



Short communication

# A digital twin for rapid qualification of 3D printed metallic components

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## ABSTRACT

The customized production of complex components by 3D printing has been hailed as a potentially transformative tool in manufacturing with important applications in health care, automotive and aerospace industries. However, after about a quarter of a century of research and development, only a handful of commercial alloys can be printed and the market value of all 3D printed products now amounts to a negligible portion of the manufacturing economy. This difficulty is attributable to a remarkable diversity in structure and properties of the printed components and susceptibility to defects. In addition, the current practice of qualifying components by prolonged trial and error with expensive printing equipment and feed stock material confine the printed products to a niche market where the high product cost and the delay in the qualification are not critical factors. Here we explain how a digital twin or a digital replica of the printing machine will reduce the number of trial and error tests to obtain desired product attributes and reduce the time required for part qualification to make the printed components cost effective. It is shown that a comprehensive digital twin of 3D printing machine consisting of mechanistic, control and statistical models of 3D printing, machine learning and big data can reduce the volume of trial and error testing, reduce defects and shorten time between the design and production.

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## 1. Introduction

The tool-less, design driven, customized production of complex metallic components by 3D printing has been hailed as a potentially transformative tool in manufacturing [1–3]. Familiar examples include printing of a complex jet engines part [4] and niche applications in biomaterial, health care and automotive industries [5,6]. However, after about a quarter of a century of research and development, only a handful of the over 5500 commercial alloys have been printed to make defect free and structurally sound components [7]. Commonly used alloys for printing include stainless steels, nickel based superalloys and alloys of aluminum, cobalt and chromium [1,8]. However, several complex alloys, such as, titanium–tantalum [9], zinc–silver [10] and titanium–molybdenum [11] have been successfully printed by carefully controlling the printing process and process variables. Excluding the specialized alloys that are designed for specific purposes such as the free machining steels and alloys for casting and rolling, many other potentially printable alloys are either not currently available in a form or shape optimized for printing or have not yet been tested. Furthermore, in the 13 trillion dollar global manufacturing industry, the market value of all 3D printed

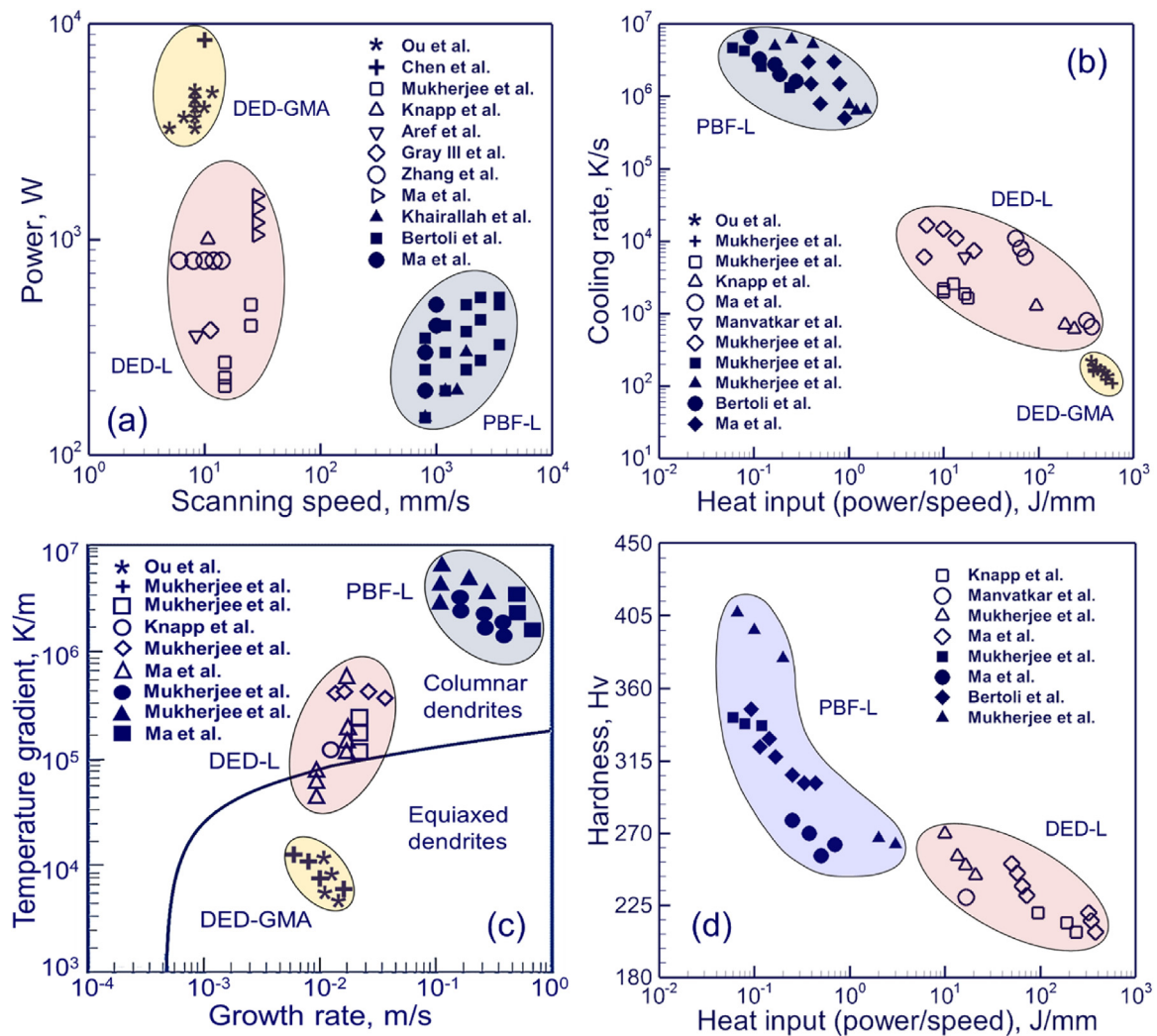
products now amounts to 7.3 billion [12] or a minuscule 0.06% of the manufacturing economy. Will 3D printing live up to the hype? Are its applications forever going to be confined to a niche market where the product cost and the time for development and qualification are not critical factors? Here, based on the available data, we examine the main fundamental metallurgical issues for printing sound parts and hinder the market penetration of 3D printing. Furthermore, we discuss how a virtual replica of the printing hardware, i.e., a digital twin consisting of a mechanistic model, machine learning, data analytics and sensing and control in a single hub can potentially overcome many of the existing issues of metal printing, improve part quality, and shorten the time needed for qualifying products.

## 2. Major metallurgical challenges

The difficulties in the market penetration of 3D printing are related to both the quality of parts and the cost of optimizing processing conditions to manufacture and qualify components. Controlling quality means being able to make defect-free parts with desirable microstructure, properties and performance efficiently. For metallic components, the processing experience controls the properties and performance of the printed components. The temperature–time history, solidification rate and temperature gradients determine the phases that form, the morphology of grains

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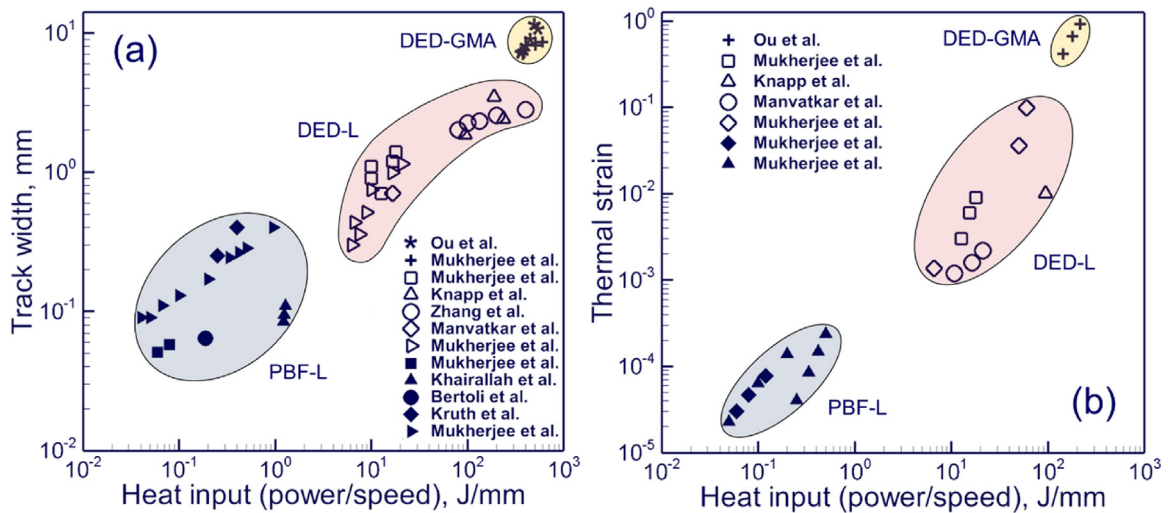
**Fig. 1.** (a) Process windows of stainless steel deposits fabricated using DED-GMA [21,22], DED-L [20,23–27] and PBF-L [18–20]. (b) Variation of cooling rate during solidification calculated on the top of the build with respect to linear heat input for DED-GMA [21], DED-L [20,23,24,29] and PBF-L [19,20,14]. (c) Comparison of temperature gradient and growth rate on the solidification map [27] for DED-GMA [21], DED-L [20,23,24] and PBF-L [19,14]. (d) Effects of heat input on hardness for DED-L [20,24,29] and PBF-L [19,14]. All data are for stainless steel 316. Values are either directly reported or calculated from the available data.

and their growth pattern, the scale of the microstructure, and the nature of the defects [13–15]. Although metallurgists have studied the relation between processing, microstructure and properties for many decades, there is no simple way to tune in to a particular microstructure. A commercial alloy has a remarkable diversity in its structure and properties depending on processing. So the starting point in controlling quality is the processing conditions.

In order to print a part, a printing process needs to be selected. Here we focus on the three most widely used printing processes [1,16,17], laser assisted powder bed fusion (PBF-L), laser assisted directed energy deposition (DED-L) and wire-arc based direct energy deposition (DED-GMA). Apart from the details of these processes, the two most important parameters of interest for controlling microstructure are heat source energy and scanning speed, both of which vary widely among these printing processes. Fig. 1(a) shows that the scanning speed in PBF-L [18–20] is around 100 times higher than those used in DED-GMA [21,22] and DED-L [23–27]. In addition, the power used in DED-GMA is around 10 times higher than those commonly employed in DED-L and PBF-L. Furthermore, in all three printing processes, significant variations exist within the reported values of power and speed as shown in the figure. Because of this wide diversity in processing conditions, alloys solidify at different cooling rates depending on the printing process and

the process variables, as shown in Fig. 1(b). As a result, parts contain diverse primary phases, secondary phases, and grain sizes in the printed components, and microstructures of metallic parts vary widely.

Solidification morphology and the orientation of crystals are important for the properties of the printed components. Grains in printed components generally exhibit various morphologies such as planar, cellular, columnar dendritic, and equiaxed dendritic depending on the spatial gradient of temperature in the molten alloy, the velocity of the solidification front, and the alloy composition [1]. Fig. 1(c) shows that metallic components printed using different printing techniques can have very different temperature gradient and growth rate, and therefore, diverse solidification morphologies. The diversity of processing conditions also becomes apparent when the properties of the printed components are examined. For example, hardness of stainless steel 316 printed using different techniques can be significantly different [14,28,29], as shown in Fig. 1(d). Printing process parameters also affect the other mechanical properties of the component, such as, yield strength, ductility and elastic and plastic behaviors [30,31]. For example, high heat source power and slow scanning speed reduce the cooling rate that results in larger grain size [1,14]. Larger grains facilitate the movement of the dislocations and thus reduce strength



**Fig. 2.** (a) The relationship of track width with heat input for DED-GMA [21], DED-L [23,24,29] and PBF-L [18,19,14,28]. (b) Effects of heat input on thermal strain for DED-GMA [21], DED-L [23,24,29] and PBF-L [14]. All data are for stainless steel 316. Values are either directly reported or calculated from the available data.

and enhance ductility [1]. Printing with thinner layers using PBF-L technique results in rapid cooling rate and makes the component harder and stronger [14]. Higher rate of material deposition in DED-L also increases the cooling rate, hardness and the yield strength of the component [24]. However, inhomogeneity in the grain structure is often a source of anisotropy in the mechanical properties of the printed metallic components. For example, Wang et al. [32] reported that stainless steel components printed using DED-L can exhibit 20% higher ductility along the build direction compared to that along the scanning direction.

Columnar grains are considered undesirable because they are detrimental to properties [1]. Apart from controlling the temperature gradient and solidification growth rates, other methods have been adapted to prevent their formation. For example, inoculants were used during PBF-L of an aluminum alloy to increase the number of nucleation sites and form equiaxed grains [7]. In another study, growth of columnar grains was disrupted by changing the scanning direction in successive layers during DED-L of a nickel based superalloy [33]. Changing the scanning pattern altered the main direction of heat flow. Since the orientations of grains are affected by both the heat flow direction and the easy growth directions for crystal growth, the orientations of the grains were significantly different in different layers. It was shown that customized heterogeneity in the microstructure of metallic components during printing enhanced both the strength and ductility of printed components simultaneously [34–36]. The aforementioned studies indicate successful ways of avoiding detrimental microstructures for the selected alloys. However, there is no known methodology to obtain desirable microstructure for all major commercial alloys. Current practice is to use trial and error to achieve the desired microstructure and properties of the printed parts.

Another important quality issue is the formation of defects such as thermal distortion, porosity and lack of fusion [1]. Thermal distortion is affected by the volume of the liquid pool that forms during printing. Large pools of molten alloy shrink more during solidification and make the component susceptible to thermal distortion [37,38]. Fig. 2(a) shows that the track width, which is an easily measurable component of the liquid pool geometry, depends significantly on the printing technique and processing conditions used. Therefore, susceptibility to thermal distortion in the printed components, represented by thermal strain, can vary for different printing techniques, as shown in Fig. 2(b). Similarly, the lack of fusion defects depend on the extent of melting that affects the

fusional overlap between the layers and hatches [39]. The choice of process variables is important for mitigating defects. In Figs. 1 and 2, heat source power and scanning speed are considered as examples of important process parameters that affect the metallurgical attributes of the printed components. Apart from the power and speed, structure, properties and susceptibilities to defect formation also depend on other process parameters such as layer thickness in PBF-L [40] and material deposition rate in DED-L [24]. For example, PBF-L components printed using thinner layers accumulate less heat and result in rapid cooling and low thermal strain [14].

Currently, optimization of structure and properties and mitigation of defects are done by trial and error testing of a matrix of process variables for different printing techniques. This brute force qualification technique has worked for welding where the equipment and feed stocks are inexpensive. However, the high price of feedstock material and printing equipment makes the trial and error method expensive when qualifying 3D printed parts. As a result, the challenges of quality and cost currently confine the printed products to a niche market where the high product cost and the delay in the qualification are not critical factors. To address these difficulties, the trial and error testing needs to be replaced by an advanced tool that takes advantage of our growing knowledge base of 3D printing as explained below.

### 3. Digital twin: a new concept in metal printing

A digital twin is a virtual replica of the hardware that has been successfully constructed and utilized for different manufacturing processes by many industries and government agencies. For example, General Electric currently possesses over 550,000 digital twins of real, physical systems in operation ranging from jet engines to power turbines [41]. Additionally, NASA and the U.S. Air Force have examined their use to increase reliability and safety of vehicle designs [42]. A digital twin of 3D printing [24,43] hardware consists of a mechanistic model, a sensing and control model, a statistical model, big data and machine learning, as shown in Fig. 3(a). The functions of each of these units and how they may assist in the production of high quality parts in a timely manner are discussed below.

A mechanistic model [23,24,14] can estimate the metallurgical attributes such as the transient temperature field, solidification morphology, grain structure, phases present, and susceptibilities to defect formation [23] based on well-established theories of engineering, science, and metallurgy. The capabilities of the

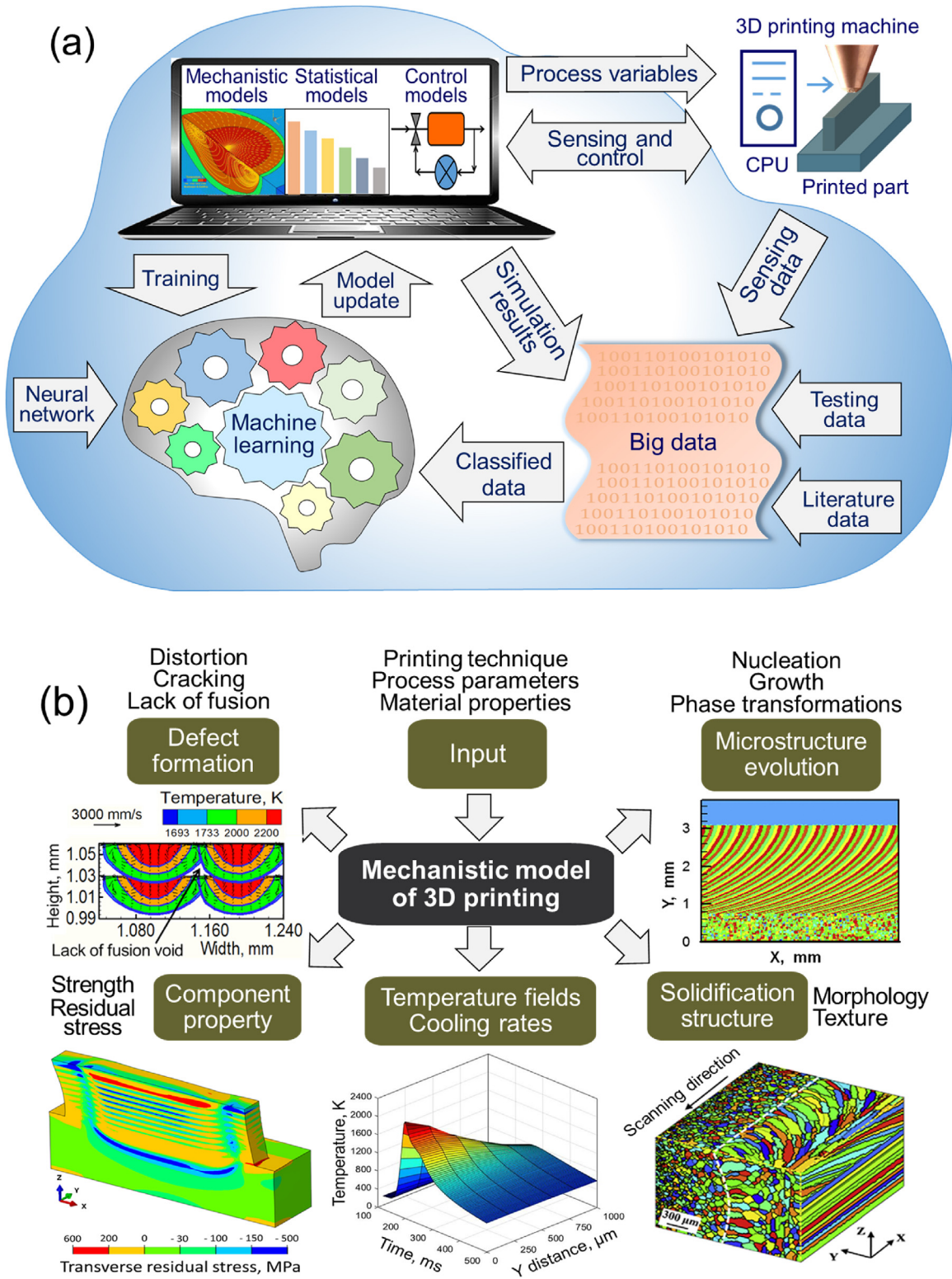


Fig. 3. Schematic representation of (a) the digital twin and (b) mechanistic model of 3D printing.

mechanistic models are summarized in Fig. 3(b). These models rely on the interaction between moving heat sources such as a laser beam, electron beam and electric arc with metallic materials that have been studied to understand fusion welding [44] and more recently 3D printing [13,24,29,33]. Starting with the calculations of transient temperature fields, calculations of simple features of microstructures [33] and properties [29] have been demonstrated.

Currently, there are six main approaches to simulate the essential metallurgical and thermo-mechanical variables in metal printing [1]. Analytical methods [45] solve Rosenthal's heat conduction equation based on several simplified assumptions to obtain temperature fields and cooling rates. However, these methods ignore the dominant mechanism of heat transfer and produce large errors. Heat conduction models [46] using finite element method

(FEM) solve the energy conservation equation and the constitutive equations of stress and strain to calculate temperature fields, build geometry, cooling rates, distortion and residual stresses. Although these models are easy to implement and can handle complex geometries, they often neglect convective flow of liquid metal and often overestimate the temperature. Heat transfer and fluid flow models [13,24] using finite difference method (FDM) solve conservation equations of mass, momentum and energy to calculate essential metallurgical variables in metal printing. Level set method (LSM) and volume of fluid method (VOF) based models track the evolution of the deposit surface [47]. Therefore, the calculated deposit geometries using these models agree well with the experiments. However, these models are computationally expensive and often applied in 2D. Powder scale models [18] using lattice Boltzmann method (LBM) and arbitrary Lagrangian-Eulerian (ALE) method solve the heat, mass and momentum conservation equations in micro-scale and thus involve free surface boundary conditions treating thermodynamics, surface tension, phase transition and wetting. Apart from temperature fields and deposit geometry, these models can accurately predict void formation, spattering and surface roughness. However, these models are computationally expensive and require advanced computational resources.

Mechanistic models can be made bi-directional, so that they can switch between input and output variables. In other words, they can compute a set of process variables necessary to achieve a desired product attribute, such as, part dimensions, microstructure, average grain size, and some simple properties. For example, if attaining a target microstructure requires a particular cooling rate, the model can compute the heat input required as shown in Fig. 1(b). The bi-directional feature of mechanistic models has been successfully demonstrated in welding [44] and can be implemented in 3D printing.

A sensing and control model can interface with multiple sensors such as infra-red cameras for temperature measurements, acoustic emission system for capturing variations in surface roughness, defects and geometric deviation and in situ synchrotron for monitoring selected geometrical features [48]. These models can be used for real time control of AM processes to produce high quality parts efficiently and repeatedly [49]. When a component is made, the model continuously evaluates the sensing data to check if they are within the acceptable limits. If any discrepancy is found, the control model adjusts the process variables to ensure compliance with the design and avoid defects. For example, both too hot and too cold liquid metals are undesirable because they are associated with defects. If the monitored temperature deviates from the normal range, the control model may adjust process variables such as the power of the heat source or the scanning speed to avoid formation of defects.

Both the mechanistic and control models are complex and their outputs may have errors due to several simplifying assumptions in the model [1], errors in input thermophysical and thermomechanical property data, especially at high temperatures, and the common numerical errors in large complex calculations. In order to minimize these errors the mechanistic and control models should be combined with the advanced statistical models. For example, there are several mechanistic models in the literature for the calculation of lack of fusion voids [39]. However, many variables affect the lack of fusion and model predictions do not always agree with the experimental data because of the complexity of the formation of these voids. A statistical model can correct the inaccuracies in the predictions of the mechanistic models based on previous results from a set of classified records within a large set of data known as the big data [49–51].

The big data is a huge collection of a variety of digital data, so large that it cannot be stored, analyzed or shared by usual means [49–51]. The big data for 3D printing primarily includes four main

types of records as shown in Fig. 3(a). First, it contains the data obtained by sensing such as the temperatures, features of the liquid pool and part geometry from multiple printing machines. Second, data from the test results of previously built components such as microstructural features, grain size, solidification texture and properties are also stored. Third, the computational results from mechanistic models and finally, data from 3D printing literature are also collected. Sometime, the data generated during the design and printing of components are also included in the big data set [52]. These data are generated from specifications of the product to comply the desired engineering requirements, new design concept associated with design data such as CAD (computer aided design) files and the evaluation of the design by testing [52].

The big data expands every time an experiment is done or a model is executed. The data are appropriately classified based on the intended purpose using advanced algorithms [49–51]. For example, if the intended purpose is to use the big data for PBF-L, data for other printing processes such as DED-L and DED-GMA should not be included. However, the data must be appropriately used for continuous improvement of model predictions based on the data gathered from new experiments, simulations, and the growing literature.

The expanding big data is classified and used continuously to decide when and how to improve the model predictions using machine learning [53,54]. Machine learning provides a dynamic ability to improve statistical and control models based on continuously growing knowledge base and provides the digital twin the agility to change with time. This capacity is particularly useful when the printing conditions or the alloy systems are changed. Generally, machine learning is achieved by implementing smart algorithms such as neural network [55] that can be developed in two steps. First, it is trained with a set appropriately classified data [55]. Second, the trained neural network is tested and validated using independent set of data excluded during training. However, big data and machine learning, increasingly deployed in various industries, are just emerging for 3D printing [49].

Building a digital twin of 3D printing is a new concept. The existing production methodologies and are unable to determine optimized conditions and alloys system that can be used to fabricate structurally sound, defect free and reliable components in a timely manner and reduce cost. Although several components of a digital twin have been reported in the literature [24,43,49,50], a comprehensive, open source digital twin of 3D printing is not available but can be constructed as described in the following section.

#### 4. Tasks to construct a digital twin of 3D printing

The following tasks need to be performed in order to construct a comprehensive, state of the art digital twin of metal printing. First, many of the aforementioned building blocks of the digital twin need to be developed or modified. For example, transient mechanistic models that run in a reasonable time need to be developed by including all important physical phenomena of the printing process and validated using experimental data for different alloys at various processing conditions. Second, sensing data on which the control models depend should be captured more accurately with enhanced resolution, accuracy and precision of the sensors. Third, the software and hardware for data management, analysis, interrogation, and decision making need to be improved further by developing smart algorithm, computational facilities and storage devices. Finally, different building blocks of the digital twin need to be integrated under one umbrella by establishing strong rapid interactions among them. For example, after the design of a component and its desired attributes are available, the mechanistic model can compute the appropriate processing conditions

to print the part. By providing a recommendation about a printing process and the parameters to produce components with near optimum microstructure and properties before printing, it can significantly reduce the volume of testing needed for qualification. While printing, the control model assures that the printed part complies with the design and adjusts the process parameters during printing to reduce defects. The results from the mechanistic model prior to printing, the sensing data obtained while printing and the test results after printing are all stored in the big data. The anticipated results from the mechanistic model are compared by machine learning with the test results after printing and the already existing results in the big data set in order to decide whether the statistical model or the control model need to be improved further.

## 5. Outlook

Building a bridge between the physical and virtual world of printing by creating a digital twin will reduce the number of trial and error tests, mitigate defects, reduce the time between the design and production and make printing of more metallic products cost effective. The awesome software and hardware capabilities of the digital age, a global pool of technologically savvy and creative workforce and a rich knowledge base of metallurgy and fusion welding are synergistic factors that make the construction of a comprehensive, open source digital twin both a promising venture and a worthwhile realistic undertaking.

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