REVIEW ARTICLE

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Modeling process-structure-property relationships for additive manufacturing

Abstract This paper presents our latest work on comprehensive modeling of process-structure-property relationships for additive manufacturing (AM) materials, including using data-mining techniques to close the cycle of design-predict-optimize. To illustrate the process-structure relationship, the multi-scale multi-physics process modeling starts from the micro-scale to establish a mechanistic heat source model, to the meso-scale models of individual powder particle evolution, and finally to the macro-scale model to simulate the fabrication process of a complex product. To link structure and properties, a high-efficiency mechanistic model, self-consistent clustering analyses, is developed to capture a variety of material response. The model incorporates factors such as voids, phase composition, inclusions, and grain structures, which are the differentiating features of AM metals. Furthermore, we propose data-mining as an effective solution for novel rapid design and optimization, which is motivated by the numerous influencing factors in the AM process. We believe this paper will provide a roadmap to advance AM fundamental understanding and guide the monitoring and advanced diagnostics of AM processing.

Keywords additive manufacturing, thermal fluid flow, data mining, material modeling

1 Introduction

Metallic powder-based additive manufacturing (AM) technologies, including selective laser melting (SLM),

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electron beam selective melting (EBSM) and laser engineered net shaping (LENS), have been drawing increasing attention over the past decade. The basic principles are to selectively add material point by point or layer by layer to produce the desired product directly from the geometry defined by computer-aided-design (CAD) data [1], as illustrated in Fig. 1 [2,3] for two of the myriad AM methods. Since no specific tools or molds are needed, AM, also known as free-form fabrication or more commonly three-dimensional (3D) metal printing, offers an excellent solution for reducing production time and cost in a variety of applications, such as personalized bio-implants [4], prototyping, and small batch production. The topological freedom granted by AM has also been shown to decrease energy and CO_2 costs, e.g., in aircraft applications, by reducing buy-to-fly ratio and operating weight [5]. Thus, AM technologies can reduce the cost and time associated with the traditional design-manufacture-test chain. Moreover, AM is playing an increasingly significant role in the repair of damaged components, especially in the aerospace industry.

Although significant progress has been made, and many appealing potential applications have been demonstrated, there are many barriers to the wide industrial adoption of metallic AM technologies. The uncertain quality of the final product is perhaps the most serious of these barriers. The underlying reasons are: A lack of understanding of the physical mechanisms governing the build process, and numerous influencing factors in the process [6]. The actual process consists of many different physical phenomena over a range of temporal and spatial scales. While it is difficult to experimentally observe the phenomena concurrently, computational modeling of AM processes can help achieve a thorough understanding in a time- and expense-efficient manner.

Many models have been developed to shed light on the underlying mechanisms of manufacturing processes and properties of additively manufactured components.

Manufacturing process models can be divided into two
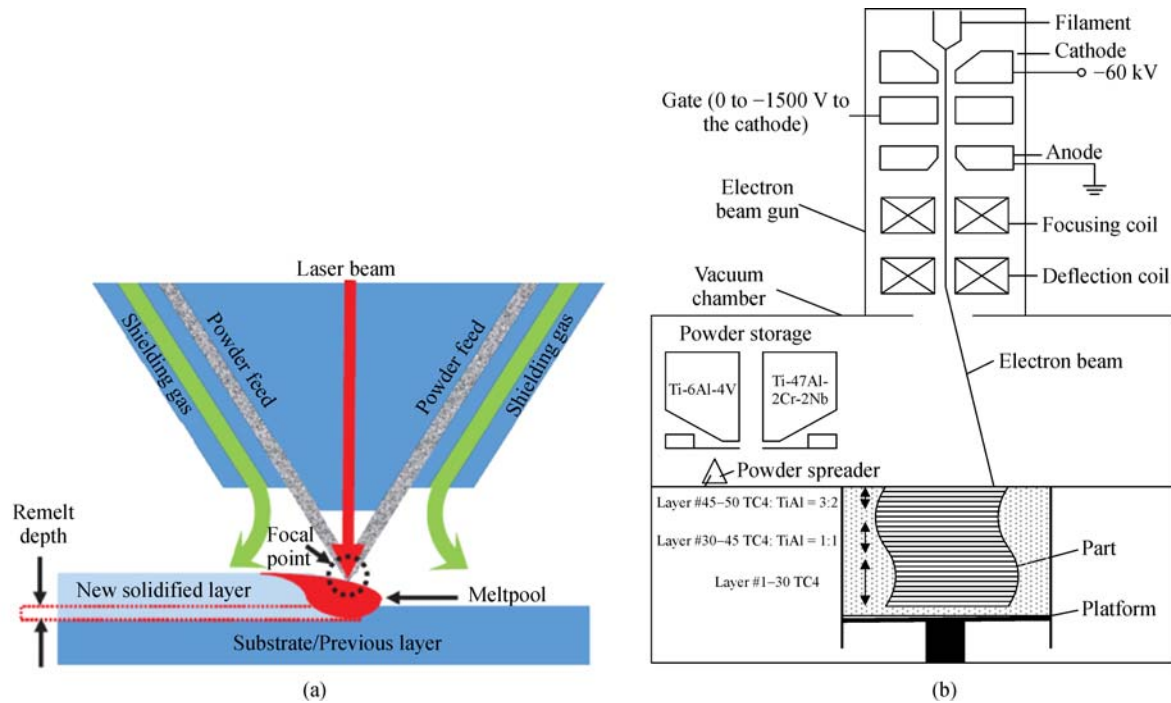
Fig. 1 Basic principles of (a) LENS and (b) EBSM. In the LENS process, a continuous stream of powder is delivered to the focal point of a laser, at the melt pool; in EBSM a bed of powder is spread before being selectively melted. Figures reused with permissions from Refs. [2,3]

major categories: Macro-scale continuum models and meso-scale powder evolution models. Large-scale continuum models enforce a number of simplifying assumptions such that the model can resolve process evolution at the product-scale. Such assumptions include treating powder clusters as an effective continuum and neglecting hydrodynamics. The simplest modeling approaches usually only implement a thermal analysis model in order to predict the temperature field, temperature history and thermal gradients for an additively manufactured material. Significant findings have been obtained from these simplistic models. A review of these macro-scale modeling works was given by Schoinochoritis et al. [7]. These macro-scale continuum models, however, are not able to resolve the flow dynamics of the molten pool within the heat affected zone or the cyclic microstructural evolution during solidification.

Meso-scale models are able to spatially and temporally resolve the evolution of individual powder particles. As a result, more detailed information, such as melt pool evolution and grain growth kinetics, can be obtained to further our understanding of the fundamental physical mechanisms. Initial work in meso-scale modeling of the SLM and EBSM processes have been focused on understanding the molten pool flow dynamics of the process [8–10]. Modeling these dynamics requires the solution of hydrodynamic models which include Navier-Stokes equations coupled to an interface capturing technique to resolve the free surface between the metal and gas/vacuum, such as

volume of fluid [11]. Recent advances in meso-scale modeling of the AM process have begun to couple these hydrodynamic models to a microstructure evolution model [12,13] extended this approach to 3D and gave valuable insight into the effect of powder layer thickness and atmospheric conditions on solidification microstructure. Although these meso-scopic modeling efforts are restricted to very simple build strategies and geometry, they offer valuable insight into the fundamental driving physics of the AM process. These insights can then be used to derive a more physically-informed macro-scale model of additively manufactured products.

While several models [14,15] have been proposed to predict the mechanical properties of AM parts, the overall efforts to predict the material response, plastic response in particular, have been challenged by highly variable and anisotropic properties. Adding to these difficulties, properties also vary significantly with a few build factors. However, attempts to calibrate and validate even specially modified versions developed to take into account the types of variations expected in AM materials have proven relatively ineffectual in terms of predictive capabilities — Too many conditions are outside the calibration domain to have confidence in the prediction.

The ultimate goal for modeling AM is to quantitatively predict the working performance of the final products deployed in functional or load-bearing capacity from the input process parameters, e.g., the properties and the service life under a certain loading conditions. Further-

more, we can control the properties and design the products in both structures and properties. In other words, the predictive models allow for optimal design of structure and properties combinations to make the most efficient use of the raw materials. For instance, in order to produce an individualized bio-implant, a design may include varied surface roughness, microstructures and even voids at different locations to optimize cell adhesion abilities, stiffness and effective densities, since the replaced tissues such as bones withstand different loads at different locations and thus require different properties.

In order to achieve this goal, we proposed a data-driven multi-scale multi-physics modeling framework (Fig. 2) to link process-structure-property-performance, which not only integrates the process and mechanical models but integrally employs data-mining techniques to close the cycle of design-predict-optimize.

2   Multi-scale multi-physics modeling of AM process

We developed a multi-scale modeling framework to understand and optimize the manufacturing process at various scales [3], which is outlined in Fig. 3. Our approach focuses on a bottom-up approach to understand the driving mechanisms of the AM process and predict the quality of AM-fabricated materials given a set of processing parameters, followed by a top-down approach to design new material structures and select process parameters. This requires the implementation and coupling of multi-physics models at multiple scales. Initial work in developing this framework includes the development of a new heat source model derived from the micro-scale electron-material interaction simulations (for EBSM), a meso-scale model simulating the evolution of individual molten pool tracks at the powder scale, and a homogeneous macro-scale model to predict the evolution of additively manufactured products.

2.1   Micro-scale modeling for heat source model

The physical mechanism of an electron beam heating materials is in essence that high-speed free electrons colliding with material atoms and transferring their translational energy to the atoms' vibration energy (thermal energy at macro-scale). We employed the Monte Carlo method to simulate electron-atom collisions [16], as illustrated in Fig. 4. By tracking the penetration trajectories and energy transfer, we can derive a physically-informed heat source model for an electron beam [3,16,17].

2.2   Meso-scale modeling

We developed a comprehensive modeling framework to model the EBSM process at the meso-scale, from spreading powder layers to selectively melting powder along the designated scan path [18]. It consists of a powder spreading model using the discrete element method (DEM) and a hydrodynamic model using the finite volume method
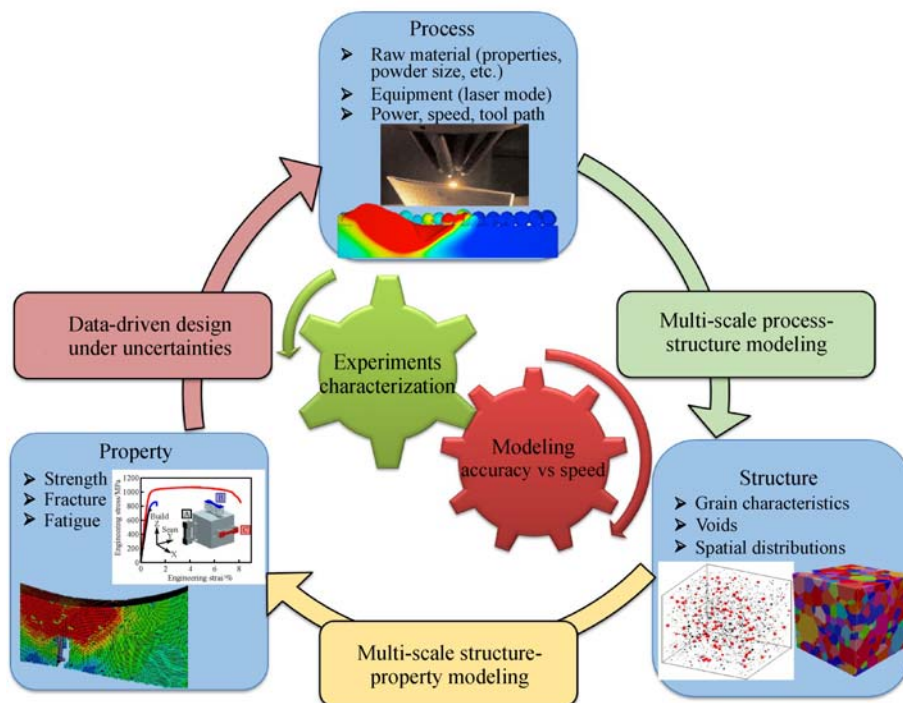

Fig. 2   A data-driven multi-scale multi-physics modeling framework
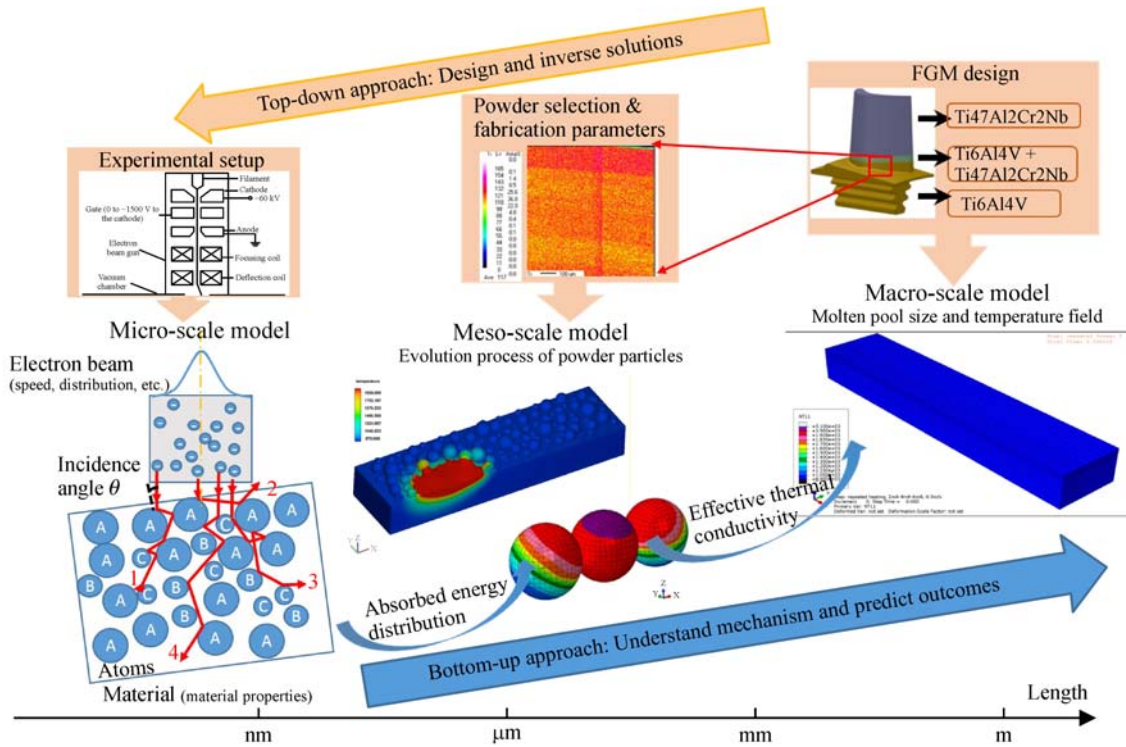
Fig. 3 Framework of multi-scale modeling to link process and structures. Figures reused with permission from Ref. [3]

(FVM), as shown in Fig. 5. The powder spreading model simulates the frictional colliding process between the rake and powder particles; the hydrodynamic model resolves the melting and subsequent molten pool flow process at the powder scale. The powder spreading model generates an initial spatial distribution of powder particles on the substrate. Upon completion of a scan path in one layer in the FVM model, the resulting solidified geometry is transferred back to the powder spreading model to spread another layer. These two procedures are repeated to model a typical multi-layer manufacturing process. A variety of factors can be incorporated to study the influence of experimental set-ups on the manufacturing process, linking equipment and process.

More importantly, our model is able to simulate the manufacturing processes of multiple tracks and multiple layers incorporating the scan path to better guide the optimization of the real processes, while single track simulations cannot. These multiple-layer multiple-track simulation results (Fig. 6) can further advance our understanding of how current and previously melted tracks and layers interact with each other to build complex products and how inter-track and inter-layer defects are formed. These seldom have been reported.

2.3 Modeling of grain growth

Assessing the properties and performance of additively

manufactured materials requires a prediction of the evolving microstructure throughout the process. The evolution of microstructure morphology and textures is in turn influenced by the thermal history of the process. As a result, a major research thrust has been devoted to coupling thermal models such as those presented in Sections 2.2 and 2.4 to a microstructure evolution model.

Compared with traditional solidification models, microstructure modeling for AM processes must account for the effects after solidification, since multiple beam scans cause repeated reheating and cooling cycles and then lead to grain coarsening. Thus, we propose to couple the cellular automata coupled finite element (CAFE) and kinetic Monte Carlo (KMC) methods to model the grain nucleation/growth and subsequent coarsening. While the CAFE method is able to give a good description of the nucleation of grains during solidification, the KMC model can be used to further evolve the predicted grain structure simulations during the reheating regime. Figure 7 demonstrates this methodology for a sample temperature history in an LENS process.

2.4 Macro-scale modeling

Macro-scale models for additive manufacturing are targeted at predicting the build process over several hours for a fully functional product spanning several centimeters in contrast to the millisecond/millimeter time
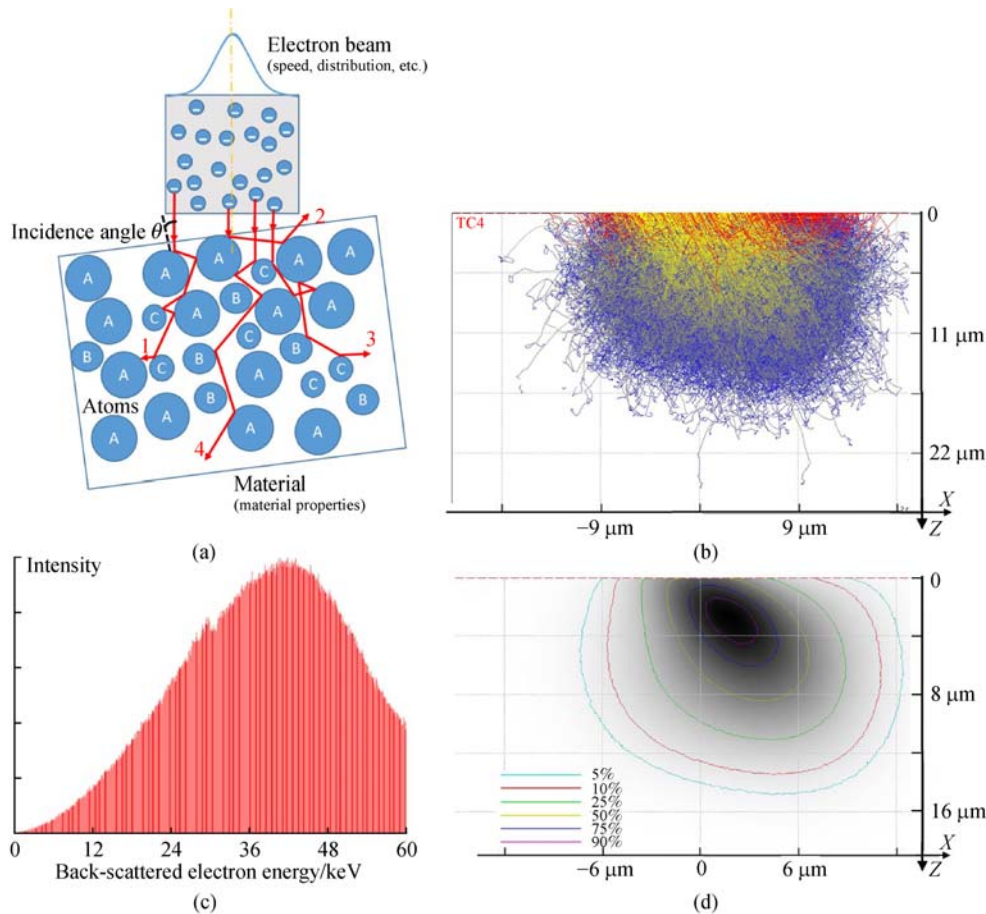
Fig. 4   Micro-scale model of electron-atom interactions. (a) Schematic of the model, simulation results of an electron beam (60 kV) irradiating a Ti-6Al-4V substrate: (b) Penetration trajectories, (c) back-scattered electron energy intensity, and (d) absorbed energy distribution in the substrate. Figures reused with permission from Ref. [3]

scale of the previously aforementioned meso-scale models. The results of such models provide a prediction of temperature field and residual stress to evaluate the performance of the final product [19–21].

Recent work at Northwestern University has been focused on combining tools used by metallurgist/materials and mechanical engineering to develop an interdisciplinary approach to modeling the AM fabrication process. A CALPHAD-based finite element heat transfer model has been developed to connect thermodynamically consistent properties prediction to AM process modeling [22]. This has the potential to open up new opportunities for design of new materials. Simulations are being performed to predict physical response of new materials under AM processing conditions. An application to a Questek custom-made steel Ferrium PH48S is shown in Fig. 8, where material properties are not readily available in an engineering handbook. The material properties are predicted using a CALPHAD-based software based on the constituents. These predictions can be fed into the thermal simulator to predict temperature histories and cooling rates at any point within the product.

3   Mechanical modeling for AM products using self-consistent clustering analysis

The use of the finite element method (FEM) to perform a direct numerical simulation (DNS) incurs computational costs to the point where it becomes inapplicable to material design and concurrent simulations [22]. In order to achieve efficiency and accuracy at the same time, our group [24,25] developed a reduced order modeling technique named self-consistent clustering analysis (SCA) for nonlinear materials with complex microstructural morphologies. This reduced order modeling method is based on a computational homogenization approach using data-clustering, where the microstructure is not accounted for directly at the macroscale, but through a coupled macro-micro formulation. The database created by sampling from prior DNS and experimental data in the offline stage is compressed by establishing clustering groups with similar mechanistic features such as the local strain concentration tensor. Since the clustering is based upon DNS and experimental data, the method can capture local
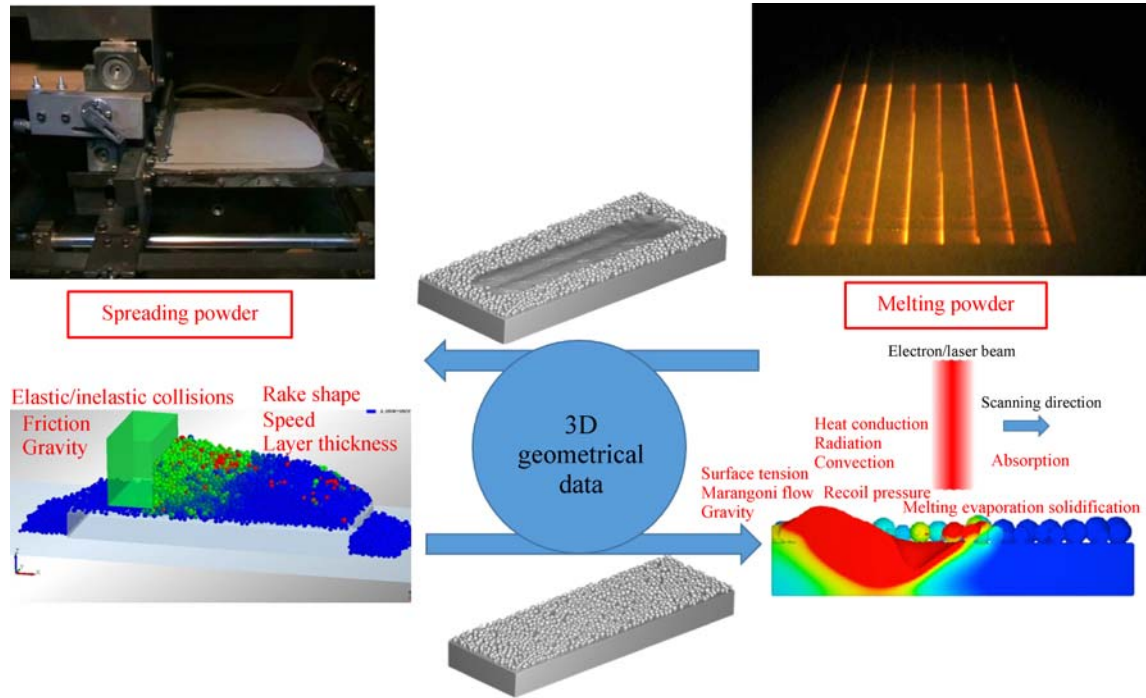
Fig. 5 Meso-scale modeling of EBSM processes from powder spreading to selective melting. Figures reused with permission from Ref. [3]
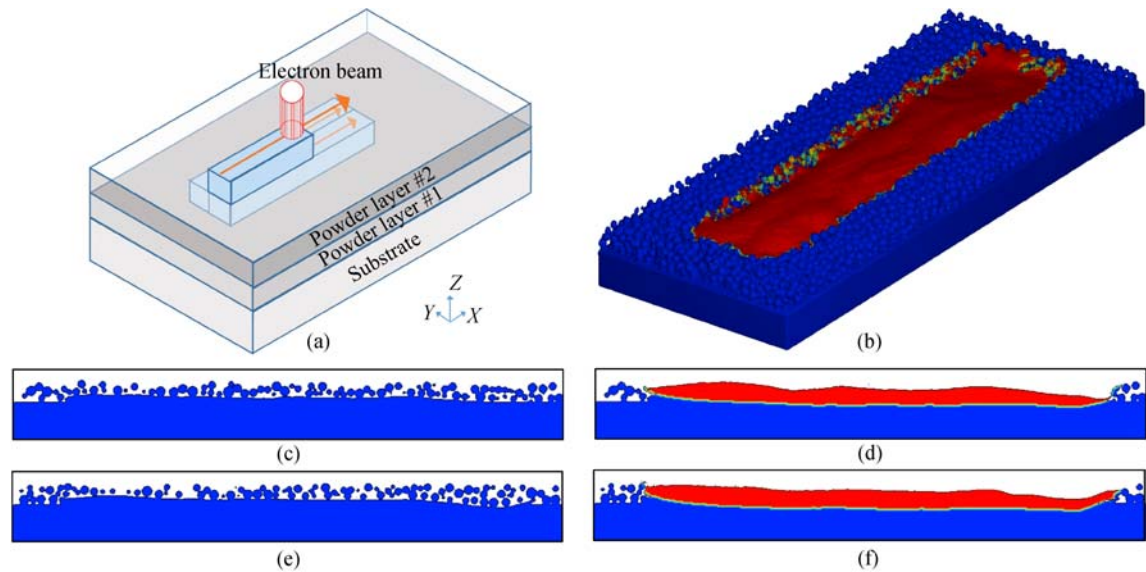

Fig. 6 (a) The schematic and (b) simulated fused zone of the 2-layer-2-track case. The cross section along the scan direction before and after manufacturing are (c) and (d) for $y = 0.4$ mm, and (e) and (f) for $y = 0.6$ mm, respectively

mechanical features and works for arbitrary microstructural morphologies, including voids and other defects, sharing the same versatility as representative volume element (RVE) analysis. For each type of microstructure characterized from the imaging process or process-structure modeling, including imperfections such as pores and inclusions, SCA can be used to create an entry

in the microstructural material database, filled by all the necessary offline clustering data. A concurrent multi-scale modeling framework can be adopted to predict the overall responses at the macro-scale for AM materials, where the responses at each macro material point will be directly computed on the fly from an associated microscale high-fidelity model in the material database.
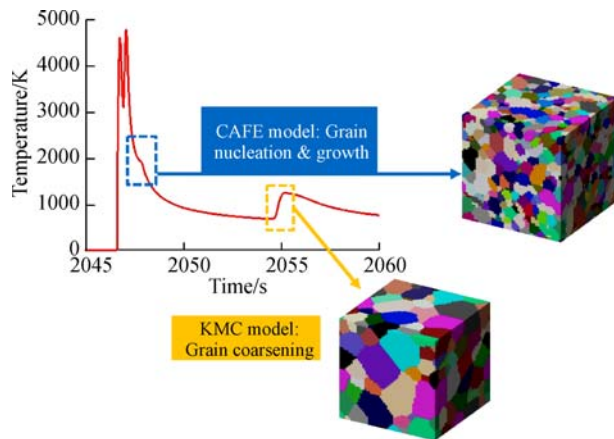
Fig. 7 Schematic for coupling CAFE and KMC methods for modeling grain evolution. A CAFE model will resolve grain nucleation and growth during solidification. KMC methods will be used to further evolve the predicted microstructure from the CAFE model to reproduce the coarsening during cyclic reheating
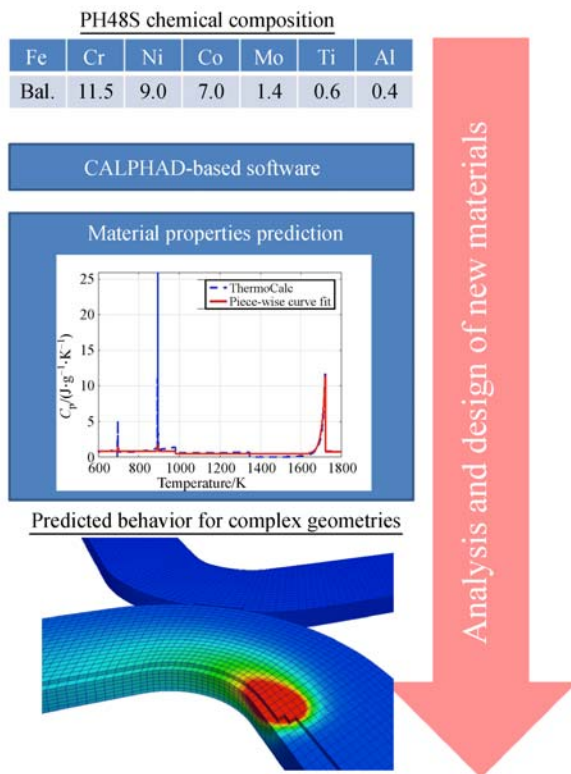

Fig. 8 Comparison of the predicted temperature history at a selected point between handbook-based property assumptions for specific heat and enthalpy change and those predicted by the CALPHAD method

We present two case studies for additively manufactured components: First, a synthetically generated polycrystal microstructure, with randomly oriented, columnar grains;

and second, a microstructure generated from an experimentally obtained image of void clusters within an AM material. In each case, the scale and microstructural features necessitates the use of a crystal plasticity constitutive model, implemented within SCA.

3.1   Polycrystal

In as-built additively manufactured materials, columnar grains extending in the build direction are typically seen; in addition, a preferred orientation, also in the build direction, is seen. A qualitatively similar microstructure has been created with DREAM.3D [26], as shown in Fig. 9(a). The response of this geometry to an applied load in either the X or Z directions is then computed using the SCA: An offline dataset (Fig. 9(b)) is used to create clusters (Fig. 9(c)); from this, the overall response (Fig. 9(d)) and local response (Figs. 9(e) and 9(f)) are computed with SCA.

In Fig. 9(d), a reference solution computed with FEM is given, to show the difference of less than 1% between the FEM and SCA solutions. While some speedup is lost when using crystal plasticity (in part because a more complicated offline computation is needed), a factor of speedup of about 2500 is still achieved.

3.2   Void cluster

A relatively large number of voids is another characteristic of AM metals in the as-built or heat-treated state, even for well-built materials. To understand the impact of a large number of voids on the fatigue response of the material, a microstructure has been reconstructed from focus ion beam (FIB)-SEM serial sectioning and meshed (Fig. 10(a)). A fast Fourier transform (FFT)-based solver computed the offline dataset required (Fig. 10(b)) to compute the clusters (Fig. 10(c)). From the clustering results, the online computation stage of SCA was used to compute the mechanical response of the material to cyclic load, using a crystal plasticity with kinematic hardening. A Fatemi-Socie fatigue indicating parameter, akin to that described in Ref. [27], is then used to determine regions or high fatigue initiation potency.

4   Data-driven material design

Our group at Northwestern University has proposed a data-driven material design framework (Fig. 11) [28]. This framework consists of three steps: (1) Design of experiments, where the input variables describing microstructure, phase properties and external conditions are sampled; (2) efficient computational analyses of each design point, constructing a material response database; and (3) machine learning applied to the database to obtain a new design or response model.
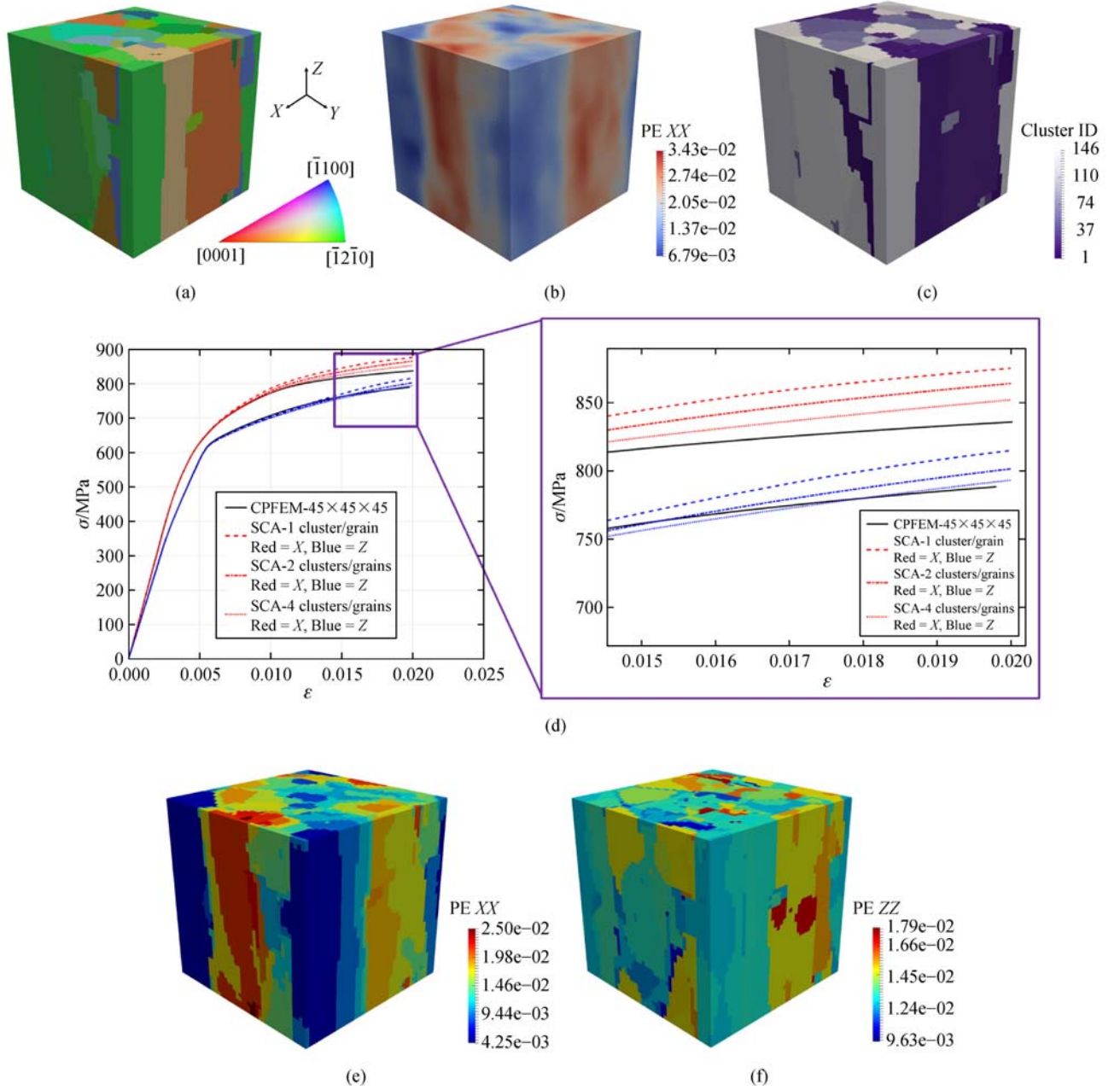
Our SCA reduced order method [24,25] alleviates the

Fig. 9   (a) Synthetically generated columnar microstructure; (b) offline data: Plastic strain; (c) clustering results; (d) overall response and comparison to a DNS simulation with FEA; (e, f) contours of plastic strain in directions X and Z on the surface of the microstructural element as computed with SCA
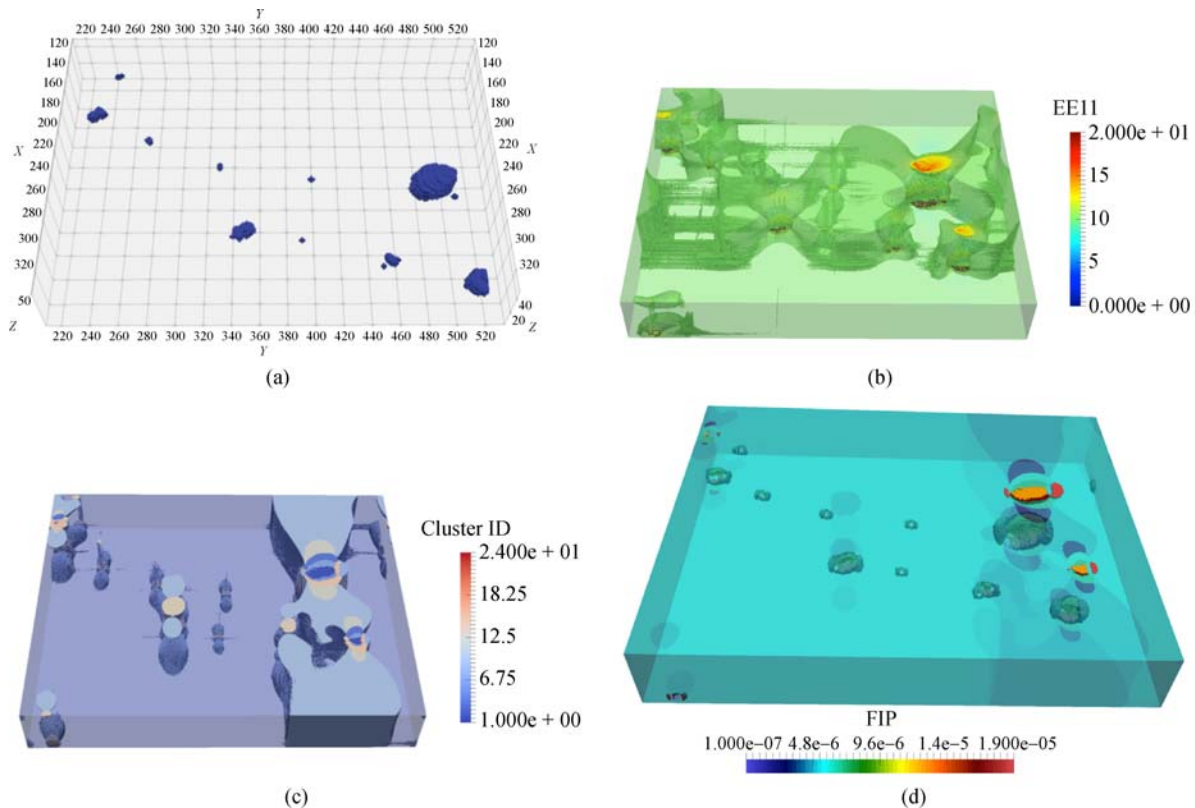
Fig. 10   (a) Voxel mesh of AM voids and (b) offline data for SCA simulation of a cluster of voids in SS316L; (c) clusters built from plastic strain; (d) fatigue indicating parameter computed with SCA

extremely high computational expense of direct numerical simulations. After efficiently constructing large response databases, we employ data mining methods, such as Kriging and neural networks [29], to obtain an optimal design. With the flexibility of adjusting processing parameters and tailing microstructures, AM is expected to benefit from our proposed data-driven design framework and achieve rapid microstructure acceleration.

5   Conclusions

In order to derive process-structure-property relationships for AM, we developed multi-scale process models and mechanistic models at several scales. These models include factors such as voids, inclusions, and grain structures, which are the differentiating features of metallic

AM. We proposed to use data-mining techniques to close the cycle of design-predict-optimize, based on comprehensive material modeling of process-structure-property relationships for AM materials.

Experimental material characterization to determine crystallographic information and volumetric defect distributions, and in-process monitoring to observe the particle melting and molten pool flow, can provide valuable validation to these models, and advance the understanding of the fundamental driving mechanisms. Moreover, close-loop control algorithms incorporating the feedback of in-process monitoring systems are to be developed to ensure the stability of manufacturing process and fabrication quality. We believe that the process-structure-property models will also provide a roadmap to guide the development of the monitoring and diagnostics of AM techniques.
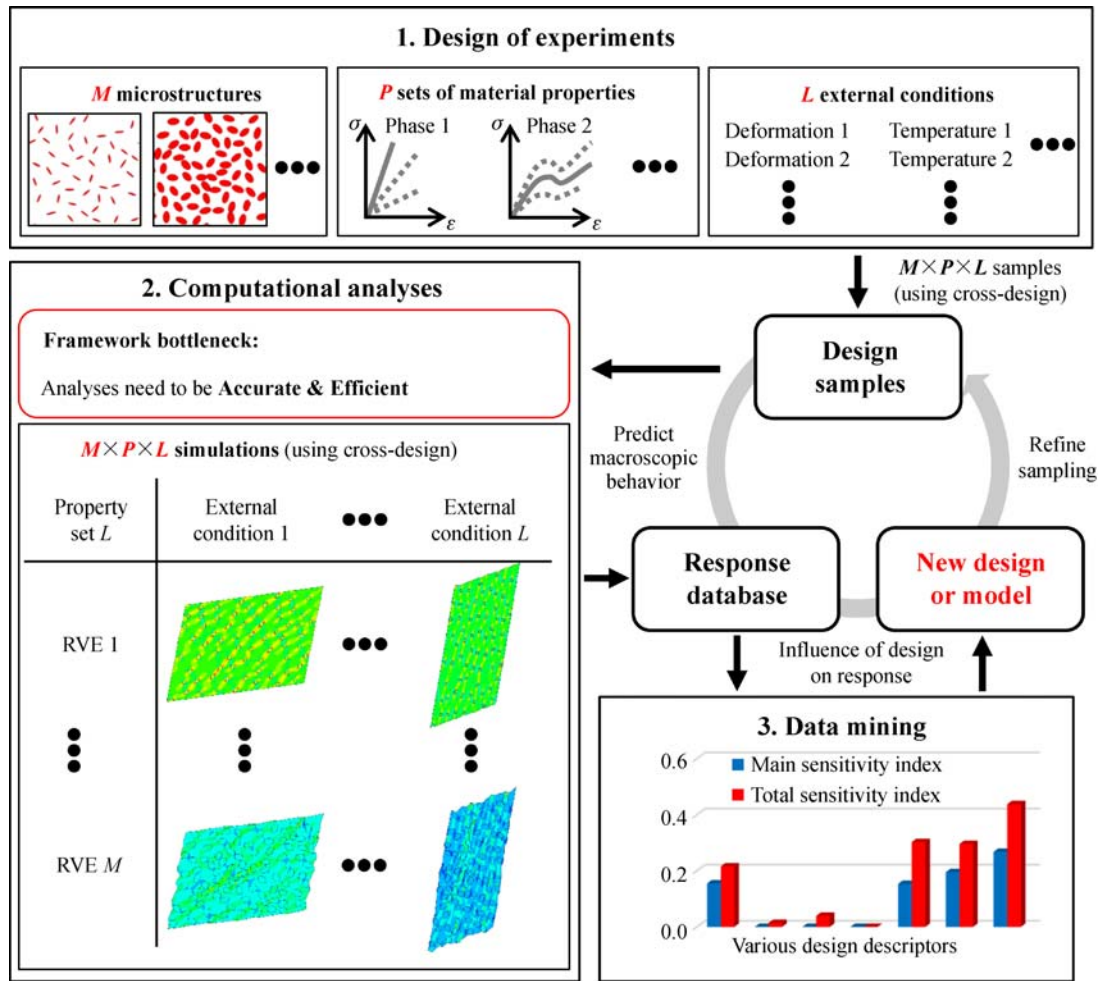
Fig. 11 Schematic of data-driven material systems design. Figures reused with permission from Ref. [28]

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