Multi-track, multi-layer dendrite growth and solid phase transformation analysis during additive manufacturing of H13 tool steel using a combined hybrid cellular automata/phase field, solid-state phase prediction models

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Abstract
Using an efficient hybrid Cellular Automata/Phase Field (CA-PF) dendrite growth model in combination with a solid-state phase transformation model, microstructure evolution and solid-state phase transformation were predicted during laser direct deposition (LDD) of H13 tool steel powder within a large domain across multiple deposition tracks and layers. Temperature and surface geometry data were provided by a comprehensive physics-based laser deposition model. The computational efficiency of the CA-PF model allows for simulating domains large enough to capture dendrite growth across an entire molten pool and into multiple neighboring LDD tracks and layers. The microstructure of the target track is strongly affected by heat from neighboring tracks including re-melting, re-solidification and solid-state phase transformation including austenitization, martensite formation and martensite tempering. Dendrite size and growth direction across the entire fusion zone, as well as predicted hardness values, are found to be in good agreement with experimental results.

Keywords Microstructure · Additive manufacturing · H13 · Predictive modeling · Solid-state phase transformation

1 Introduction

1.1 Laser direct deposition
Laser direct deposition (LDD) of metals is a multi-track, multi-layer additive manufacturing (AM) process where fine metal powders are blown into the same focal point as the laser, either coaxially [1] or off-axis [2]. The laser directs enough energy at the focal point to create a molten pool, thereby melting the incoming powder that is directed at the molten pool. As the molten pool and directed powder stream travel together at the laser travel speed, the back of the molten pool experiences very rapid solidification, while the addition of powder builds up the surface of the part.

AISI H13 tool steel is extensively used in toolings for hot work and cold work. Its high hardness, strength, and resistance to thermal fatigue cracking at an elevated temperature make it ideal for use in high-pressure die casting tooling, hot forging dies, extrusion dies, and plastic injection molding dies [3]. Traditionally, H13 tooling is cut from blocks with a long lead time to obtain parts, but in recent years, AM has facilitated the creation of conformal cooling where coolant passages are printed within the tool to allow superior heat removal to previously inaccessible areas [4, 5]. Additionally, complex die surfaces with loops, deep trenches and metal savers are increasingly difficult and costly to subtractively manufacture, while AM tooling requires only finishing machining and/or electrical discharge machining (EDM).

While AM provides many advantages such as the creation of complex shapes and no required tooling, it also carries many disadvantages, aside from the cost, which are less well understood. With subtractive manufacturing, the material properties of a machined part are mostly carried over from the stock material. Since the material properties of stock materials are well understood and well regulated, the material properties after subtractive manufacturing are well controlled. However, with laser or e-beam AM processes for metals, the AM part undergoes local melting and solidification throughout the building process, resulting in unknown and widely varying microstructure.
The traditional choice for developing material properties of AM processes is experimentation and measurement. However, the huge number and ranges of experimental variables that affect material properties (not to mention the numbers of processes, materials and AM machines available) make this approach very time-consuming and expensive.

The alternative choice, physics-based numerical simulation, is a more desirable way. The foundation of predicting material properties is an accurate prediction of the resultant microstructure and phase transformation after an AM process is performed, all of which require accurate temperature calculation [6–9]. Microstructure prediction involves simulating dendrite growth [10–12]. A quick literature search will reveal that the two most popular numerical methods for simulating dendrite growth are the Cellular Automata (CA) and Phase Field (PF) methods.

Cellular Automata models specialize in the simulation of micro-scale dendrite growth as well as meso-scale grain growth. The strength of these models lies in their computational efficiency, but their accuracy is completely dependent on the accurate determination of growth velocity of the solid/liquid interface. In a typical example [13], the growth velocity of the interface is calculated based on the undercooling as predicted by an analytical model such as the Kurz et al. (KGT) model [14], which assumes equilibrium solidification conditions and a parabolic dendrite tip shape. This restricts the model’s accuracy to that of the analytical model, which ought to be applied only to steady-state situations, limiting the simulation to qualitative prediction. As another example, a more recent model implicitly calculates the growth velocity at the solid/liquid interface by solving the transport equations for both solid and liquid phases while holding a solute concentration boundary condition at the interface [15–19], but is only quantitatively accurate for domains of low Péclet number [20–22].

Early CA models used to predict dendrite growth were limited to pure materials and binary alloys. Several attempts have been made to expand these approaches to more complex material systems such as multi-component and/or multi-phase alloys [21, 23–25], but most of them have made simplifying assumptions, which limit their applicability. Tan and Shin [26] developed a 3D CA model to predict grain growth during laser melting processes of austenitic stainless steel. More recently, Gu et al. [27] presented a 3D CA model with a quantitative prediction of dendrite growth in ternary alloys applicable at low cooling rates and near steady-state growth conditions, but it is not applicable at cooling rates associated with laser melting processes [28].

The Phase Field method is a more elegant solution with a much higher computational cost. It is established on a set of thermodynamically based partial differential equations, with a diffuse solid/liquid interface defined by the parameter $\phi$ [29–33]. This modeling method has been widely used to study growth kinetics for different multicompontent alloys on very small scales due to the high computational cost [34–40]. Suzuki et al. [41] presented the most influential multi-component PF model (expanded from their two-phase binary PF model [42]). Because the PF equations are thermodynamically based, the CALPHAD method has widely been used, in conjunction with the PF equations, to calculate the Gibbs energy of the system. This makes PF easily applicable to ternary alloys [34, 35, 37, 43, 44] and higher-order systems [45, 46], and realistic multi-phase microstructure patterns have been obtained.

The major disadvantage of the PF method is the extremely high computational cost. Compared to the CA method, the PF method requires a very fine mesh to characterize the diffuse interface, greatly limiting the domain size of PF models. Adaptive mesh refinement methods have only slightly alleviated the computational cost [47–49].

A novel CA-PF model [50] that combines the strengths of the CA and PF methods was proposed by the authors’ group to accurately predict the solidification and dendrite growth of multi-component alloys on a scale large enough to capture an entire molten pool. This model has been used for the quantitative prediction of dendrite growth and micro-segregation during solidification of multi-component alloys over areas large enough to visualize molten pools in laser cladding [7] and laser welding of austenitic stainless steel [26]. In this paper, the model has been expanded to include simulation of multi-track and multi-layer additive processes, including re-melting and re-solidification of previously deposited tracks. To the authors’ best knowledge, this is the first time the solidification and dendrite growth of an entire molten pool of a ternary alloy undergoing fast transient cooling has been modeled with the influence of multiple tracks and layers typical of AM processes.

In addition to melting and solidification processes, solid-state phase transformation can also have a strong effect on the material properties of AM parts and cannot be neglected. Hypoeutectic steels can undergo dramatic solid phase transformation during rapid heating and cooling caused by multiple heating cycles from neighboring tracks. A solid-state phase transformation model [9, 51] was also merged with the CA-PF model to calculate the tempering effects of the heating and cooling cycles inherent to laser-based additive processes.

The CA-PF model and the solid phase transformation model discussed in this paper get their needed temperature and surface geometry field data from a validated, comprehensive multi-physics thermal model [1, 52] that was developed in-house. This model considers multi-phase heat transfer from conduction, convection and radiation, as well as free-surface tracking of the molten pool surface via the level-set method [53]. The details of this thermal model are skipped for brevity, as it is well described in Ref.
The major contribution of this work is to elucidate the microstructure and phase evolution involving re-melting, re-solidification and solid-state phase transformation for an entire cross section of an LDD track during a multi-track and multi-layer LDD process using the integrated computationally efficient CA-PF and solid phase transformation models in combination joined with temperature and geometry data from a comprehensive thermal model.

2 Numerical models

This work combines the simulation capabilities of the CA-PF model, as presented by Tan et al. [50], with the solid phase transformation model presented by Bailey et al. [9] for the purpose of predicting melting, solidification, dendrite growth and solid phase transformation during multi-track and multi-layer LDD of H13 tool steel.

2.1 CA-PF model

A flowchart, shown in Fig. 1, helps describe the working of the CAPF model. Temperature data from the thermal model (described in detail in Sect. 3.1) are provided to the CAPF model. The CA portion of the model uses the temperature data to calculate the solute diffusion within the CA domain and determine the initial shape of the solid/liquid interface. Then, for each interface cell within the CA domain, the CA model sends and receives data to and from the PF model which calculates the growth kinetics along the solid/liquid interface.

2.1.1 Cellular automata

The discretized domain of the CA model consists of regular square cells where each cell can be assigned one of three states: liquid, interface or solid. Dendrite growth occurs when increasing numbers of cells change their states from liquid to interface and then to solid. The state change of each cell is determined by the decentered square algorithm [54] such that a nucleus grows by a square envelope whose corner aligns with the crystallographic orientation θ, as shown in Fig. 2.

The growth of the envelope is governed by Eq. (1),

$$ L = \sum_i V(t_i) \Delta t $$

where $L$ is half the length of envelope diagonal, $V(t_i)$ is the velocity of the solid–liquid interface at time $t_i$, and $\Delta t$ is the time step. As the square envelope expands during growth, it will contact neighboring cells. If the “contacted” cell is liquid, it will be reassigned as an interface cell. The crystallographic orientation of the “parent” cell will then be passed on to the new interface cells, and the new “daughter” cells’ envelopes will center at the corners of the parent cell’s envelope (Fig. 2b). The child cells will then expand with their own velocities that may be different from that of the parent envelope (Fig. 2c). Their growth will cause other neighboring liquid cells to become interface cells as they grow sufficiently large. The solid fraction, $f_s$, of each cell is governed by Eq. (2),

$$ f_s = \frac{L}{\Delta x (|\sin \theta| + \cos \theta)} $$

where $\Delta x$ denotes the mesh size of the CA model. Once $f_s$ reaches 1, the interface cell is considered solid and is no longer included in the calculations of interface cells.
Two alloying components must be considered in a ternary system. During solidification at the interface, a certain amount of each solute is rejected into the liquid, while each solute also diffuses throughout the liquid. This solute diffusion and rejection of each alloying component is governed by

\[
\frac{\partial C_{e,i}}{\partial t} = \nabla \cdot (D_{e,i} \nabla C_{e,i}) + \frac{\partial S}{\partial t} \left( C_{L,i}^i - C_{S,i}^i \right) (i = 1, 2) \tag{3}
\]

where \(D_{e,i}\) and \(C_{e,i}\) are the equivalent diffusion and composition coefficients for liquid, interface and solid cells, and \(C_{L,i}\) and \(C_{S,i}\) are the liquid/solid concentrations at the interface.

The normal vector \(\beta\) at the solid–liquid interface, as shown in Fig. 3, and the interface curvature, \(K\), are needed to calculate the growth kinetics of each interface cell; \(\beta\) for an interface cell is calculated by using Raghavan’s algorithm [55]. As shown in Fig. 3, a circle is drawn inside a 7 × 7 cell area centered on the cell of interest. Point C is the mass center of the solid within the circle and is calculated based on a weighted average of the solid fractions of the cells. The normal vector \(\beta\) is determined by the angle between point C and point A of the interface at cell.

The calculation of the curvature \(K\) is based on the work of Martorano et al. [56]. First, as illustrated in Fig. 4, line segments are used to approximate the curve of the interface within a 3 × 3 cell area centered on the cell of interest. A second-degree polynomial is calculated from the midpoints of each line segment within the 3 × 3 cell area. The normal vector \(\beta\) is the polynomial’s vertical axis, \(y'\). The curvature can then be calculated from the polynomial.

Once the temperature and concentration fields are calculated within the CA domain and the interface normal vectors and curvatures of the interface cells are known, the growth kinetic values of interface velocity \(V\) and the interface concentrations \(C_{L,i}\) and \(C_{S,i}\) can be calculated by the PF model.

### 2.1.2 Phase field model

The sole purpose of the phase field model is to provide the CA model with accurate local growth kinetics at each interface cell along the solid/liquid interface. It is assumed that the local interface growth at a given interface cell can be approximated as 1D growth as long as the direction is always normal to the interface. Therefore, a 1D phase field model is sufficient for calculating the local growth kinetics along the interface.

The PF model may be expressed by Eqs. (4) and (5) [37, 42, 43, 57, 58].

\[
\frac{1}{M_{\phi}} \frac{\partial \phi}{\partial t} = \varepsilon^2 \nabla^2 \phi - \frac{\partial f}{\partial \phi} \tag{4}
\]

\[
\frac{\partial C_i}{\partial t} = \nabla \cdot \sum_j^n \left( D_{ij} \nabla C_j \right) + \nabla \cdot \sum_j^n \left( M_{ij} \frac{\partial^2 f}{\partial C_j \partial \phi} \nabla \phi \right) \tag{5}
\]

Here, the order parameter of the phase field is represented by \(\phi\), \(M_{\phi}\) is the phase field mobility, \(\varepsilon\) is the gradient energy coefficient, and \(f\) represents the free energy density. The concentration of each component \(i\) of the alloy is \(C_i\), while \(D_{ij}\)
and $M_{ij}$ are the $(i, j)$th components of the material diffusion and mobility matrices, respectively.

If this system is solved in 1D, it would simulate the solidification of a planar interface. Yet locally, the curvature of a dendrite strongly affects the velocity of the interface. For example, an interface with a positive curvature, such as the tip of a dendrite, will solidify much faster than a planar interface since the rejected solute cannot diffuse away and is trapped by an inward–curving interface. A 1D planar PF model would underestimate the growth near the tip of a dendrite and overestimate the growth near the root of the dendrites.

Therefore, the 1D PF model (Eqs. (4) and (5)) has been reformulated into a polar coordinate system with radius $r = 1/K$.

$$\frac{1}{M_{\phi}} \frac{\partial \phi}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) - \frac{\partial f}{\partial \phi} \tag{6}$$

$$\frac{\partial C_{i}}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \sum_{j}^{n} \left( D_{ij} \frac{\partial C_{i}}{\partial r} \right) \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \sum_{j}^{n} \left( M_{ij} \frac{\partial f}{\partial C_{i}} \frac{\partial \phi}{\partial r} \right) \right) \tag{7}$$

The effect of interface curvature is incorporated into the model through this 1D polar formulation. The polar coordinate formulation takes into account the unique circular shape of each interface cell by using the local curvature of the interface cell as calculated in the CA model. Thus, the solidification velocity of the interface is dependent on the local curvature and the concentration gradient(s) of the solute(s). A detailed description of all relevant PF equations required in the CA-PF model is presented by Tan et al. [50]. For multicomponent alloys, more than one phase may form upon solidification. To determine which phases will form, the PF model is linked to a CALPHAD database which is based on the Gibb’s energy of the system.

### 2.1.3 CA-PF combination

The PF model needs the interface curvature, concentration field and the local temperature to replicate the local solidification conditions in order to calculate the growth kinetics for an interface cell in the CA model. For diffusion-controlled dendrite growth, the concentration distribution is the dominant factor for determining interface velocity. The concentration distribution can be accurately described with a 1D concentration profile using a number of points along the interface cell’s normal vector as shown in Fig. 5. These concentration values are interpolated from the CA model’s concentration fields. For example, the solute concentrations of point 1 are interpolated from the values of cells B, C, D and E. A typical cell size for the CA model’s mesh is 0.5 µm, while a typical cell size in the 1D PF model is 0.25 µm. The 1D concentration profile can then be fitted to an exponential curve as described by Eq. (8).

$$C_{i}(x) = C_{\infty,i} + \left( C_{L,i} - C_{\infty,i} \right) \exp(-A_{i}x) \tag{8}$$

Here, $C_{L,i}$ is the concentration at the interface, $C_{\infty,i}$ is the concentration far from the interface, and $A_{i}$ is a variable that defines the exponential strength of the concentration profile, and $x$ is the distance from the interface into the liquid in the normal direction. The concentration value at the interface, $C_{L,i}$, is known from the last CA time step, the concentration value far from the interface, $C_{\infty,i}$, is found at distance into the melt far enough away from the interface that the value does not change significantly, and $A_{i}$ is determined from the concentration values of the 1D profile. The interface concentrations, $C_{L,i}$, and $A_{i}$ are then used by the PF model, along with the local temperature and curvature, to determine local growth velocity and equilibrium concentrations at the interface.

To correctly set up the PF model, the mid-point of the PF interface ($\phi = 0.5$) must be positioned at $r = 1/K$ in the polar coordinate domain. The temperature used in the PF model is assumed to be isothermal at temperature $T$ of the CA interface cell. The isothermal assumption is valid because the variation in temperature along the normal vector

![Fig. 5 1D concentration profile along cell A’s normal vector is interpolated from the CA model to the PF model (adapted from [50])](image-url)
is much smaller than the variation in solute concentration across the distance the interface advances during one CA time step.

With the values of temperature and curvature and the concentration profile provided by the CA model, the PF model can precisely predict the progression of the solidification interface. This velocity of the PF solidification interface is the interface velocity, $V(t_i)$, needed in the CA model (Eq. (1)), and is the main purpose of the PF model. Several time steps are required for the PF model to reach convergence from the initial concentration profile as given by the CA model. Once convergence has been reached, the interface velocity of the PF model is given to the CA model, along with values of the solid and liquid interface concentrations $C_{LI}$ and $C_{SI}$ taken from the PF model’s converged 1D concentration profile. By applying the PF model everywhere along the interface, the CA model can determine the overall growth of the dendrite via de-centered square algorithm Eq. (2), and the macroscale diffusion within the liquid via Eq. (3). With the CA model and the PF model working together, the dendrite growth can be predicted over a large area with accurate growth kinetics of multi-component alloys and with the efficiency of a CA model and the precision of a PF model.

### 2.2 Solid-state phase transformation model

Both microstructure characteristics (grain size, secondary dendrite arm spacing (SDAS), etc.) and solid phase have strong influences on the material properties of a part. Although solid phase transformation kinetics is a characteristic of microstructure, it is not trivial to predict solid phase from dendrite growth simulation data. Therefore, the CA-PF model has been expanded to include solid-state phase transformation prediction capabilities. A full description of the solid phase transformation model is provided by Bailey et al. [9], while an abbreviated description is presented here.

Three temperature-dependent processes are included in the model: heating, cooling and tempering. To simulate the heating cycle, a 2D kinetic model was developed by Skvarenina and Shin [59] based on Ashby and Easterling’s work [60]. This model was expanded to include the tempering effect by Lakhkar et al. [61]. Bailey et al. [51] further expanded the model to 3D and included cooling effects.

Rapid heating and cooling are defining characteristics of laser-based manufacturing processes. The heating cycle is explained graphically in Fig. 6. As temperature increases past the eutectoid temperature (727 °C) depicted by point b in Fig. 6, all high-carbon pearlite regions will transform into austenite. The ferrite regions are slower to transform to austenite because of a lack of carbon. As temperature further increases, carbon from the newly formed austenite regions will diffuse into the low-carbon ferrite regions, transforming them into austenite. As temperature increases, carbon diffusion also increases. If the temperature increases beyond the austenitization temperature (850 °C for H13 steel), all remaining ferrite will transform into austenite, as depicted by point c in Fig. 6. For slow heating cycles, carbon diffusion cannot be neglected when modeling the solid-state phase transformation. However, the rapid heating of laser-based processes makes modeling the carbon diffusion irrelevant. In the present model, all material with a temperature above the austenitization temperature is assumed to have transformed to 100% austenite. For temperatures between the eutectic and austenitization temperatures, the lever rule defined by Callister and Rethwisch [62] is used to determine the fraction between austenite and ferrite.

In this model, the rapid cooling cycle uses Sheil’s additive rule and follows Kang and Im’s implementation of the Johnson–Mehl–Avrami–Kolmogorov (JMAK) model [63] and the implementation of Woodard et al. [64] of the Koistinen–Marburger (KM) equation. The details of this model are presented by Bailey et al. [9, 51].

The multi-track and multi-layer nature of LDD requires the use of a tempering model [61]. Below the eutectoid temperature, pearlite and ferrite phases are stable, while martensite can be tempered at temperatures between 100 °C and the eutectoid temperature. During LDD, the peak temperature during a single track reaches far above the eutectoid temperature, resulting in rapid cooling and a track that is mostly martensite. However, as the laser deposits additional tracks next to and above this track, the
heat from these tracks will cause the martensite to temper significantly. This tempering effect must be considered when modeling the solid-state phase transformation of multi-track and multi-layer LDD.

In the tempering model, any martensite phase fraction higher than zero in a given cell will experience tempering if the temperature rises above 100 °C while remaining below the eutectoid temperature 727 °C. Between 100 °C and 250 °C, a certain fraction of the martensite phase fraction will transform to ε-carbide and ferrite, while cementite and ferrite are formed between 250 °C and 727 °C. The fraction of martensite, \( f_m \), that is transformed into these tempered phases is calculated based on the JMA equation:

\[
f_m = 1 - e^{-\beta m}
\]

Here, \( n \) is a constant set at 0.109 [61]. For non-isothermal processes, the \( \beta \) term is governed by the differential equation,

\[
\frac{d\beta}{dt} = k + \frac{Q}{RT^2} \beta \frac{dT}{dt}
\]

where the activation energy, \( Q = 1.97 \times 10^5 \), and \( k = 5.11 \times 10^9 \) are constants.

The fractions of ε-carbide \( f_e \) and ferrite \( f_f \) that form between 100 °C and 250 °C from the phase fraction of tempered martensite \( f_m \) are given by

\[
f_e = \frac{f_mC_{H13} - C_a}{C_e - C_a} = f_m - f_a
\]

where the carbon concentration of H13, \( C_{H13} = 0.4\% \), and the carbon concentrations of ε-carbide and ferrite are \( C_e = 8.55\% \) and \( C_a = 8.22\% \), respectively. Similarly, cementite \( f_c \) and ferrite \( f_f \) form between 250 °C and 727 °C, according to Eq. (12)

\[
f_c = \frac{f_mC_{H13} - C_a}{C_c - C_a} = f_m - f_a
\]

with a carbon concentration of cementite, \( C_c = 6.7\% \).

Once all the phase fractions are calculated, the hardness field can be calculated by the weighted average of the hardness of each phase according to Eq. (13).

\[
H = \sum f_i H_i
\]

While the solidification as predicted by the CA-PF model occurs very rapidly during cooling near the solidus and liquidus temperatures, the solid phase transformation occurs over a much longer temperature span and time including heating, cooling and multi-track and multi-layer tempering. Although these two pieces of the model are solved simultaneously and use the same domain and mesh size, they have a separate timescale and time steps.

### 2.3 Material

To predict solidification microstructure and dendrite growth with the CA-PF model during additive manufacturing of H13 tool steel, this complex tool steel alloy is first approximated as a ternary alloy. The composition of H13 tool steel is given in Table 1. The top three elements are iron, chromium and molybdenum. Therefore, the ternary system to be implemented into a CALPHAD subroutine is the Fe–Cr-Mo system, as studied by Andersson and Lange [66] with appropriate Gibb’s energy coefficients for equilibrium states for liquid and the iron image result for face-centered cubic (FCC) crystal structure (austenite) solid phase. For simulations in this paper, the initial concentrations of chromium and molybdenum were set at 5.0 and 1.5 wt.%, respectively.

### 3 Simulation and results

In this work, simulations are run using the hybrid Cellular Automata/Phase Field and solid state phase prediction models and compared with experimental results. To help clarify, Fig. 7 gives a graphical summary of some of the simulations and experimental results. The simulation and experimental images shown in Fig. 7 are shown in detail throughout Sect. 3.

#### 3.1 AM thermo-fluid dynamics modeling results

The temperature data used by the CA-PF model in this work were calculated using a validated, comprehensive multiphysics laser direct deposition (LDD) thermal model [1, 52]. For the situation presented in this study, tracks are built in parallel with the operating parameters listed in Table 2 as presented in [9]. Each track is offset 0.300 mm from the previous track. The next layer is then deposited 0.300 mm above the surface of the previous layer. For multi-track deposition, it was found that the geometry of the third track accurately represents the geometry of each additional track [9]. Therefore, the quasi-steady state temperature field and geometry

| Element | Composition |
|---------|-------------|
| C       | 0.32–0.45   |
| Cr      | 4.75–5.5    |
| Mn      | 0.2–0.5     |
| Mo      | 1.1–1.75    |
| Ph      | 0.03 max    |
| Si      | 0.8–1.2     |
| S       | 0.03 max    |
| V       | 0.8–1.2     |
| Fe      | balance     |

The composition of H13 tool steel [67] in wt.%
predicted by the LDD model of a third track simulation are provided to the CA-PF model. The temperature field and track geometry, as predicted by the LDD model, are shown in Fig. 8.

The 3D temperature field and track geometry of both the molten pool and the solidified track are used as input parameters for the 2D CA-PF model. The term track geometry indicates the overall shape and surface profile of the track. This is predicted for both the molten pool (before the metal solidifies) and the solidified track geometry. The molten pool geometry will be transient due to vigorous fluid flow within the molten pool. The thermal model predicts this transient geometry, and these data are used in the CA-PF model. The temperature and geometry data are read into the CA-PF model at the beginning of the CA-PF analysis. The 2D CA-PF analysis domain is 430 µm high and 300 µm wide, and the initial location of the analysis plane is at the heart of the molten pool (the bright region in Fig. 8) where the analysis plane has the maximum amount of liquid before solidification begins. As time progresses, the 3D temperature field is brought forward (relative to the 2D CA-PF analysis plane) in the laser travel direction and at the laser travel speed. At each time step of the CA-PF simulation, the temperature for the CA-PF simulation is interpolated from the LDD model’s 3D temperature field at the current relative position of the 2D CA-PF analysis plane. As the CA-PF 2D domain moves through the molten pool toward the solid region, solidification begins and dendrites will start to grow within the CA-PF analysis plane, according to the thermodynamic conditions of the domain. A track’s simulation is complete when all of the 2D CA-PF domain is solidified. To simulate multi-track and multi-layer dendrite growth, the CA-PF region is shifted laterally by the track spacing (0.300 mm in this paper) for each track and each layer, and then the next track begins again with the 2D CA-PF analysis plane in the heart of the molten pool. Areas of the second track that were previously solid and now have a temperature higher than the melt temperature are reset as liquid and are subsequently re-solidified during the second track’s simulation.

In this paper, four tracks were simulated: two on the first layer and two on the second layer. The locations of each of these simulations are depicted in Fig. 9. The microstructure is first predicted by the CA-PF model in the red box labeled “CA-PF initial simulation domain location.” After the dendrite growth simulation of the first track is complete, this predicted microstructure is then used as the initial microstructure for the second simulation at the location 2 indicated

### Table 2

| Parameter                  | Value     |
|----------------------------|-----------|
| Laser power                | 350 W     |
| Laser travel speed         | 14.8 mm/s |
| Powder flow rate           | 8.5 g/min |
| Track spacing              | 0.3 mm    |

In this paper, four tracks were simulated: two on the first layer and two on the second layer. The locations of each of these simulations are depicted in Fig. 9. The microstructure is first predicted by the CA-PF model in the red box labeled “CA-PF initial simulation domain location.” After the dendrite growth simulation of the first track is complete, this predicted microstructure is then used as the initial microstructure for the second simulation at the location 2 indicated...
in Fig. 9. The small black boxes indicate the locations of the lower left-hand corners of each simulation location. Simulations 3 and 4 then use the previous simulations’ predicted microstructure as their initial microstructures, resulting in the final microstructure predicted in the green region labeled “CA-PF final simulation domain location.”

The background temperature field shown in Fig. 9 (a head-on view of the LDD simulation) represents the 2D temperature as interpolated from the 3D temperature data from the LDD model at a certain point in simulation time. The area in the top half of Fig. 9 labeled “Current track Melt pool” represents the temperature and geometry of the molten pool. The order of the four simulations, as they appear in Fig. 9, is not the order in which each track is deposited, but the order of microstructure evolution. In other words, the microstructure in simulation is formed first and gets affected by the deposition in the adjacent track as in simulation 2. Therefore, the microstructure in simulation 2 is modeled using the microstructure formed in simulation 1 and the temperature history in simulation 2. Therefore, the microstructure of the multi-track, multi-layer deposition will go through the evolution shown in simulations 1, 2, 3 and 4. Obviously, a track in the position of simulation 4 as shown in Fig. 9 would be the first of the four tracks to be deposited, but has gone through the evolution of simulations 1, 2 and 3 before the final microstructure is formed. This is the only track that is being considered in the microstructure prediction simulations as noted by the text “CA-PF final simulation domain location” in Fig. 9. The temperature field of each neighboring track will strongly affect the final microstructure predicted at this location. Therefore, the four locations noted in Fig. 9 depict the positions of the temperature field relative to the final simulation domain location as deposition occurs for each neighboring track. Each of the four simulations required about 20 h of computation on Intel Xeon CPU E5-2660 v3 with 20 cores at 2.6 GHz. This does not include the computational cost of the thermal model results which can be found in reference [68].

### 3.2 Single-track results

Results for the first track, Simulation 1, are shown in Fig. 10 through Fig. 12. The coordinate system of the CA-PF model, as shown in Fig. 10, is not the same as the coordinate system of the thermal model shown in Figs. 8 and 9. However, the x/y plane of the CA-PF model is always parallel to the y/z plane of the thermal model. The first track simulation begins at the heart of the molten pool with the temperature profile shown in Fig. 10. The values of some of the isotherms have
been adjusted to show the boundary of the molten pool and the location of the mushy zone.

As the temperature begins to drop, randomly oriented seeds are randomly placed at the back of the molten pool and grains will begin to grow in the direction of the temperature gradient, as shown in Fig. 11. The first solidified phase here is austenite with a face-centered cubic structure. The dendrites with crystallographic orientations that are closely aligned with the temperature gradient will grow more quickly, blocking the dendrites with less favorable

Fig. 9 Head-on view of direct deposition track with temperature distribution in Kelvin. Laser travel is in the X direction (out of the page)

Fig. 10 Initial temperature field (in Kelvin) and phases before dendrite growth begins for the first track (simulation 1)
orientations. The competitive growth is clearly seen in the zoomed-in image of Fig. 11, as well as the detailed microstructure predicted by the CA-PF model. Once the temperature cools sufficiently, the melt in the entire 2D CA-PF domain will completely solidify, as shown in Fig. 12.

In any directional solidification process, grains with a favorable orientation will have an advantage over less favorable orientations, but this is only an advantage, not an absolute outcome. The competitive growth phenomenon will reliably produce large-scale trends, as seen in Fig. 11. Near the left side of the left figure are shown a majority of orientations at or near 0° or 90° growing in the y-direction, while grains on the right side of the left figure are growing diagonally and are primarily 30° to 60° orientations. The overall trend is obvious, but some grains may beat the odds and successfully grow in unfavorable directions. In Fig. 11, a grain with an orientation close to 0°, indicated by a yellow oval, grows in unfavorable conditions where the temperature gradient is close to 45°. However, in Fig. 12 it is shown that the same grain is eventually blocked by grains with orientations close to 45°.

It is noted that all simulations from the CA-PF model are 2D. True grain growth is indeed a 3D phenomenon, and a 3D simulation will always be superior to a 2D simulation without regard to computational cost. It is well known that the computational cost of a 3D simulation is usually several orders of magnitudes higher than that of a 2D simulation. Simulations performed in 2D have provided valid and useful data for decades and cannot be overlooked in their usefulness. However, one must be careful in choosing how to perform a 2D simulation of a 3D process [40].

Generally, in solidification conditions during welding or additive manufacturing, dendrites will grow toward the heat source. If the solidification speed of the grains is
similar or slower than the heat source’s travel speed, the grains will appear equiaxed in a cross section perpendicular to the heat source’s travel direction when in fact the grains are columnar in their growth direction. This will result in a misleading and inaccurate microstructure. However, if the grains’ solidification speed is much faster than the heat source’s travel speed (as is the case in the conditions in this work), the grains will grow quickly toward the center of the molten pool, resulting in accurate columnar grains as viewed in a cross section perpendicular to the heat source’s travel direction. This phenomenon is clearly explained by Tan and Shin [26].

### 3.3 Multi-track, multi-layer results

After the first track is finished, the resulting microstructure (top left image of Fig. 13) is used as the initial microstructure of the second track, simulation 2. When the temperature is above the melting temperature, the solidified material in the corresponding region will be assigned as the liquid. Then

![Fig. 13 Predicted solidification microstructures for simulations 1 through 4 showing the angle of each dendrite between 0° and 90°](image)
as the temperature in simulation 2 drops, dendrites again begin to form along the bottom of the molten pool. Once solidification of the second track is complete, the resulting microstructure (top right image of Fig. 13) is used as the initial microstructure of the third track (simulation 3), and the third track’s final microstructure (bottom left image of Fig. 13) is used as the initial microstructure of the fourth track (simulation 4). The final predicted microstructure of the multi-track, multi-layer laser direct deposition simulation is shown in the bottom right image of Fig. 13.

Fig. 14 Microstructure from 2-layer experimental results. The region for Fig. 15 is shown as a box.
The final predicted microstructure, after all four simulations, should match the microstructure of the multi-layer, multi-track experimental microstructure shown in Fig. 14 through Fig. 16. Figure 14 is a microscope image of a cross section of a two-layer multi-track LDD sample workpiece. The substrate and both layers are clearly shown. The box in Fig. 14 represents the area of an SEM image shown in Fig. 15.

Melt boundary lines were added to Fig. 15 to indicate the melt boundaries of each laser track. The box “Detail A” represents the area of the zoomed-in SEM image at the bottom of Fig. 16. Shown at 750× zoom, the SEM image in Fig. 16 shows the dendritic details of the LDD microstructure as well as the melt boundaries between the tracks. The direction of dendrite growth is clear along the melt boundaries. This actual microstructure is compared with the top image in Fig. 16, a zoomed-in image of the final predicted microstructure after all four CA-PF simulations (Detail B of Fig. 13).

In comparing these two images, it is clear that the locations and curves of the molten pool boundaries agree, as do the average size and orientations of the dendrite arms near the molten pool boundaries. The arrows in Fig. 16 assist in illustrating the agreement of directional growth between the predicted and experimental dendrites. The measured primary dendrite arm spacing for both the predicted and experimental dendrites agrees well at around 2 µm. The CA-PF model accurately predicts the directional dendrite growth...
during LDD via multi-track and multi-layer solidification simulations.

3.4 Solid phase transformation results

In addition to predicting dendrite growth during solidification, the CA-PF model has been expanded to include solid phase transformation prediction for hypoeutectoid steels. As noted above, austenite is the solidified phase, but H13 steel can undergo dramatic phase transformations during the repeated cooling and reheating cycles, which are typical in AM. Austenite is not stable at room temperature and the newly solidified material will quickly transform into other phases before the material reaches room temperature. Typical to LDD, quickly cooling austenite will transform to martensite, a body-centered tetragonal phase that has a very strong influence on the material hardness, strength and distortion. Additionally, previously formed martensite is easily tempered by the heat of neighboring tracks in multi-track, multi-layer situations, resulting in additional phase transformation.

**Fig. 17** Predicted martensite phase fraction of each track after each simulation
The post-cooling results of the solid phase transformation model for all four tracks are shown in Fig. 17 in terms of the martensite phase fraction. For the first track, it is clear that the solidified and cooled material is nearly 100% martensite. This is expected since the entire molten pool solidifies as austenite and transforms to martensite due to the rapid cooling. The second track, as expected, also consists of nearly 100% martensite. Even though not the entire region of the second track undergoes melting from the heat of its neighboring track, it does reach a temperature higher than the austenitization temperature, thereby transforming every phase (along with newly solidified material) to austenite and then to martensite upon cooling.
A region within the third track undergoes a heating cycle from its upper neighbor, where the peak temperature is not high enough to cause austenitization but is high enough to temper the existing martensite, as can be seen in the lower half of the third track image of Fig. 17 where the phase fraction of martensite has dropped below 90%. Additionally, the heat from a more distant neighboring track further tempers the martensite in the fourth track’s region, resulting in an even lower phase fraction of martensite below 80%.

According to the model, the tempered martensite forms three phases: ferrite, ε-carbide and cementite. The phase fraction of cementite is shown in Fig. 18 where it can be seen that the degree of tempering increases between tracks three and four.

To validate the solid phase transformation model, the hardness field was calculated for the domain shown in Figs. 17 and 18 according to Eq. (13) and compared to the experimental sample’s measured hardness. Using a Vickers
The hardness in the region of the sample shown in Fig. 14 was tested across a 12 x 10 grid where each indentation was spaced 0.075 mm across a 0.900 x 0.750 region under 200 g load for 13 s, as shown in Fig. 19. The measured hardness field data are shown in Fig. 20, while the predicted hardness field data and the measured hardness field data are compared in Fig. 21. Note that Detail C represents the same region in Figs. 19, 20 and 21.

From the measured hardness field data in Fig. 20, it is shown that the top layer of deposited material is rather hard, ranging between 570 and 600 HV, which matches well with the predicted value of 589 HV. This corresponds to published data on typical H13 working hardness of 52–54 HRC [67]. Due to tempering from the top layer, the lower layer is softer, ranging between 550 and 430 HV. Additionally, it can be seen from the measured hardness field in Fig. 20 that the hardness field within the lower layer is horizontally periodic. Between 0.20 mm and 0.35 mm along the y-axis, there are three softer regions spaced along the x-axis at 0.15 mm, 0.45 mm and 0.70 mm where the maximum amount of tempering occurs from each top-layer track. The measured and predicted hardness in these soft spots matches well at around 435 HV. Overall, the predicted hardness data match well with measured hardness data, as can be seen from Fig. 21, validating the phase data shown in Figs. 17 and 18.

4 Conclusions

The CA-PF model was expanded and used to simulate a multi-track and multi-layer LDD process, including melting, solidification, dendrite growth and solid-state phase transformation. Using the CALPHAD method, the material, H13 tool steel, was modeled as a ternary alloy consisting of Fe, 5.0 wt.% Cr and 1.5 wt.% Mo. The simulated deposition of multiple tracks and layers showed that the dendrite growth direction and scale across an entire weld pool (430 µm x 300 µm) matched very well with experimental results. In addition to microstructure simulation, the model also predicted that during the deposition of a single track, the resultant solid-state phase is nearly all martensite due to the rapid cooling typical of laser-based additive processes. However, after multiple neighboring deposition tracks caused high- and low-level heating cycles to affect the target track, the previously formed martensite was significantly tempered to softer phases resulting in a reduction down to 80% martensite phase fraction and a reduction in hardness of 150 HV.

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Declarations

Competing interests The authors have no relevant financial or non-financial interests to disclose.

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