the bottom and the sides of the melt pool to a value equal to \( V_b \) at the rear of the melt-pool surface. In the case of dendritic growth, due to the effects of preferred crystallographic direction, the dendrite growth velocity is not always equal to the velocity of the solid–liquid interface \( (V_n) \). A relationship between the growth velocity \( (V_{hkl}) \) of the dendrite tip along a specific crystallographic direction \( [hkl] \) and the heat source travel speed \( (V_b) \) was derived by Rappaz et al. [6], as given by

\[ |\vec{V}_{hkl}| = |\vec{V}_b| \cdot \frac{\cos \theta}{\cos \psi_{hkl}}, \]  
(7)

where \( \psi_{hkl} \) is the angle between the normal \( (\vec{n}) \) to the melt-pool interface and the \( [hkl] \) direction (Fig. 2).

For the face-centered cubic (fcc) nickel-base superalloys studied in present work, the six \( (100) \) directions are the preferred directions of growth. At a given location of the melt-pool interface, it is assumed that the dendrite trunk which is selected from among the six possible \( (100) \) variants is the one that is the closest in orientation to the direction of maximum temperature gradient (i.e., the direction of the normal to the melt-pool interface).

![Fig. 2. Schematic representation of the angular relationships between the solidification interface normal (\( \vec{n} \)) and the \( x-y-z \) reference system and between the normal (\( \vec{n} \)) and the \( [hkl] \) dendrite growing direction (\( \vec{V} \)).](image)

In other words, the minimum value of the angle-\( \Psi_{hkl} \) determines the orientation \( [hkl] \) (where \( [hkl] \) is one of the six \( (100) \) directions) of the dendrite trunk that is selected at a given location of the melt-pool interface [6]. This dendrite trunk selection criterion corresponds to a minimum growth velocity of the dendrite tip, as one can see in Eq. (7). The minimum growth velocity also leads to a minimum undercooling of the dendrite tip since the undercooling increases with increasing growth velocity over the dendritic stability range, as indicated by Rappaz et al. [7].

In order to calculate the angle-\( \Psi_{hkl} \) and subsequently the growth velocity \( (V_{hkl}) \), one needs to determine the angles \( \theta \) and \( \phi \) that are used to specify the direction of the normal \( (\vec{n}) \) to the melt-pool interface (where \( \phi \) is the angle between the \( y \)-axis and the projection of \( \vec{n} \) on the \( y-z \) plane). Based on Fig. 2, the components of the unit vector of the normal \( (\vec{n}) \) to the melt pool interface are given in the \( x-y-z \) reference system by

\[ \vec{n} = (\cos \theta \quad \sin \theta \cos \phi \quad \sin \theta \sin \phi). \]  
(8)

By comparing Eq. (8) with Eq. (5), one can obtain \( \theta \) and \( \phi \) in the following expressions:

\[ \theta = \arctan \left[ \left( \frac{(\partial f/\partial y)^2 + (\partial f/\partial z)^2}{(\partial f/\partial y)^2} \right)^{0.5} \right], \]  
(9)

\[ \phi = \arctan \left( \frac{\partial f/\partial z}{\partial f/\partial y} \right). \]  
(10)

(see Appendix B for details of calculations of \( \theta \) and \( \phi \)). The unit vector describing the \( [hkl] \) crystallographic direction in the \( x-y-z \) reference system can be expressed with its components \( u_x, u_y \) and \( u_z \) as
\[ \vec{u}_{hh} = (u_x, u_y, u_z). \]  

(11)

Thus, after determining the values of \( \theta \) and \( \phi \), the angle \( \Psi_{hh} \) characterizing the orientation of a specific (100) variant with respect to the normal (\( \vec{n} \)) can be obtained through Eqs. (8) and (11) as follows:

\[ \cos \Psi_{hh} = \vec{u}_{hh} \cdot \vec{n} = u_x \cos \theta + \sin \theta (u_y \cos \phi + u_z \sin \phi). \]

(12)

Finally, the velocity ratio \( V/V_{th} \) can be calculated from Eq. (7).

2.3. Computation

Based on the above model, a computer program was written using the FORTRAN programming language for the model computations. For a specific set of melt-pool geometrical parameters \( (w, l, h, z) \), the melt-pool shape (i.e., the surface of the solidification front) was first computed. Next, the angles \( \Psi_{hh} \) of the six potentially active (100) dendrite directions were computed for a matrix of points on the melt-pool interface according to a specific substrate crystal orientation with respect to the laser scanning direction. The dendrite growth direction at a specific point on the melt-pool interface was determined by the minimum of these angles \( \Psi_{hh} \) and identified by the computer program, and the ratio of the dendrite growth velocity to the laser beam travel velocity was subsequently computed. By changing the melt-pool geometrical parameters \( (w, l, h, z) \) and substrate crystal orientation with respect to the laser scanning direction, one can, using this model, systematically study the effects of melt-pool geometry and crystal orientation on crystal growth and microstructure developments in laser surface-melting and other similar solidification processing of single-crystal alloys.

3. Experimental procedure

An Optomec LENS™ 750 system was used in this study for the laser surface melting experiments. The LENS machine consists of a continuous-wave Nd:YAG laser, a controlled environment glove-box, a motion control system and a powder feed system (no powder feeding was utilized for the surface melting experiments in the present investigation). The Nd:YAG laser has a circular beam of 0.5–1-mm-diameter at the focal zone with a Gaussian intensity distribution and a maximum output power of 750 W. The oxygen level in the Ar-gas atmosphere glove box was below 30 ppm during the laser processing. The LENS system is equipped with a melt-pool sensor that provides a 2-D infra-red image of the molten pool on the substrate surface. The melt pool image can be used for the determination of melt-pool geometrical parameters.

A typical commercial single-crystal nickel-base superalloy, the CMSX-4 alloy, was chosen for the experiments for consideration of practical applications. The nominal composition of this alloy is Ni–9Co–6.5Cr–5.6Al–1Téli–6.5Ta–3Re–0.6Mo–0.1Hf (in wt%). The as-grown crystal obtained from Concorde Castings (Eastlake, OH) was cut into specimens of approximately 9 (width)×4.5 (thickness)×20 (length) mm used in the laser surface melting experiments, with the (001) orientation normal to the surfaces of the specimen. For the investigation described in this paper, laser surface melting was performed along the [100] crystallographic direction on the (001) substrate surface. The substrate surfaces to be laser-processed were ground with 600-grit SiC paper and cleaned in methanol before laser surface melting. Experiments were conducted under different processing conditions by changing the laser power and travel velocity (Table 1). Although the melt-pool geometrical parameters can be obtained from a 3-D melt-pool heat and fluid flow simulation computation, as mentioned previously, the heat and fluid flow modeling is beyond the objective of this work. Therefore, in this study the melt-pool geometrical parameters were determined by the following experimental methods. The melt-pool half-width \( (w) \), depth \( (h) \) and the \( z \) angle were directly measured from the photomicrographs of the transverse cross-sections. The melt-pool length parameter \( (l) \) was determined from the 2-D video image of the melt pool or from direct measurements of the melt-pool traces (ripple formation) on the top surface of the melt track. Samples for microstructure analysis were mounted and polished using standard metallographic techniques and etched with a solution containing \( \text{HCl} (100 \text{ ml}), \text{HCl} (100 \text{ ml}) \) and \( \text{CuCl}_2 \) (5 g).

4. Results and discussion

For convenience of results presentation and comparison, in the computations presented in Sections 4.1–4.3, the melt-pool geometrical parameters \( (w, l, h) \) excluding the angle \( z \) are represented by their relative values using \( w \) as the reference parameter. Thus, in the \( x-y-z \) reference frame defined in Fig. 1, on the melt-pool interface corresponding to the solidification front, the value of

<table>
<thead>
<tr>
<th>Track No.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power (W)</td>
<td>200</td>
<td>200</td>
<td>375</td>
<td>500</td>
</tr>
<tr>
<td>Velocity (mm/s)</td>
<td>4</td>
<td>2.5</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td>( w ) (mm)</td>
<td>0.52</td>
<td>0.52</td>
<td>0.5</td>
<td>0.56</td>
</tr>
<tr>
<td>( h ) (mm)</td>
<td>0.194</td>
<td>0.235</td>
<td>0.19</td>
<td>0.215</td>
</tr>
<tr>
<td>( l ) (mm)</td>
<td>0.52</td>
<td>0.51</td>
<td>1.35</td>
<td>1.65</td>
</tr>
<tr>
<td>( z ) (°)</td>
<td>75</td>
<td>62</td>
<td>69</td>
<td>73</td>
</tr>
</tbody>
</table>
$x/w$ varies from $-l/w$ to zero, the value of $y/w$ varies from a minus unit to a unit, and the value of $z/w$ varies from $-h/w$ to zero. Effects of variations in the geometrical parameters were studied by changing the ratios $l/w$ and $h/w$ and the value of the angle $\alpha$.

### 4.1. Effect of variations in $l/w$

Fig. 3(a) and (b) shows the computational results of dendrite growth velocities and directions on the melt-pool solidification interface for a melt pool of the geometrical parameters $l/w=1.5$, $h/w=1$ and $z=75^\circ$ produced when the laser surface melting is conducted along the [100] crystallographic direction on the (001) plane of the single-crystal substrate. The same substrate crystallographic orientation conditions with respect to the laser scanning direction are used for all the computational results and discussion in this paper, and will not be mentioned hereafter. From the dendrite growth direction graph (Fig. 3(b)) plotted in the $y$–$z$ plane, four regions corresponding to four growth directions can be seen. In the bottom region of the melt pool, the [001] growth direction is chosen. For the side regions of the melt pool, either the [010] or the [100] growth direction is favored. In the rear part of the melt pool (corresponding to the region closest to the origin in the $y$–$z$ cross-section plane), the [100] dendrites grow along the laser beam travel direction. At the boundaries between the regions, the possibility of the dendrite to grow along either direction is the same since in each case the value of the angle $\Psi$ is equal. From the contour graph (Fig. 3(a)) depicting the distribution of the dendrite growth velocities during the melt-pool solidification, which is also plotted in the $y$–$z$ plane, it can be seen that from the bottom and the sides of the melt pool to the rear part of the melt-pool interface the dendrite growth velocity increases gradually, with a maximum growth velocity equal to the beam travel velocity ($V_b$) in the [100] growth region. Fig. 4(a) shows the variation of dendrite growth velocity along the melt-pool boundary line in the $x$–$z$ plane (under the same melt pool geometrical conditions as given in Fig. 3). The relative melt-pool depth ($z/w$) along the boundary line is also shown in

![Fig. 3](image-url)

Fig. 3. Dendrite growth velocities (a) and directions (b) on the melt pool solidification interface for a melt pool of the geometrical parameters: $l/w=1.5$, $h/w=1$ and $z=75^\circ$ with the (001)/[100] substrate orientation.

![Fig. 4](image-url)

Fig. 4. (a) Variation of dendrite growth velocity along the melt-pool boundary line in the $x$–$z$ plane, together with the variation of the relative melt-pool depth on this line; (b) variation of dendrite growth velocity along the melt-pool trace line in the $x$–$y$ plane, together with the variation of the relative melt-pool width on this line ($l/w=1.5$, $h/w=1$ and $z=75^\circ$).
this figure for reference. It is clearly seen from the computational results that the ratio of dendrite growth velocity to the beam velocity \( \frac{V}{V_b} \) increases from zero at the bottom of the melt pool to exactly a unit at the rear of the boundary line. The beginning point of the dendrite growth velocity equal to the beam travel velocity corresponds to the transition of dendrite growth direction from [001] to [100]. At the transition point on this boundary line, the values of \( \theta \) and \( \psi_{100} \) (the angle between the normal to the boundary line and [100]) and \( \psi_{001} \) (the angle between the normal and [001]) are all the same, which is 45°. Fig. 4(b) shows the variation of dendrite growth velocity along the melt-pool trace line on the top surface (x-y plane), together with the variation of the relative melt-pool width \( \frac{y}{w} \) on this same surface (under the same melt-pool geometrical conditions as given in Fig. 3). The results shown in this figure are only for the -y side of the melt pool due to symmetry in this case. The computational results indicate that the ratio of dendrite growth velocity to the beam velocity \( \frac{V}{V_b} \) increases from zero at the side of the melt pool to a unit at the rear of the melt-pool surface. Similarly, at the transition point of the dendrite growth direction from [010] to [100] where the dendrite growth velocity starts to equal the beam travel velocity, the angles \( \theta \), \( \psi_{100} \) and \( \psi_{010} \) have the same value of about 48° in this case.

When the \( l/w \) value is reduced from 1.5 to a unit (corresponding to a circular shape on the top surface) and the other geometrical parameters remain unchanged, based on the computational results shown in Fig. 5, the main characteristics of the dendrite growth velocity distribution and the pattern of dendrite growth directions do not change much. However, in comparison with Fig. 3, the area of the [100] growth region is increased while the areas of the [001], [010], and \[010\] growth regions are decreased. Accordingly, the area with a maximum velocity ratio in the contour graph of dendrite growth velocity is increased. These changes occur due to the variation in the slope of the melt-pool interface in the length direction (x-axis direction) caused by the change in the \( l/w \) value. As the \( l/w \) value is decreased from 1.5 to 1.0, the slope of the melt-pool interface in the x-axis direction is increased, resulting in a bigger area with the angle \( \theta \) smaller than 45° where the [100] dendrites grow.

On the contrary, the area of the [100] growth region will be decreased when the \( l/w \) value increases. In actual situations, the \( l/w \) value increases with increasing processing speed \( V_b \). As the \( l/w \) value increases to a...
critical value, no dendrite will grow along the [100] direction. Theoretically, according to the model proposed in the present paper, the critical \( l/w \) value \( (l/w)_c \) for the [100] dendrite growth to disappear is related to the angle \( \alpha \) by the following expression:

\[
\frac{l}{w}_c = \tan \alpha.
\]  

(13)

(The above equation can be derived by the following relation: \( \tan \beta = w/l \cdot \tan \alpha \), where \( \beta \) is the angle between the substrate surface and the tangent of the melt-pool interface in the \( x-z \) plane. No dendrites grow along the [100] direction when \( \beta \leq 45^\circ \).) For \( \alpha = 75^\circ \), Eq. (13) gives a critical \( l/w \) value of 3.72. Fig. 6(a) and (b) shows the computational results of dendrite growth velocities and directions on the melt-pool solidification interface for a melt pool of the geometrical parameters \( l/w = 4, h/w = 1 \) and \( \alpha = 75^\circ \). From the dendrite growth direction graph, only the [001], [010] and \([010]/C22\) dendrite growth regions can be observed, and the [100] dendrite growth region no longer exists. As seen in the contour graph of the velocity ratio \( (V/V_b) \), the maximum value of the velocity ratio and the change in velocity with location over the whole melt-pool interface is reduced due to the disappearance of the [100] dendrite growth. Fig. 7(a) and (b) shows variations of the velocity ratio along the melt-pool boundary lines in the \( x-z \) plane and in the \( y-z \) plane (top surface), respectively. In comparison to Fig. 4, as the melt-pool shape becomes more elongated and the \( l/w \) value is larger than the critical value, the velocity ratio is always less than a unit. But the maximum velocity ratio is invariably at the trailing point of the melt-pool surface with a coordinate of \( (l/w, 0, 0) \) in the \( x-y-z \) reference frame. Under the conditions of laser scanning along the [100] direction on the (001) substrate plane, based on the 3-D melt-pool shape Eq. (1) and the velocity ratio Eq. (7), the maximum velocity ratio can be derived to be a function of the geometrical parameters \( l, w \) and \( \alpha \), which is given by the following equations:

\[
\frac{V}{V_b}_{\text{max}} = \frac{w}{l} \cdot \tan \alpha \quad (\text{for } l/w \geq \tan \alpha),
\]  

(14)

\[
\frac{V}{V_b}_{\text{max}} = 1 \quad (\text{for } l/w < \tan \alpha),
\]  

(15)

\[\text{Fig. 7. (a) Variation of dendrite growth velocity along the melt-pool boundary line in the } x-z \text{ plane, together with the variation of the relative melt-pool depth on this line; (b) variation of dendrite growth velocity along the melt-pool trace line on the } x-y \text{ plane, together with the variation of the relative melt-pool width on this line (} l/w = 4, h/w = 1\text{ and } \alpha = 75^\circ\).} \]
For $\alpha = 75^\circ$ and $l/w = 4$, Eq. (14) gives the maximum velocity ratio of 0.93, which is shown in Fig. 7.

4.2. Effect of variations in $h/w$

Fig. 8 shows the results of dendrite growth directions and velocities on the melt-pool solidification interface for a melt pool of the geometrical parameters $l/w = 1.5$, $h/w = 0.48$ and $\alpha = 75^\circ$. Compared to Fig. 3, the relative area of the [001] growth region on the melt-pool interface is greatly increased and the relative areas of the [100], [010] and [010] growth regions are all significantly decreased in Fig. 8 when the $h/w$ value is reduced from a unit to 0.48 with other geometrical parameters remaining the same. As the area of the [100] growth region is decreased, the area with the highest growth velocity ratio in the velocity-ratio contour graph is also reduced. These changes in computational results can be simply explained according to the change in the 3-D melt-pool shape. The decrease in the melt-pool depth, with other geometrical parameters fixed, leads to a reduction in the slope of the melt-pool interface in both the $x$ and $y$ directions which promotes the [001] dendrite growth.

Fig. 9 shows the dendrite growth direction and velocity results for a melt pool of the geometrical parameters $l/w = 4$, $h/w = 0.6$ and $\alpha = 75^\circ$, which are in contrast to those given in Fig. 6 obtained for a set of geometrical parameters $l/w = 4$, $h/w = 1$ and $\alpha = 75^\circ$. In these cases, as the $l/w$ value is larger than its critical value for disappearance of the [100] dendrite growth, the reduction in the $h/w$ value can only influence the relative areas of the [001], [010] and [010] growth regions, increasing the [001] growth region and decreasing the other two regions. It is interesting to note that, unlike the variation in the $l/w$ value, the variation in the $h/w$ value cannot determine the existence or elimination of a specific growth region, although it can change the relative areas of the growth regions on the melt-pool interface. Furthermore, as indicated in Eqs. (14) and (15), the maximum ratio of dendrite growth velocity to the beam velocity in the melt pool is independent on the $h/w$ value.

4.3. Effect of variations in the angle $\alpha$

Fig. 10 shows the results of dendrite growth directions and velocities on the melt-pool solidification interface for a set of geometrical parameters $l/w = 1.5$, $h/w = 1$ and $\alpha = 90^\circ$. This set of geometrical parameters gives a semi-circular cross-section in the $y-z$ plane and represents a melt-pool shape that can be derived from the
Rosenthal solution to the three-dimensional temperature field induced by a point heat source moving along the surface of a semi-infinite solid, as mentioned previously. In this computation, the angle $\alpha$ is approximated by $\alpha = 89.99^\circ$ since the tangent of a $90^\circ$ angle is infinite. In comparison to Fig. 3, the change of the angle $\alpha$ from $75^\circ$ to $90^\circ$ only influences the relative areas of the four dendrite-growth regions. A larger $\alpha$, which also induces a larger $\beta$ (the angle between the substrate surface and the tangent of the melt-pool interface in the $x$-$z$ plane), increases the slope of the melt pool interface in both the $x$ and $y$ directions, thus promoting the dendrite growth along the [100], [010] and [010] directions and accordingly depressing its growth along the [001] direction.

On the contrary, the dendrite growth along the [001] crystallographic direction is promoted and its growth along other directions is depressed on the melt-pool interface as the value of the angle decreases. As mentioned previously, the [100] dendrite growth disappears when $\beta = 45^\circ$. Based on the relationship between $\beta$ and $\alpha$: $\tan \beta = \frac{w}{l} \tan \alpha$, the critical $\alpha$ value ($\alpha_c$) for disappearance of the [100] dendrite growth can be expressed as $\alpha_c = \arctan \left( \frac{l}{w} \right)$.

For $l/w = 1.5$, Eq. (16) gives a critical value $\alpha_c = 56.3^\circ$. Fig. 11(a) and (b) shows the computational results of dendrite growth directions and velocities on the melt-pool solidification interface for the geometrical parameters $l/w = 1.5$, $h/w = 0.48$ and $\alpha = 55^\circ$, which are in contrast to those given in Fig. 8 obtained for a set of geometrical parameters $l/w = 1.5$, $h/w = 0.48$ and $\alpha = 75^\circ$. Fig. 12. Dendrite growth velocities (a) and directions (b) on the melt pool solidification interface. Melt-pool geometrical parameters: $l/w = 1.5$, $h/w = 0.48$ and $\alpha = 45^\circ$.

Fig. 13. The influence of $\alpha$ values on the maximum velocity ratio as a function of the $l/w$ ratio.
It should be pointed out here that the relationship \( h/l < 0.5 \tan \alpha \) must be satisfied in order for the value of \( D \) to be positive according to Eq. (2). As seen from the dendrite growth direction graphs, the decrease of the \( \alpha \) value from 75° to 55°, with other parameters remaining unchanged, leads to the elimination of the [100] dendrite growth region and decreases in the relative areas in the [010] and [010] growth regions. Accordingly, the distribution of the \( V/V_b \) ratio is changed, with the maximum dendrite growth velocity being less than the beam travel velocity. Further decrease in the \( \alpha \) value to 45° or below will result in the disappearance of the [010] and [010] growth regions. Fig. 12 shows the dendrite growth direction and velocity results for a melt pool of the geometrical parameters \( l/w = 1.5, h/w = 0.48 \) and \( \alpha = 45° \). In this case, only the [001] growth region can be seen, i.e., an unidirectional dendrite growth along the [001] crystallographic direction is achieved on the melt-pool interface. These results indicate that not only single-crystalline solidification of multiple crystallographic growths but also unidirectional growth single-crystalline solidification can be possible through proper control of the 3-D melt-pool shape.

As given in Eqs. (14) and (15), the maximum velocity ratio is a function of the geometrical parameters \( \alpha \) and \( l/w \). Fig. 13 shows the influence of the \( \alpha \) value on the maximum value of the \( V/V_b \) ratio on the melt-pool interface. For \( \alpha = 90° \), no matter what value of the \( l/w \) ratio, the maximum velocity ratio is always a unit. As the angle \( \alpha \) decreases, the critical value of the \( l/w \) ratio for disappearance of the [100] dendrite growth is reduced rapidly. The maximum value of the \( V/V_b \) ratio at a specific \( l/w \)

![Fig. 14. Comparisons of experimentally observed transverse-section microstructures with the computed microstructure patterns for \( P=200 \) W, \( V_b=4 \) mm/s (a) and \( V_b=2.5 \) mm/s (b).](image-url)
ratio decreases also with decreasing value when the $l/w$ ratio is larger than its critical value. These results demonstrate the most pronounced influence of the $z$ value on the dendrite growth direction and velocity in the single-crystalline melt-pool solidification.

4.4. Experimental verification

Fig. 14 shows the transverse-section microstructures of melt tracks made at low processing velocities and their comparisons with the computed microstructure patterns. The melt pool observed at the low processing velocities was close to a circular shape in the top surface. As can be seen in Fig. 14, the observed melt-pool shape in the transverse cross-section is a segment of an ellipse except some irregularity in the melt-pool boundary, which further demonstrates the validity of the assumption used in the mathematical model. The irregularity observed in the melt-pool boundary was caused by non-uniform melting due to different microstructure components (primary phase vs. eutectic) and segregation in the single-crystal substrate. As shown in Fig. 14, the observed transverse-section microstructure is composed of four regions with dendrite growth directions in the $[001]$, $[100]$, $[010]$ and $[010]$ direction, respectively, which agrees well with what the computational model predicts. The sizes of the observed four growth regions in the microstructure also match reasonably well with the predicted ones. The slight discrepancy between the computed and observed sizes of growth regions is believed to come from the following three main sources: (i) the inaccuracy of substrate orientation brought by specimen cutting and positioning of laser-melted track; (ii) the local irregularities in an actual 3-D melt-pool shape caused by various factors such as the non-uniform melting, which differ from the mathematical formulation of the melt pool; and (iii) the error brought in the determination of melt-pool geometrical parameters. In addi-

![Fig. 15. Comparisons of experimentally observed transverse-section microstructures with the computed microstructure patterns for $V_b = 30 \text{ mm/s}$, $P = 375 \text{ W}$ (a) and $P = 500 \text{ W}$ (b).]
tion, a few small, isolated stray grains can be found in the microstructures, mostly in the [100] growth region.

Fig. 15 shows the transverse-section microstructures of melt tracks made at a high processing velocity (30 mm/s) and their comparisons with the computed microstructure patterns. The observed transverse-section microstructure at the high travel velocity is composed essentially of three regions with dendrite growth directions in the [001], [010] and \[\frac{1}{2}0\] directions, respectively, although more stray grains can be seen in the microstructure obtained under these conditions. Again, the computed microstructure patterns agree well with the experimentally observed microstructures, irrespective of the stray grains observed in some areas. As is known, nickel-base single-crystal superalloys are susceptible to stray grain formation during welding [4,5]. The increased propensity for stray grain formation at the high travel velocity (thus a high dendrite growth velocity in the melt pool) is probably related to an increased extent of constitutional supercooling ahead of the solidification interface. In addition, a few cracks can be seen in the area of stray grains in the microstructures obtained at the high travel velocity, as shown in Fig. 15. These cracks were identified to be solidification cracks [4], and are often associated with stray grains. The misoriented stray-grains have high-angle grain boundaries that can be easily wetted by a low-melting eutectic liquid during the later stage of solidification. When processing with a high travel velocity, the increased thermal stresses lead to solidification cracking along these boundaries of stray grains.

5. Conclusions

A mathematical model was developed for the 3-D melt-pool geometry and single-crystalline melt-pool solidification in laser surface melting. The 3-D melt-pool geometry corresponding to the solidification interface is described by four geometrical parameters (w, l, h, a). The model can be used to compute the dendrite growth pattern and velocity distribution on the 3-D melt-pool solidification interface of a set of geometrical parameters and of any substrate orientation relative to the laser scanning direction. Results indicate that the melt-pool geometrical parameters have profound influences on the dendrite growth velocity and growth pattern in the melt pool. For the (001)[100] substrate orientation, variations in l/w and a can influence both the number of selected (100) growth variants and the relative sizes of their growth regions while the variation in l/w can only influence the relative sizes of the growth regions. Unidirectional dendrite growth along the [001] crystallographic direction can be achieved in the single-crystalline melt-pool solidification for an a value of 45° or below. The maximum ratio of dendrite growth velocity to the beam velocity in the melt pool is related to the values of a and l/w. The desired dendrite growth velocity and microstructure can be obtained through proper control of the 3-D melt-pool geometry. Good agreement was obtained between the predicted and experimentally observed microstructures.

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Appendix A. Derivation of the 3-D melt-pool shape equation

The 3-D melt-pool shape in the case of laser surface melting is assumed to be a segment of an ellipsoid. The segment of an ellipsoid, whose sections in the y–z and x–z planes are shown in Fig. A1, can be defined in the following equation:

\[
\frac{x^2}{A^2} + \frac{y^2}{B^2} + \frac{(z - D)^2}{(h + D)^2} = 1 \quad (z \leq 0),
\]

(A.1)

Fig. A1. Sections of the 3-D melt pool in (a) y–z plane and (b) x–z plane.
where $A$, $B$, and $(h+D)$ are the half-axes of the ellipsoid in the $x$-, $y$-, and $z$-directions, respectively. In the $y$–$z$ plane ($x=0$), Eq. (A.1) becomes

$$\frac{y^2}{B^2} + \frac{(z-D)^2}{(h+D)^2} = 1.$$

Taking the differential of Eq. (A.2), one obtains

$$\frac{y}{B^2} + \frac{(z-D)}{(h+D)^2} \frac{dz}{dy} = 0.$$  \hspace{1cm} (A.3)

For point $P$ shown in Fig. A1, $y = w$, $z = 0$, and $dz/dy = -\tan \alpha$, and by inserting these values into Eqs. (A.2) and (A.3), the following equations are obtained:

$$\frac{w^2}{B^2} + \frac{D^2}{(h+D)^2} = 1,$$  \hspace{1cm} (A.4)

$$\frac{w}{B^2} - \frac{D \tan \alpha}{(h+D)^2} = 0.$$  \hspace{1cm} (A.5)

From Eqs. (A.4) and (A.5), one obtains $D$ and $B$ in the following expressions:

$$D = \frac{h^2}{w \tan \alpha - 2h},$$  \hspace{1cm} (A.6)

$$B = \frac{w(h + D)}{(2hD + h^2)^{0.5}}.$$  \hspace{1cm} (A.7)

Similarly, considering a corresponding point $Q$ in the $y$–$z$ plane ($y = 0$), one can obtain $A$ and the angle $\beta$ in the following expressions:

$$A = \frac{l(h + D)}{(2hD + h^2)^{0.5}},$$  \hspace{1cm} (A.8)

$$\tan \beta = \frac{\tan \alpha}{l/w}.$$  \hspace{1cm} (A.9)

By defining the solidification interface as in the side $x \leq 0$ for Eq. (A.1), the melt-pool shape equation corresponding to the solidification front can be written as

$$x = f(y,z) = -A \left[ 1 - \frac{y^2}{B^2} - \frac{(z-D)^2}{(h+D)^2} \right]^{0.5} (z \leq 0).$$  \hspace{1cm} (A.10)

### Appendix B. Details of computations of the angles $\theta$ and $\phi$

In the actual computations, Eqs. (9) and (10) cannot be used directly for the calculations of the angles $\theta$ and $\phi$ in the following situations. Separate considerations and modifications of the equations need to be made in these cases.

1. For $y = 0$, Eq. (10) cannot be executed computationally because of $\partial f/\partial \psi = 0$. Thus, $\phi = 90^\circ$ needs to be set for $y = 0$.
2. For $y > 0$, since the value computed from Eq. (10) is negative, the following equation needs to be used for $\phi$:

$$\phi = 180^\circ + \arctan \left( \frac{\partial f/\partial \psi}{\partial f/\partial \phi} \right).$$  \hspace{1cm} (B.1)

3. For $x = 0$ (in the $y$–$z$ plane), $\theta$ and $\phi$ cannot be computed directly from Eqs. (9) and (10) since both $\partial f/\partial \psi$ and $\partial f/\partial \phi$ are an infinite. In this case, the following equations can be used instead to compute $\theta$ and $\phi$:

$$\theta = 90^\circ,$$  \hspace{1cm} (B.2)

$$\phi = 90^\circ + \arctan \left( \frac{dz}{dy} \right).$$  \hspace{1cm} (B.3)

### References


