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Building blocks for a digital twin of additive manufacturing

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ABSTRACT

Properties and serviceability of additively manufactured components are affected by their geometry, microstructure and defects. These important attributes are now optimized by trial and error because the essential process variables cannot currently be selected from scientific principles. A recourse is to build and rigorously validate a digital twin of the additive manufacturing process that can provide accurate predictions of the spatial and temporal variations of metallurgical parameters that affect the structure and properties of components. Key building blocks of a computationally efficient first-generation digital twin of laser-based directed energy deposition additive manufacturing utilize a transient, three-dimensional model that calculates temperature and velocity fields, cooling rates, solidification parameters and deposit geometry. The measured profiles of stainless steel 316L and Alloy 800H deposits as well as the secondary dendrite arm spacing (SDAS) and Vickers hardness measurements are used to validate the proposed digital twin. The predicted cooling rates, temperature gradients, solidification rates, SDAS and micro-hardness values are shown to be more accurate than those obtained from a commonly used heat conduction calculation. These metallurgical building blocks serve as a phenomenological framework for the development of a digital twin that will make the expanding knowledge base of additive manufacturing usable in a practical way for all scientists and engineers.

1. Introduction

Properties and serviceability of metallic components produced by laser-assisted additive manufacturing (AM) depend on their geometry, microstructure and defects [1–5]. The evolution of microstructure and geometry is affected by the transient temperature fields, cooling rates and solidification parameters [6,7], which, in turn, depend on the process variables, alloy and specific AM process. Building a structurally sound and reliable component requires specification of an optimum set of process variables that affect the transient temperature fields, geometry and cooling rates.

Since there are many interrelated process variables, the selection of an optimized combination capable of producing a structurally sound, reliable component is challenging. The temperature fields and molten pool geometry are difficult to monitor and control in real time during AM. As a result, the structure and properties of components are routinely optimized by adjustment of many process variables by trial and error without any guiding scientific framework. Nearly all of the previous studies rely purely on empirical techniques in which select process parameters are varied while all others are held constant for achieving acceptable properties [8]. Post-process analyses determine the geometry, microstructure and mechanical properties of the as-built component. This approach is time consuming, expensive, and provides no assurance of attaining the optimal structure and properties of the component.

A recourse is to develop a phenomenological framework, or a digital twin [1], capable of predicting the most important variables that affect the metallurgical structure and properties of the components based on scientific principles. Ideally, the framework would enable users to specify any combination of AM process parameters and obtain the important metallurgical variables such as the transient temperature fields, molten pool geometry, temporal and spatial variations of cooling rates and solidification parameters rapidly. In principle, this digital twin of the AM process, when adequately validated with experimental data, would replace or reduce expensive, time-consuming physical experiments with rapid, inexpensive 'numerical experiments'. In the initial phase, such a model would consider all of the important AM process variables as input and provide the transient, three dimensional,

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temperature and velocity fields, cooling rates, solidification parameters and geometry of the deposit as output. From these outputs, non-dimensional numbers, such as the thermal strain parameter, would be computed for further insight into the process [9–11].

Existing AM process models have their inherent advantages and disadvantages for specific applications. Finite element method based heat conduction models [12–14] are able to calculate deposit geometry and temperature distributions, from which heating and cooling rates can be extracted. However, these models neglect the effects of convective flow of molten metal inside the pool during the calculations of temperature distributions. This causes inaccurate predictions of melt pool shape, which leads to inaccuracies in cooling rates. For example, Manvatkar et al. [15] showed that by ignoring the effect of convection, the cooling rates in AM were overestimated by a factor of two. Svensson et al. [16] also noted that the use of a heat conduction equation did not adequately represent experimental cooling curves. Current heat transfer and fluid flow models [15,17] consider the Marangoni convection inside the pool by using a flat-surface assumption, allowing accurate estimation of the temperature and velocity distributions, cooling rates and solidification parameters. However, this assumption causes the predicted deposit geometry to deviate from experimental data. Level Set Method (LSM) [18] and Volume of Fluid (VOF) [19] method both track the evolution of the free surface of the deposit, thus, calculate the bead geometry. This advantage is offset by the fact that they are computationally intensive and often used for only two-dimensional calculations.

Here, we seek to develop and experimentally verify important building blocks for a first-generation digital twin of AM by developing a computationally efficient, comprehensive model with abilities to predict deposit geometry, transient temperature, velocity distributions and solidification parameters in three dimensions. An analytical sub-model based on mass conservation combined with consideration of powder catchment efficiency obtains an initial prediction of the deposit geometry with curved surfaces. A 3D transient heat transfer and fluid flow model provides a crucial building block needed for the prediction of all the important metallurgical variables that affect the structure and properties of the components. This model calculates temperature and velocity distributions, cooling rate and solidification parameters for a single-layer deposit. Experimental validation of the computed deposit geometry is undertaken for stainless steel 316L and Alloy 800H to demonstrate the applicability of the phenomenological digital twin to both alloy systems. Based on the calculated cooling rates, secondary dendritic arm spacing and hardness of SS 316L are calculated and compared with the corresponding experimental results. The actual tailoring of the final component's properties based on the predictive model is still a long way in the future and is outside the scope of this manuscript.

2. Theoretical calculations

2.1. Analytical calculations of the deposit geometry

Previous research on predicting single layer cladding geometry includes the use of parabolic and sinusoidal curves fitting [20], numerical algorithms [21], in-situ sensing [22], neural networks [20,23] and ANOVA techniques [24]. However, the curve-fitting calculations often rely solely on experimental observations and do not consider relevant phenomena such as mass conservation and material properties. In order to model the directed energy deposition (DED) process, the surface of the front edge of the deposit must be considered in three-dimensions. Experimentally, the leading edge of the deposit is located in front of the laser beam axis, which is likely due to a combination of powder-stream distribution and molten liquid spreading. Based on the success of parabolic function fits to 2D clad surfaces [20], an ellipsoidal function seems a natural extension for a 3D deposit surface. Behind the leading edge of the deposit, this profile reduces to an elliptical surface, such that the surface shape can be described for leading edge as,

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}=1 \tag{1}$$

and behind the leading edge as,

$$\frac{y^2}{b^2}+\frac{z^2}{c^2}=1 \tag{2}$$

where a, b, and c are the principal axes of the ellipsoid, as depicted in Fig. 1. Taking advantage of the symmetry of the deposit along the x-z plane, half of the ellipsoid is used in the calculations to reduce computational costs. Physically, the values of b and c represent the deposit half-width and height, respectively, as shown in Fig. 1.

To calculate the values of a, b, and c, several simplifying assumptions are made:

1) The distribution of the blown powder stream is radially symmetric, and hence the values of a and b are equivalent.
2) For a particular alloy, the contact angle and the ratio of the height to half width (c/b) is constant.
3) The maximum deposit half-width is a fraction, f_m, of the laser beam radius, r_b. The value of f_m is calculated using heat balance,

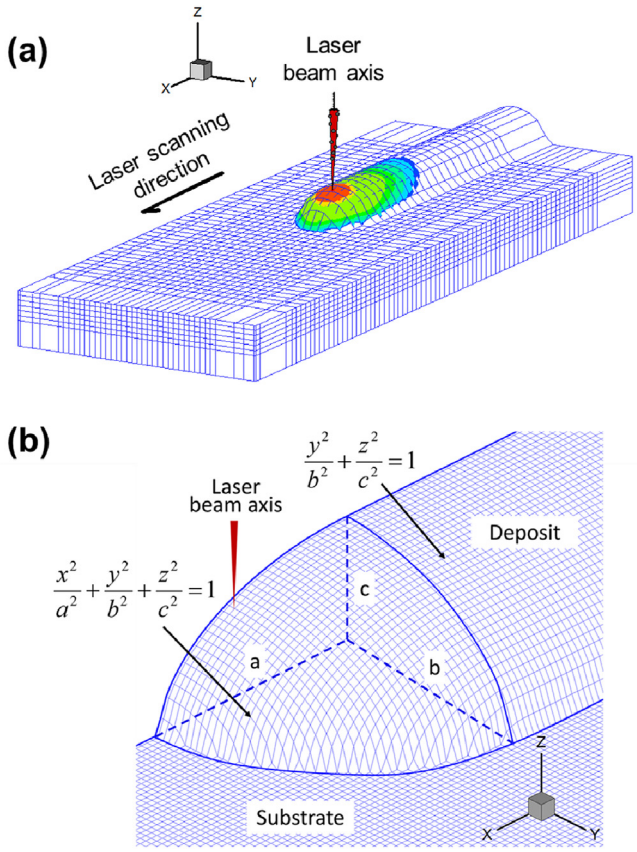

Fig. 1. (a) Schematic overview of the digital twin model. (b) Details of solution domain for the half-ellipsoid deposit indicating the position of the laser beam axis. Deposit is split along the symmetry plane for computational efficiency.