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Data-Driven Microstructure and Microhardness Design in Additive Manufacturing Using a Self-Organizing Map

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ABSTRACT

To design microstructure and microhardness in the additive manufacturing (AM) of nickel (Ni)-based superalloys, the present work develops a novel data-driven approach that combines physics-based models, experimental measurements, and a data-mining method. The simulation is based on a computational thermal-fluid dynamics (CtFD) model, which can obtain thermal behavior, solidification parameters such as cooling rate, and the dilution of solidified clad. Based on the computed thermal information, dendrite arm spacing and microhardness are estimated using well-tested mechanistic models. Experimental microstructure and microhardness are determined and compared with the simulated values for validation. To visualize process–structure–properties (PSPs) linkages, the simulation and experimental datasets are input to a data-mining model—a self-organizing map (SOM). The design windows of the process parameters under multiple objectives can be obtained from the visualized maps. The proposed approaches can be utilized in AM and other data-intensive processes. Data-driven linkages between process, structure, and properties have the potential to benefit online process monitoring control in order to derive an ideal microstructure and mechanical properties.

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1. Introduction

Accelerating the process and materials design in additive manufacturing (AM) has been investigated in the current literature (e.g., Refs. [1–3]). In this respect, multiscale and multiphysics modeling and simulation are vital, because they have the potential to significantly reduce the cost and time expended in experiments [4,5]. Many efforts have been made to model and simulate AM processes in order to predict process–structure–property (PSP) relationships [6–9]. Meanwhile, it is critical for model validation and verification to employ highly controlled experimental measurements, which include online monitoring of the process, microstructure characterization, and mechanical testing [10–12].

However, merely combining experiments with simulations cannot achieve the desired acceleration in AM process and materials design, because it is difficult to understand and utilize the high-dimensional datasets produced by simulations and experiments. There is an essential need for supportive data science approaches that efficiently integrate the iterations between experiments and multiscale simulation. Popova et al. [13] used data science approaches to understand the process–structure linkages in AM, and used a proposed data science workflow in an attempt to understand the relationships between process conditions and synthetic grain structure. An integration of physics-based and data-mining approaches for temperature field prediction in AM has been proposed [14,15]. A surrogate model based on a functional Gaussian process was calibrated by means of three-dimensional (3D) finite-element analysis (FEA) and experimental thermal image data [14,15]. Salloum et al. [16] undertook high-dimensional dataset compression by using adaptive Alpert tree wavelets in the laser-engineered net shape (LENS) process. The self-organizing map (SOM), which was proposed by Kohonen [17,18], is an unsupervised machine learning algorithm based on neural networks that is able to map high-dimensional data to two-dimensional (2D) planes while preserving topology [19,20]. Compared with an artificial neural network

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(ANN), which is commonly used for regression problems, the main advantage of the SOM is that it can visualize high-dimensional data in the form of a low-dimensional map, which helps researchers to visually identify underlying relations between the features. As a tool to visualize high-dimensional datasets, the SOM is beneficial for the cluster analysis of real-life design problems as well [21].

In this study, an SOM is used to visualize high-dimensional data in AM; these data are obtained from well-designed experimental measurements and multiphysics models. The SOM is introduced to find the relationships among laser power, mass flow rate, energy density, dilution, cooling rate, dendrite arm spacing, and microhardness in AM. In addition, the design windows of process parameters under multiple objectives can be obtained from the visualized SOM. A schematic diagram of this work is shown in Fig. 1 [22].

2. Experimental dataset

Single tracks of Inconel 718 powder were deposited on an AISI 1045 carbon steel disc using a 1020 nm high-powered continuous wave laser. The beam diameter at its focus is 3 mm. The laser power was set to be constant, while the mass flow rate was incremented from 3.35 to 27.2 g·min^{-1} in 2.65 g·min^{-1} increments. At each mass flow rate, the laser power was incremented from 1000 to 2000 W in 200 W increments, resulting in 60 single tracks. The detailed process parameters and conditions can be found in our previous paper [10]. Materials characterization in this case included CR measurements, dilution measurements, dendrite arm spacing measurements, and hardness testing. An infrared thermal camera was used to determine the cooling rate from the solidus to liquidus temperature of the steady-state melt pool, as detailed in Ref. [10]. After etching the clad cross-section, dilution and dendrite arm spacing can be identified and quantified. Vickers microhardness measurements were taken to obtain the averaged microhardness. A summary of the experimental efforts as well as a chart detailing the dilution are provided in Fig. 2. Details of experiments can be found in Ref. [22].

3. Physics-based simulation dataset

A computational thermal-fluid dynamics (CtFD) model was developed to simulate the directed energy deposition (DED) process [23]. The current paper does not describe the modeling equations, but rather provides a few features to offer an understanding of the CtFD model and process–structure models. The non-isothermal Navier–Stokes (N–S) equations, which include mass, momentum, and energy equations, were solved to obtain the temperature field and liquid metal flow in the melt pool [24,25]. A physics-based arbitrary Lagrangian–Eulerian (ALE) method was utilized to track the free surface of the melt pool [23]. The melt pool dimensions, dilution, and cooling rate at the liquid–solid interface can be computed based on the steady-state melt pool temperature field. Dendrite arm spacing is evaluated by the Hurt formula [26]. Vickers hardness (HV) can be determined by the

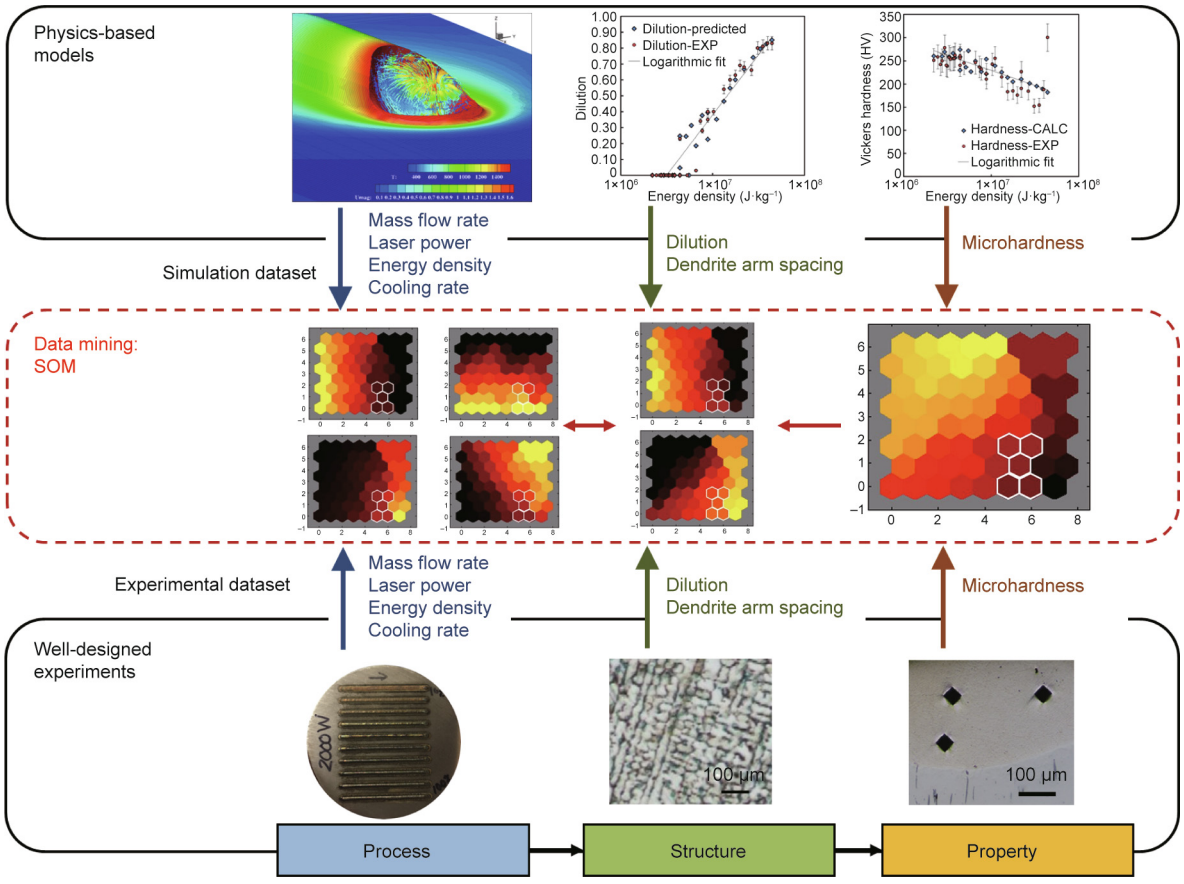

Fig. 1. A schematic description of the workflow typically employed in current computational efforts (top row) and of experimental efforts (bottom row), along with a description of how this can be augmented with a data-mining approach to recover high-value PSP linkages of interest to material innovation efforts. CALC: calculated; EXP: experiment.

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