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Viewpoint article

Building digital twins of 3D printing machines☆

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ABSTRACT

Geometrical conformity, microstructure and properties of additively manufactured (AM) components are affected by the desired geometry and many process variables within given machines. Building structurally sound parts with good mechanical properties by trial and error is time-consuming and expensive. Today's computationally-efficient, high-fidelity models can simulate the most important factors that affect the AM products' properties, and upon validation can serve as components of digital twins of 3D printing machines. Here we provide a perspective of the current status and research needs for the main building blocks of a first generation digital twin of AM from the viewpoints of researchers from several organizations.

1. Introduction

Microstructure and mechanical properties of additively manufactured (AM) components are affected by many process variables such as the heat source power, power distribution, scanning speed, powder/wire feed rate, hatch spacing and substrate preheat [1,2]. Building structurally sound components with good mechanical properties based solely on experiments is time-consuming and expensive due to the need for numerous experiments with various combinations of process variables [3–5]. An alternative is to synthesize the available knowledge base of AM and welding to build a digital replica of the AM hardware. The digital twin needs to integrate the major physical components of the evolution of microstructure and properties into a tractable numerical framework: energy interaction with powders, heating and cooling rates, solidification parameters, phase transformation kinetics, evolution of residual stresses and distortion, and defects [6,7]. The visual abstract shows the anatomy of such a digital twin in more details.

There are many advantages of building a digital twin such as (i) minimizing expensive trial and error optimization to save time and money, (ii) shortening the path for product qualification, and (iii) reducing/alleviating defects. The goal of the current viewpoint paper is to examine the current status and research needs for the building blocks of a digital twin: (a) heat and material flow simulation, (b) simulation of solidification, grain structure and texture evolution, (c) modeling of microstructure and properties, and (d) calculations of residual stresses and distortion. Note that this article is not intended to provide a comprehensive review of all existing computational models, rather the authors' view of the components necessary to build a first generation digital twin for AM systems.

2. Modeling of heat transfer - the foundation for understanding structure and properties

Modeling of heat transfer and material flow can provide the transient temperature fields, heating and cooling rates, solidification parameters and the dominant heat flow directions [3,6]. These quantities are critical for the prediction of structure and properties, texture, residual stresses, distortion and many types of defects [2]. Both the temperature field in the entire part and the flow conditions in the liquid metal pool must be calculated by solving the equations of conservation of mass, momentum, energy in transient three-dimensional form with appropriate boundary conditions [3,4,8]. A comparison of numerical techniques commonly used for the heat transfer calculations is summarized in Table 1.

The computational domain is divided into small control volumes or cells, and it changes with time as the part is built layer upon layer. At

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Table 1
A comparison of commonly used techniques for the modeling of heat transfer in additive manufacturing.

Method	Selected features	References
Finite element method (FEM)	Widely used, computationally efficient, can accommodate large and complex computational domains, but ignores convective heat transfer	[16,55]
Finite difference method (FDM)	Computationally efficient but less so than FEM for large and complex domains, meso-scale, and widely used for transient heat and fluid flow calculations	[3,4]
Level set method (LSM)	Computationally intensive, meso-scale, tracks free surface profile of melt pool, but tends to suffer from non-conservation of mass	[17]
Volume of fluid (VOF) method with FDM	Computationally intensive, meso-scale, tracks free surface geometry with mass conservation maintained but at less sharp interface than LSM	[19,20]
Lattice Boltzmann method (LBM) and Arbitrary Lagrangian-Eulerian (ALE)	Most computationally intensive but suitable for massively parallel computing, meso-scale, capable of tracking detailed melting of individual powder particles using VOF	LBM [18] and ALE [6]

any given time, all cells are assigned temperature dependent thermophysical properties of either a solid, powder, liquid or gas. At every time step the properties of the cells change because of changes in the material of the cell and/or its temperature. The governing equations are discretized into algebraic equations which are solved by an appropriate technique to obtain enthalpies (temperatures), and three components of liquid alloy velocities [3,4].

Fig. 1(a) shows the typical computed temperatures and velocities in the liquid pool [3]. The results show large velocities of liquid alloy in a small melt pool in the range of 400–600 mm/s [3] driven by the spatial gradient of temperature [9]. These large velocities indicate convective heat transfer as the main mechanism of heat transfer within the liquid pool during AM [3–5,8,9]. Fig. 1(b) shows the computed thermal cycles at the mid-height and mid-length of the alternate layers in a nine-layer structure [3]. In each of these cycles, the first peak corresponds to a position of the laser beam just above the monitoring location and the subsequent peaks occur during the deposition of the subsequent layers. Fig. 1(c) shows that the calculated cooling rate for a laser directed energy deposition of AISI stainless steel (SS) 316 agrees well with the experimental data [10]. Higher heat input results in somewhat slower cooling because of the larger size of the melt pool.

Moreover, the temperature gradient, G, and the solidification growth rate, R, provide useful information about the evolution of solidification structure [11,12]. In particular, the local cooling rate ($G \cdot R$) is related to the scale of microstructure and G/R influences the morphology of the solidification front [12]. Higher G/R indicates a higher tendency for plane front solidification. The effect of heat input [13] on the ratio G/R is shown in Fig. 1(d). Among different engineering alloys, the temperature gradient in the melt pool is the smallest with Inconel® Alloy 718 (IN 718) deposits followed by that for Ti-6Al-4V and SS 316 alloy deposits [14]. As a result, the SS 316 deposits exhibit the highest G/R followed by that of Ti-6Al-4V and IN 718 alloy deposits.

Various simplifications are used to make the heat and fluid flow calculations tractable [3]. They include two-dimensional approximations [15] and three dimensional calculations ignoring convective heat transfer [16] and three-dimensional convective calculations assuming a flat top surface [3,4]. As shown in Table 1, efforts have also been made to model the free surface profile by either the level-set method [17] or

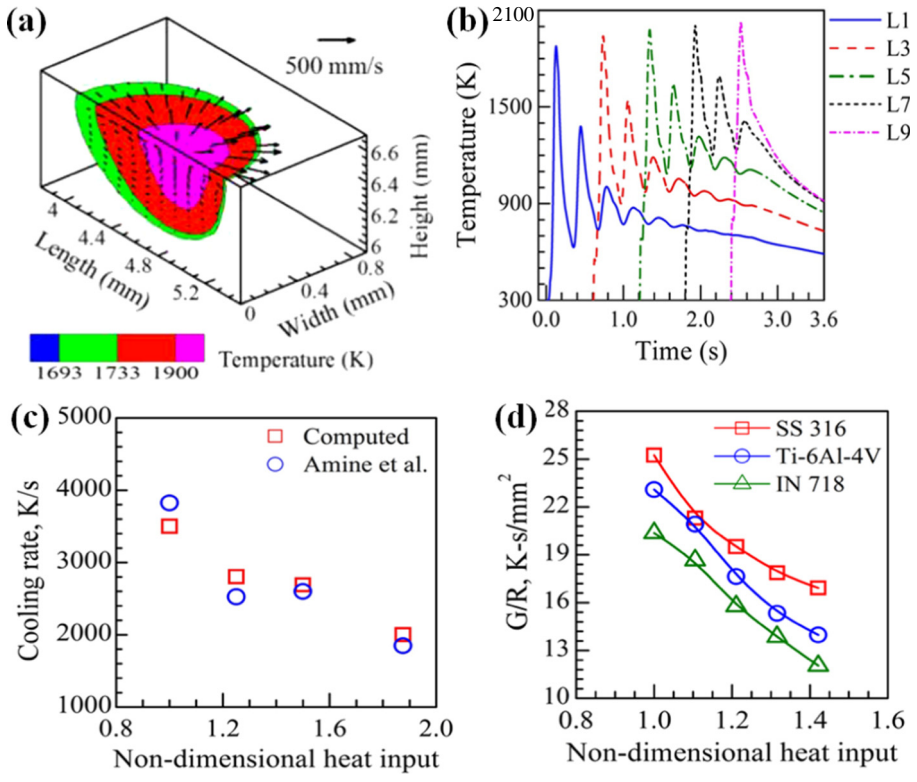

Fig. 1. (a) Computed temperature and velocity fields during laser directed energy deposition AM [3]. (b) Computed thermal cycles during AM [3]. (c) A comparison of the experimental [10] and computed cooling rates [3]. (d) Computed G/R values for the AM of three common alloys [13]. The non-dimensional heat input is defined as the ratio of laser power by the scanning speed divided by the ratio of reference laser power to the reference scanning speed. It provides a measure of the energy deposited per unit length of the deposit.

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