

Linking process, structure, property, and performance for metal-based additive manufacturing: computational approaches with experimental support

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Received: 9 November 2015 / Accepted: 8 December 2015 / Published online: 5 January 2016
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Abstract Additive manufacturing (AM) methods for rapid prototyping of 3D materials (3D printing) have become increasingly popular with a particular recent emphasis on those methods used for metallic materials. These processes typically involve an accumulation of cyclic phase changes. The widespread interest in these methods is largely stimulated by their unique ability to create components of considerable complexity. However, modeling such processes is exceedingly difficult due to the highly localized and dras-

tic material evolution that often occurs over the course of the manufacture time of each component. Final product characterization and validation are currently driven primarily by experimental means as a result of the lack of robust modeling procedures. In the present work, the authors discuss primary detrimental hurdles that have plagued effective modeling of AM methods for metallic materials while also providing logical speculation into preferable research directions for overcoming these hurdles. The primary focus of this work encompasses the specific areas of high-performance computing, multiscale modeling, materials characterization, process modeling, experimentation, and validation for final product performance of additively manufactured metallic components.

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Keywords Additive manufacturing · Non-equilibrium processes · Multiscale modeling · Materials design · Process–structure–property

1 Introduction

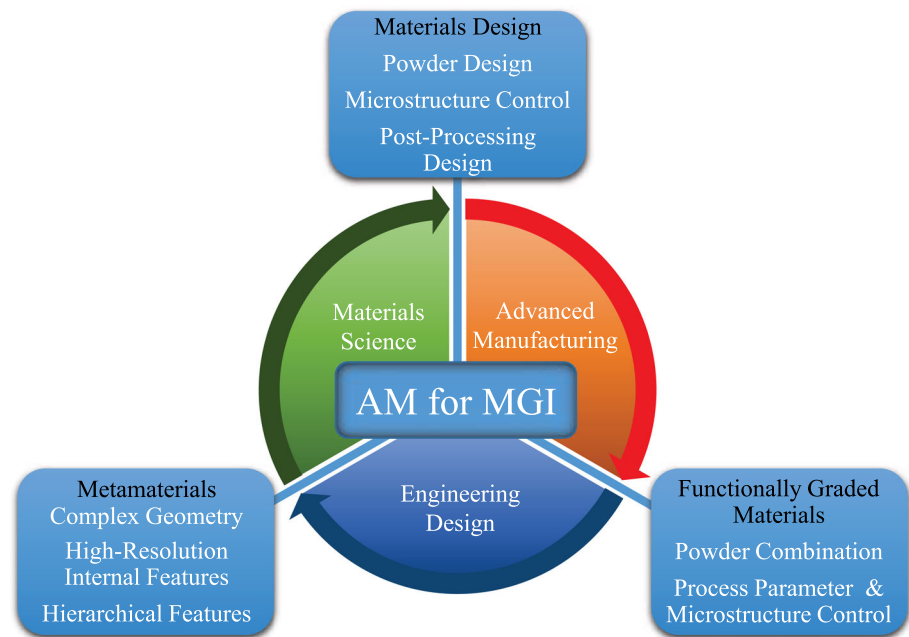
Additive manufacturing (AM) comes in many different varieties for numerous material systems including polymeric materials, biological materials, and metallic materials. However, AM for metallic components has risen to be one of the major research thrusts in materials science and mechanical engineering over the past decade. One of the primary reasons that these manufacturing methods have become so popular is because of their unique ability to create complex components that may otherwise be impossible to manufacture. The impact of these methods can be observed in many scientific disciplines, e.g., advanced manufacturing, mechanical engineering, materials science, component/systems design, aerospace engineering, and bio-medical engineering. AM

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Fig. 1 Opportunities and impact areas of AM for the MGI



also offers strong societal impact through enablement of entrepreneurship and patient-specific medical applications. For the present work, the authors confine the focus of the manuscript to metallic powder-based AM and thus the term “AM” from this point forward will refer to these particular forms of AM. Moreover, it will be assumed when discussing “metal-based AM” that the authors are referring to those methods that involve metal powder as the raw material.

In 2011, the White House set forth the Materials Genome Initiative (MGI) [53], a multi-agency initiative designed to accelerate the discovery and deployment of advanced materials at a substantially reduced cost. The advanced capabilities of AM empower it to have a natural extension to the MGI (see Fig. 1). Processes falling under the umbrella of AM have created a foundation that has the potential to revolutionize the design capabilities for novel components and engineering systems. A stable framework for rapid design and improved time-to-market of materials for enhanced bulk material properties, a fundamental objective of the MGI, is closer to fruition than ever before. AM offers a unique opportunity for materials design through a combination of process control and compositional optimization via an integration of powder metallurgy, physical metallurgy and mechanical metallurgy. The enhanced capability provided by AM for topological optimization and manufacturing components with complex geometries greatly facilitates design and creation of functionally graded materials, which is a challenging endeavor for conventional subtractive manufacturing due to gradient structures, internal features, and interface layers. Additionally, a likely high-impact research direction in AM that will become popular in the near future is design of metal-based metamaterials that have properties superseding metallic materials

found in nature. The numerous capabilities of AM paired with a coupled top-down and bottom-up design methodology positions it to become a key tool in the MGI’s ultimate goal of accelerated discovery of new advanced materials. A top-down approach to comprehensively understand the AM process will allow us to implement a bottom-up methodology to design novel materials.

Patient-specific implants and prosthetics are perhaps the most obvious of medical applications of AM. Everyone has a unique body structure and therefore mass production of prosthetics and metallic implants is not always a viable solution, e.g., jaw replacement. For cases when patient-specific alternatives are desirable, a simple 3D scan can be used to obtain the necessary component geometry followed by AM processing with no special tooling required. Additionally, AM provides the possibility of directly printing functional products with embedded electronics for various applications, many of which are uniquely suited for biological applications. This reduces the amount of time for a patient to receive the final product while also being far more economical than using more traditional processes requiring additional tooling and rework by way of high-precision machining processes.

Extending the life of existing products and engineering systems is of particular importance for aerospace and defense related applications. AM can play two roles in this area: (1) improved design and manufacturing of the materials and/or prototypes and perhaps even more so through (2) component and systems repair. As there is no need for product-specific dies and tooling, AM can be used to repair damaged or failed components on-site with minimal lead time. Even full size AM machines are not excessively large and could be

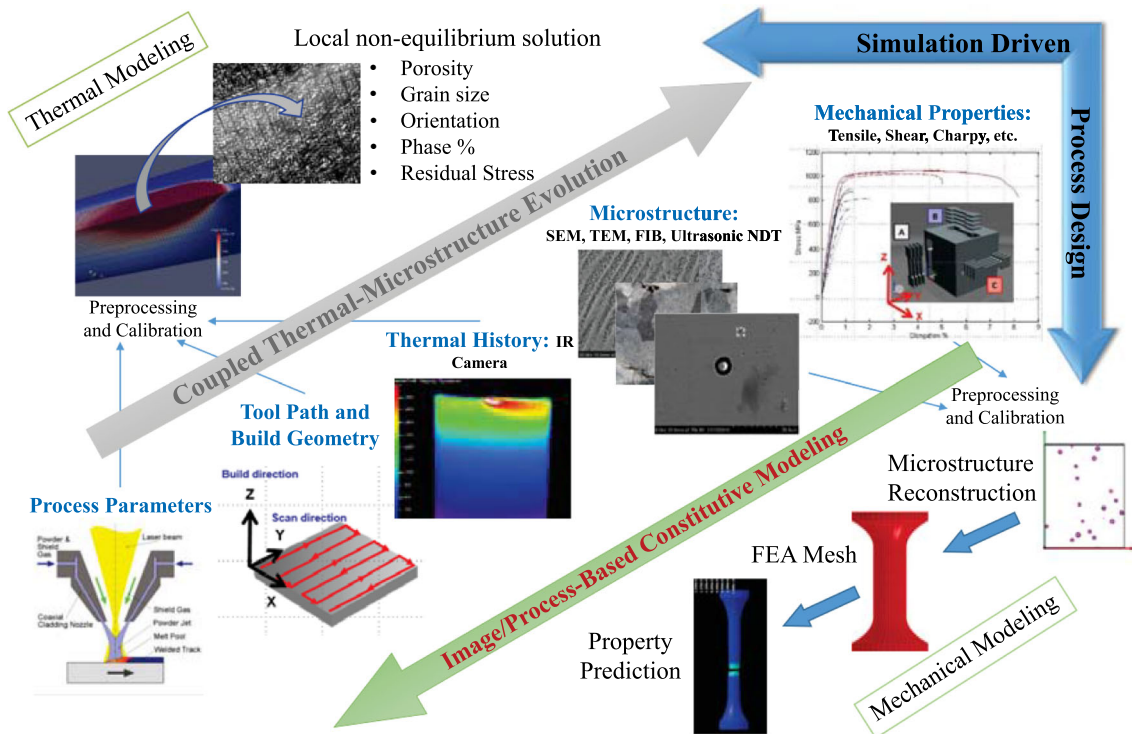


Fig. 2 Simulation driven process/product design strategy for AM processes

developed in such a way that portability will not be a major concern.

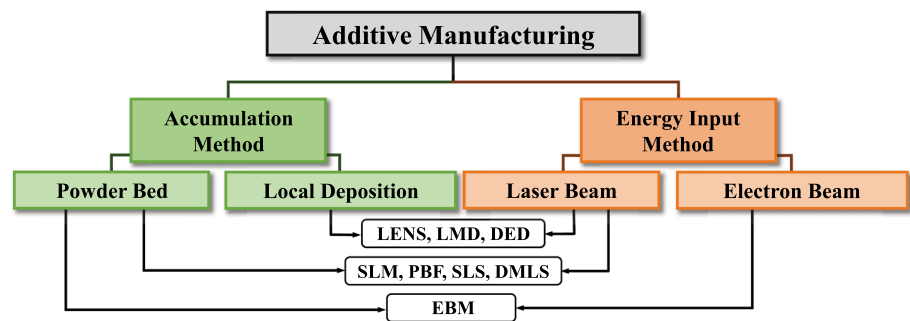
Digital manufacturing is a digital framework for concurrent virtual design of materials, components, materials systems, and manufacturing process chains simultaneously within the paradigm of process–structure–property–performance (see Fig. 2). This form of design is much more economical than guess-and-check experimental methods, which generally have poor sustainability properties in the form of excessive material waste, high energy consumption, and sometimes years of experiments before a viable solution is determined. As digital manufacturing becomes more prevalent for industrial applications, the manufacturing methods for which this framework can be applied must be examined. AM fits perfectly into a digital manufacturing framework due to process flexibility and excellent compliance to complex geometrical features. The aforementioned patient-specific applications provide a great example of how digital manufacturing and AM can be coupled effectively. One can imagine a situation in which a patient-specific implant that includes specific design constraints is needed. The biological feature can be scanned and imported as a CAD file, then sent into a simulation-based analysis preprocessor, followed by topological optimization, and finally a virtual design loop which iteratively develops a robust and practical set of process parameters along with material composition for the desired application. The process is so flexible in fact

that once the topology, material composition, and process have been successfully designed, the part can be produced with minimal to no human interaction. This also improves the viability of AM in distributed manufacturing networks and cloud manufacturing.

AM will no doubt have a positive impact on driving both entrepreneurship and innovation by reducing design and production costs. One way in which this has already been made a reality is through the development of desktop versions of AM machines. While the current versions of personal AM machines are typically for polymeric-based materials, there is the potential for metallic-based AM machines to become available in the near future. Designers from any level of experience can capitalize on this new technology with minimal training. The level of simplicity in operating AM machines allows it to be used as a platform for innovation and design in educational atmospheres as well; many high schools and universities have already invested in assorted versions of these machines in order to encourage student interest in the fields of science and technology.

While the benefits and impact of using AM to create metallic components is quite clear, the governing physics that drive the process to be so versatile also greatly complicate our ability to fully characterize the effect of the process on final product performance. The lack of predictability in the final product tends to reduce the level of confidence that can be expected with more traditional manufacturing process

Fig. 3 Metal-based AM processes with associated methods of accumulation and energy input. *LENS* laser engineered net shaping, *LMD* laser metal deposition, *DED* directed energy deposition, *SLM* selected laser melting, *PBF* powder bed fusion, *SLS* selected laser sintering, *DMLS* direct metal laser sintering, *EBM* electron beam melting



methodologies, e.g., metal forming and cutting. This has resulted in a delay in the use of AM for metallic components and could be a potential bottleneck that may ultimately lead to a premature decline in AM research. This indicates that there is a strong need for robust and efficient computational tools that can improve predictive capabilities in these processes. This will ensure a fruitful future for AM and will accelerate the emergence of high-quality AM products that can have a high economical and societal impact. The question that needs to be answered is, what can the computational mechanics community do to aid the development and widespread usage of AM?

The purpose of the present work is to shed light on the intricacies of AM processes to a wide audience of computational and experimental researchers with the hope of inspiring the pursuit of collaborative research amongst each other and within the many facets of AM. While this article addresses the current challenges and directions of AM research (including novel conceptual contributions from the authors), the present work is not meant to be a complete technical guide to AM as the details and governing equations can be observed through the citations found within the text. The target research areas in AM along with short-term and long-term goals for the computational and experimental research communities will be discussed. The manuscript is divided into the following primary sections: Sect. 2 will describe the methods used for AM of metallic materials, Sect. 3 will focus on experimental AM process and AM materials characterization, Sect. 4 showcases computational challenges and the current approaches used to obtain an understanding of AM processes, materials, and products, Sect. 5 will discuss the short-term and long-term goals for the computational community to realize for continued growth of AM processes as seen from the perspective of the authors, and Sect. 6 contains the conclusions of the work.

2 AM methods for metallic components

Metal-based AM processes can be separated into a number of categories based on the methods implemented to create the 3D components. In the present work, the categories of

additive manufacturing will be dissected based on (1) the method of accumulation and (2) the method of energy input. The term “method of accumulation” refers to the strategy selected for depositing particles on the substrate while the “method of energy input” is referring to the type of heat source used in order to fuse the particles to the layer substrate. From a practical analysis point-of-view, these two categories are the most fundamental drivers of the overall physics encountered during processing, regardless of the spatial and temporal scales in question. In other words, although a single modeling method may be adequate for multiple processes, all necessary or simplifying assumptions should start by assessment of these two primary categories (see Fig. 3).

2.1 Methods of accumulation

For the metal-based AM methods discussed in this work, the metal begins in powder form, with each particle typically being on the order of 20–100 μm in diameter. Therefore, it is necessary to develop methods for transferring the particles to the substrate in order to prepare for the process of fusing the new particle layer to the substrate. While each of the currently utilized methods have value, there are both similarities and unique considerations afforded by the differences in the accumulation methods.

2.1.1 Selective processes

Selective processes, also known as powder bed processes, e.g., selective laser melting (SLM) and electron beam melting (EBM), use a mechanical system to apply a flat layer of particles with a preselected thickness to a substrate prior to application of an energy input. Once the material has been applied to the surface, an energy input method selectively fuses the new particles to the previously fused layer substrate. Therefore, each layer of particles in the powder bed accumulation method is a 2D slice of a 3D component, but there will be additional unused powder in each layer. The accumulation of these slices create a 3D component that is then resting within the powder bed. The component is then

pulled from the powder bed and the excess powder is removed in order to yield the final product.

Powder bed based AM technologies, especially SLM, are some of the most popular among the many AM technologies. One major advantage of powder bed based AM is the outstanding ability to fabricate components with highly complex geometries. In particular, the powder bed acts as a supporting mechanism that improves the feasibility of fabricating cantilever-type structures. Another major advantage is the relatively small residual stress in the final products; the powder bed in selective processes acts to reduce thermal gradients, cooling rates, and residual stress by insulating the build and removing convective heat transfer. Additionally, preheating the powder bed before the selective melting stage can yield favorable reductions in the residual stress. The most notable drawbacks of these processes are the low utilization rate of the powder and the potential size of the component, which is limited by the manufacturing chamber size. For example, in order to manufacture a part with a weight of 5 pounds, approximately 100 pounds of powder must be prepared.

2.1.2 Local deposition processes

Local deposition processes, e.g., Laser Engineered Net Shaping (LENS) and Direct Metal Deposition (DMD), are vastly different from powder bed processes with respect to the methodology behind transferring particles to the substrate. In this method, the powder is applied to the substrate using a nozzle that sprays the particles into the focal point of the energy input source. The focal point of the energy input source is the location where the material is to be fused and therefore local deposition processes require a prediction/assumption of the approximate location of the previous layer in order to obtain optimal particle-substrate fusion.

In comparison with selective processes, the local deposition processes have a high or even perfect utilization rate of the powder and more flexibility in the manufacturable size because powder is only supplied where necessary. Not only can larger parts be created with this method, the ability to provide component modification and repair are unique qualities of local deposition processes. On the other hand, the major drawbacks are the high residual stresses, distortion (sometimes causing fracture of the component), and limited ability to fabricate cantilever-type structures. It is worth noting that the use of the pressurized carrier gas leads to higher porosity and oxidation.

2.2 Methods of energy input

A tremendous amount of energy is required in order to create a 3D component from metallic particles. In AM processes this energy is applied locally to the particles, which can be used

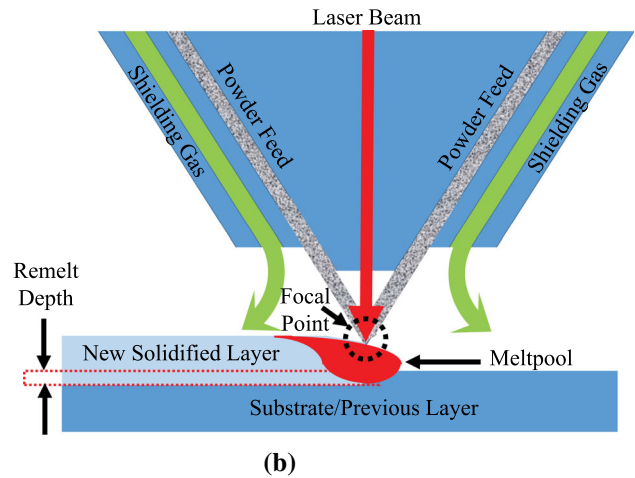
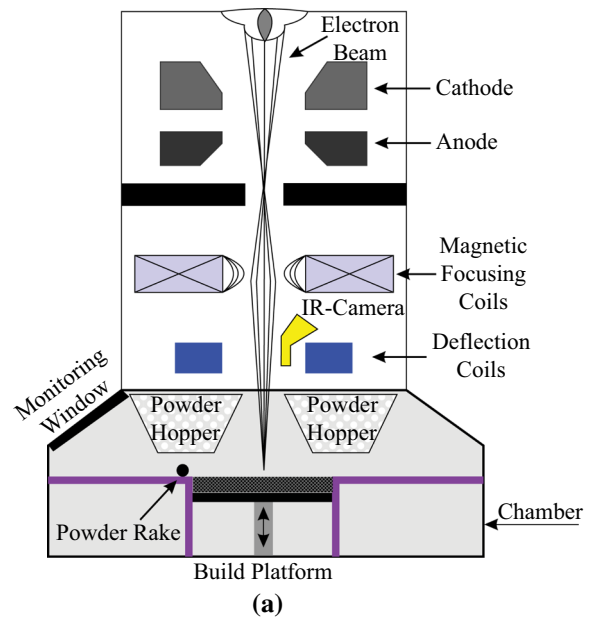


Fig. 4 Equipment used for different types of AM processes. **a** Schematic diagram of electron beam melting (selective-powder bed) equipment. **b** Schematic diagram of Laser Engineered Net Shaping (local deposition) equipment

to reduce the amount of energy needed when compared to other casting/forging processes; in particular, AM processes allow for remanufacture of damaged components in order to reduce waste associated with component replacement. The localized nature of the process requires a highly controllable and high intensity energy source in order to achieve adequate energy density to force phase changes in the metallic particles while also giving acceptable spatial resolution of additively manufactured components. There are currently two primary choices of the energy input method, i.e., laser beam and electron beam, each unique in its underlying physics. Figure 4 showcases some of the primary equipment used for different types of energy inputs.

2.2.1 Laser beam

Laser-based AM (see Fig. 4b) uses a mobile laser head to create the 2D planar sections discussed in the previous subsections. The laser beam is capable of emitting photons to a focal point located on a substrate and the collision of these photons with the surface produce enough heat to change the phase of the particles/substrate. State-of-the-art laser technology allows for numerous control methods including modulation and pulsing, fine-scale adjustments to spot diameter and a wide range of power output settings.

Lasers can be employed to heat a large variety of materials, providing extensibility of laser-based AM processing methods to a vast number of practical applications. It is also relatively easy to control the scan strategy of the laser beam, either by mirror deflections or a moving fiber laser bead; these two advantages combined are primary contributing factors that have led to laser beams being the most widely used heat source in AM and other manufacturing areas. Additionally, the focal point of the laser beam can be extremely small ($20\mu\text{m}$ [26]), which improves the ability of the process to fabricate fine-featured structures to an impressive resolution. The drawbacks of laser-based AM are the low absorption rate of the transmitted energy and the relatively low scan speed (0.2m/s [40]) induced by the mechanical inertia. Moreover, laser-based AM methods have difficulty in manufacturing materials with high melting points and high thermal conductivity.

2.2.2 Electron beam

Electron-based AM uses a scanning electron beam in order to create a 3D component out of 2D planar sections, but the physical mechanisms of both heating and control of the electron beam are different from those used in laser-based methods. As schematically shown in Fig. 4a, the electrons are emitted by the electrical heating filament and then accelerated at a voltage of about 60 kV. The high-energy electrons can be focused to create an electron beam with a diameter of approximately $350\mu\text{m}$, which is controlled by a focusing coil. The focusing coil is turned off and a defocused electron beam is used during the preheating step, whereas the focused electron beam (provided by the focusing coil) is used to obtain a high energy density for the melting step [21].

Scanning of the electron beam is controlled through the deflection coil. The scan speed can be extremely high, on the order of tens of meters per second (sometimes even higher), because of the lack of mechanical inertia. The entire process takes place in a vacuum chamber, which effectively prevents contaminations from surrounding air (oxidation) and reduces porosity. Furthermore, the powder bed can be preheated to reduce both the thermal gradients and, as a result, the residual stresses. The fundamental mechanism of the energy transfer

from the electron beam to the material is penetration of the electrons followed by collision with the particle/substrate atoms. A detailed description and modeling procedure for these interactions can be found in [84]. It should be noted that the penetration ability of the electron beam is stronger and the absorption rate is higher than that possible with laser-based methods. Therefore, the use of electron beam based AM has advantages over laser-based methods in terms of the ability to manufacture materials with both high melting points and good thermal conductivity. Compared with laser-based AM technologies, the electron-based technologies have an advantage in fabricating high reflectivity and high melting point materials, e.g., Ti-Al alloys and Tungsten, because of the high energy absorption.

Unfortunately, electron beams are not applicable to materials with poor electrical conductivity and there is notable complexity in the process of focusing and deflecting the electron beam; these two disadvantages are the primary reasons that EBM is not as widely used as SLM. Another major drawback of electron beam based processes is the limitation of the size of the product. Large vacuum chambers allowing high volume parts to be produced are very expensive. Moreover, the deflection angle cannot be too large or dimensional accuracy of each scan will be unsatisfactory, which again limits the size of the chamber.

3 AM process mechanics and materials characterization

Characterization of the AM process mechanics, as well as the effects of these mechanics on the final product material behavior, is necessary in order to obtain insight that can drive design of both process and product. This characterization is the primary starting point for selection of numerical schemes directed at prediction of as-built AM material microstructures and relating conformation and composition to performance, i.e., process–structure–property relationships.

3.1 AM process mechanics

Understanding the fundamental mechanics inherent to a given process, whether it is deformation based, subtractive, or additive, is the key to process control, process optimization, and process innovation. As previously stated, AM processes incorporate a heat source that drives a phase transformation of the material being processed. Thus, the primary process mechanics are related to an extremely localized phase transformation that accumulatively becomes a final product. The current priority in AM is to develop the capability of controlling the powder-scale phase and microstructure evolution to produce a high quality final product. Design/control of the local microstructure evolution is limited only by the

controllable process parameters and an understanding of the effect of those parameters on structure, properties and performance. The most fundamental controllable process parameters are: (1) input source power, (2) energy source velocity/position, (3) surface area of the energy input, e.g., laser spot size, (4) mass flowrate (local deposition processes), (5) composition, size distribution, and packing density (powder bed processes) of the powder material, and (6) the hatch spacing and layer depth. Establishing a comprehensive understanding of the fundamental physics driving the complex microstructure and phase evolution is imperative to regulating AM processes; this will inform us on how to optimize process parameters to produce a desirable final product quality.

A number of different physical phenomena, and interactions between these phenomena, directly influence the AM process, and consequently alter the local and global product properties and performance. While it is well-understood that the fundamental driving forces are inherently connected to the selection of process parameters, the exact correlation between the physical phenomena and the process parameters is poorly understood. The primary culprit of the lack of understanding is the inability to establish high-resolution and accurate in situ experimental monitoring methods for AM processes. Although detailed quantitative data related to the real-time physical processes taking place in AM are not presently available, the inherent physical mechanisms driving the complex microstructures can still be explored using ex situ experimental observation (see Sect. 3.2).

A typical physical mechanism seen during the process is the rapid melting and solidification of the metallic powder, which is primarily driven by thermodynamic and hydrodynamics forces. Melting of the powder particles lead to the formation of a melt pool, incorporating fluid dynamic forces such as surface tension. Surface tension effects can cause surrounding powder particles to be drawn into the melt pool, whereas surface tension gradients can introduce additional convective forces from Marangoni effects, significantly impacting the smoothness and continuity of the ensuing melt track [83]. Rayleigh instabilities within the melt pool can also result in a discontinuous melt track, which is known as balling [28]. Lastly, sufficient remelting of the previously solidified layers is required for sufficient bonding of the current layer; this impacts the flow behavior of the melt pool and ultimately influences the melt track formation. These forces combined with the highly localized solidification dynamics significantly impact the surface finish of the final product. Further complications arise when the energy density becomes high enough to cause evaporation within the melt pool. The evaporation effects in conjunction with the rapid solidification of the metal powders can cause gas entrapment within the product, creating both internal porosity and surface defects.

These are just a sample of the physical mechanisms occurring during the build process. Other forces that can also play an important role in the final product quality are the residual stresses resulting from highly localized temperature gradients, which are influenced by the absorption of the beam energy, thermal diffusion between powder particles and the surrounding powder bed/bulk material (substrate or previously solidified layers), convective heat loss, and radiation of heat. Aside from implying the number of complexities that impact final product performance for AM materials, the inherent physical mechanisms known to occur during AM processing establishes these methods as multiscale problems. Determining and understanding the dominant physical mechanisms can better our ability to predict the optimal process parameters to obtain the material structure and properties for a particular product application.

3.2 Experimental materials characterization of additively manufactured products

Experimental materials characterization of additively manufactured samples is similar to that of some traditional manufacturing methods. Therefore, microstructure characterization techniques used for materials manufactured by traditional methods can still be applied to AM materials. However, due to the unique attributes of AM, three major properties require special attention in materials characterization. The first is the density of as-fabricated alloys, i.e., voids/porosity, since the alloys are manufactured using alloying powders. The second is the anisotropic microstructure, e.g., defect distribution, oxide inclusions, grain orientation, attributed to the occurrence of reheating cycles via the back-and-forth motion of the laser/electron beam power source. The third is the surface roughness, which can be reduced by undergoing surface finishing in the post-processing stages. It should also be noted that residual stress is of particular importance for many applications [78] but the study in the present work related to experimental characterization will be limited to the three aforementioned properties.

The selection of density measurement techniques can have significant influence in quantifying the effect of process parameters on the bulk porosity of as-built AM alloys. For example, Kamath et al. [29] used both Archimedes method and Scanning Electron Microscopy (SEM) in order to predict the effect of laser power and laser speed in the SLM process on the density of as-built alloys, which were found to yield qualitatively similar results but were quantitatively dissimilar. As shown in Fig. 5, most of the currently available microstructural characterization techniques can be directly applied to the additively manufactured alloys, which are part of Materials by Design[®] and Accelerated Insertion of Materials [50–52, 81]. The size and volume distributions of grains and phases as a result of the complex thermal history are of

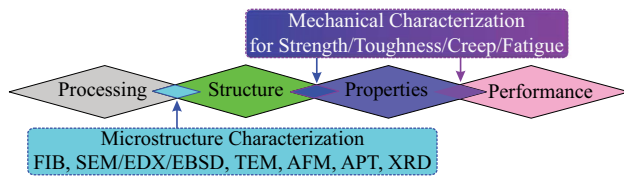


Fig. 5 Common materials characterization experiments used for additive manufacturing. *FIB* Focused Ion Beam, *SEM* Scanning Electron Microscopy, *EDX* Energy-Dispersive X-ray spectroscopy, *EBS* Electron Backscatter Diffraction, *TEM* Transmission Electron Microscopy, *AFM* Atomic Force Microscopy, *APT* Atom Probe Tomography, *XRD* X-ray Diffraction

particular interest due to their impact on the final properties. Figure 6 shows the simulated temperature profile (Fig. 6a) and the heating and cooling rate (Fig. 6b) of one spot in an additively manufactured component using EBM. The model setup is shown in Fig. 7 and uses a symmetry boundary condition on all side surfaces and the bottom surface while the top surface incorporates the effects of heat loss due to radiation. The model dimensions and process parameters along with material properties used for the simulation can be found in Tables 1 and 2, respectively. A combination of experimental measurements and robust thermal modeling procedures are highly desirable in order to provide a comprehensive understanding of the localized thermal history in AM products. The integrated experimental-computational approach will also be beneficial for simulation of microstructural evolution based on physical metallurgical models.

In addition, understanding the microstructural inhomogeneity generated by AM processing will greatly assist in connecting process parameters to microstructural evolution, and thus providing the potential for microstructure design through in situ laser/electron beam process control. It is noteworthy that among the microstructure characterization techniques, Focused Ion Beam (FIB) assisted 3D tomography with resolution on the submicron level is a powerful and often used method for characterizing anisotropic features within the microstructure as well as pore distribution and size [49]. Typically, 3D tomography based on optical microscopy can observe the distribution of large size grains and large voids at the micron scale [47,48]. Alternatively, 3D tomography based on FIB/SEM can be utilized to study the sub-micron void distribution, and thus understand causation of crack initiation and fracture [49,72]. Due to the complex thermal distribution observed during development of AM samples, the material microstructure usually shows strongly inhomogeneous features that can be associated to both size and distribution of both the grains and defects. Figure 8 (Fig. 6 in Zhu et al. [88]) illustrates such a feature observed in Ti6.5Al3.5Mo1.5Zr0.3Si titanium alloy fabricated by a laser-based local deposition process [88]. Evidently, the introduced inhomogeneity of the microstructure will have substantial influence on the generation of

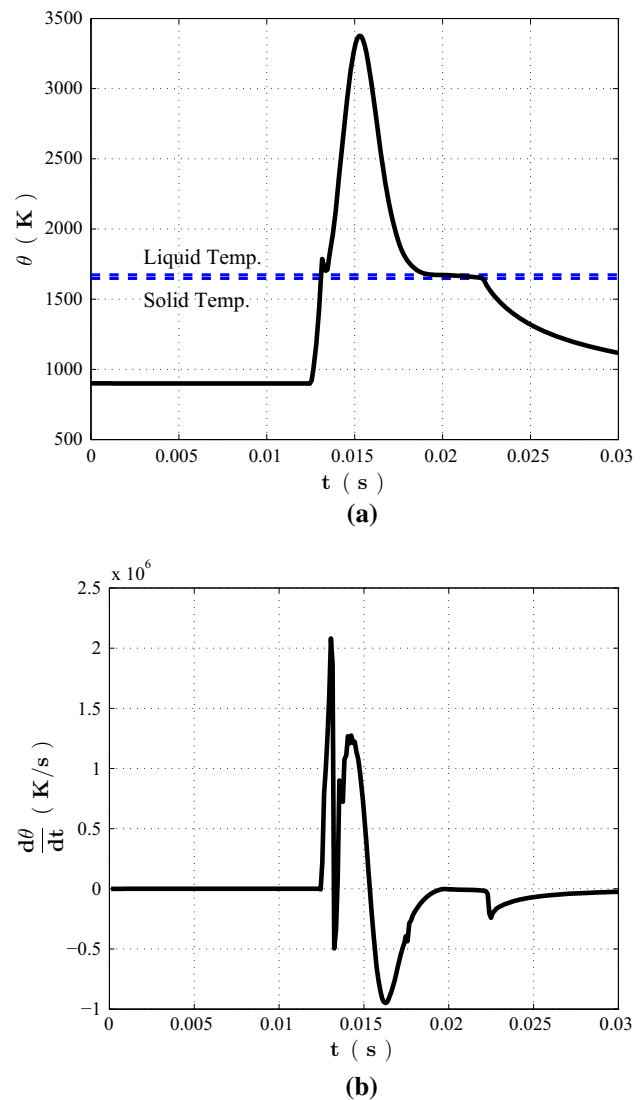


Fig. 6 Response of a selected node in the powder bed example model. **a** Thermal history for selected node. **b** Temperature rate history for selected node

anisotropic mechanical properties in the additively manufactured alloys. Therefore, in contrast to the investigation of alloys manufactured by other techniques, mechanical characterizations of the as-built alloys by AM to determine anisotropic properties are especially important for the purpose of improving materials performance [70,88,89].

Aside from the anisotropic microstructure and porosity of the as-fabricated alloys in AM, another challenging issue related to microstructure characterization and mechanical properties is surface roughness, which can lead to severe fatigue failure. Although the traditional method of using Atomic Force Microscopy (AFM) or optical profiling systems may work for 2D section measurements of the surface roughness, 3D characterization methods to investigate the surface roughness are still arduous [57]. In the study of

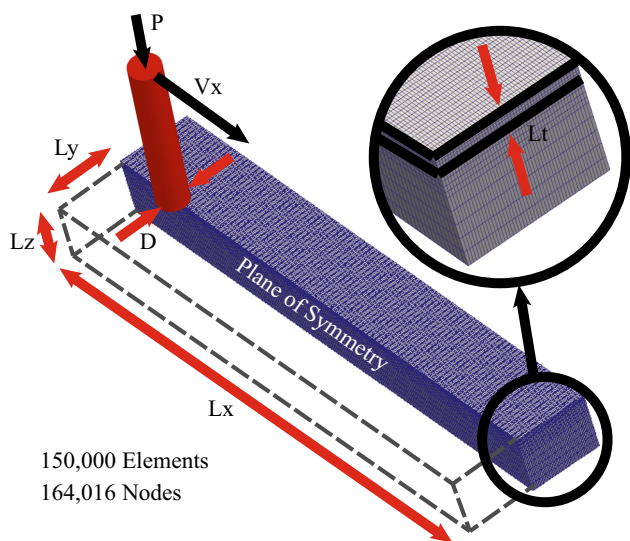


Fig. 7 Model setup for powder bed FEA study (L_x length, L_y width/2, L_z height, L_t layer thickness, V_x scan speed, P electron beam power, D electron beam diameter)

microporosity effects on fatigue properties by Xue et al. [82], it was clearly shown that the source of cracks not only include defects on rough AM product surfaces, but also near the surface within the volume of the specimens. Some research studies have been dedicated to reduce the surface roughness, and thus attempting to improve fatigue resistance of the fabricated components in AM. For example, Pyka et al. [57] developed a novel protocol for surface modification of 3D Ti alloy-based open porous structures using a combined technique of chemical etching and electrochemical polishing.

The experimental characterization of AM materials provides a tremendous amount of motivation for computational research. Although many AM processing techniques utilize post-processing methodologies, e.g., Hot Isostatic Pressing (HIP) and surface roughness refinement, in order to improve the material microstructure and performance, the as-built microstructural conformation is the initial condition for any post-processing methods and thus warrants thorough investigation. Moreover, if the process–structure–property relations can be understood for AM processes, materials, and products, post-processing could potentially be removed entirely; removal of post-processing improves applicability of AM to

Table 1 Dimensions and process parameters for powder bed FEA study

L_x (mm)	L_y (mm)	L_z (mm)	L_t (mm)	V_x (mm/s)	P (W)	D (mm)
4.0	0.5	0.4	0.05	100	60	0.35

Table 2 Material properties of stainless steel 316L [3] used in the powder bed FEA study

T_S (K)	T_L (J/g K)	C_P (J/g K)	ΔH_L (g/mm ³)	ρ	k_{powder} (W/mm ²)	k_{bulk} (W/mm ²)
1648.15	1673.15	0.5	272.5	0.008	0.0003	0.0214

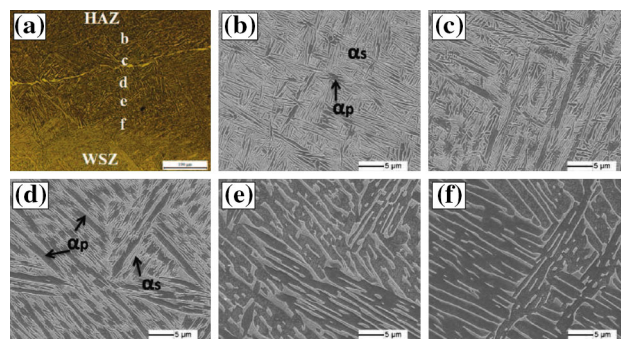


Fig. 8 Microstructure of Ti6.5Al3.5Mo1.5Zr0.3Si titanium alloy fabricated by a laser-based local deposition process [88]. **a** The overview of Transition zone between heat affected zone (HAZ) and wrought substrate zone (WSZ). **b–f** Microstructure of the corresponding positions bf in (a). α_s is lamellar secondary α -hcp phase, α_p is the primary α phase

more applications, reduces time to market for materials and products, and could potentially lead to the highly desirable mass production of AM products.

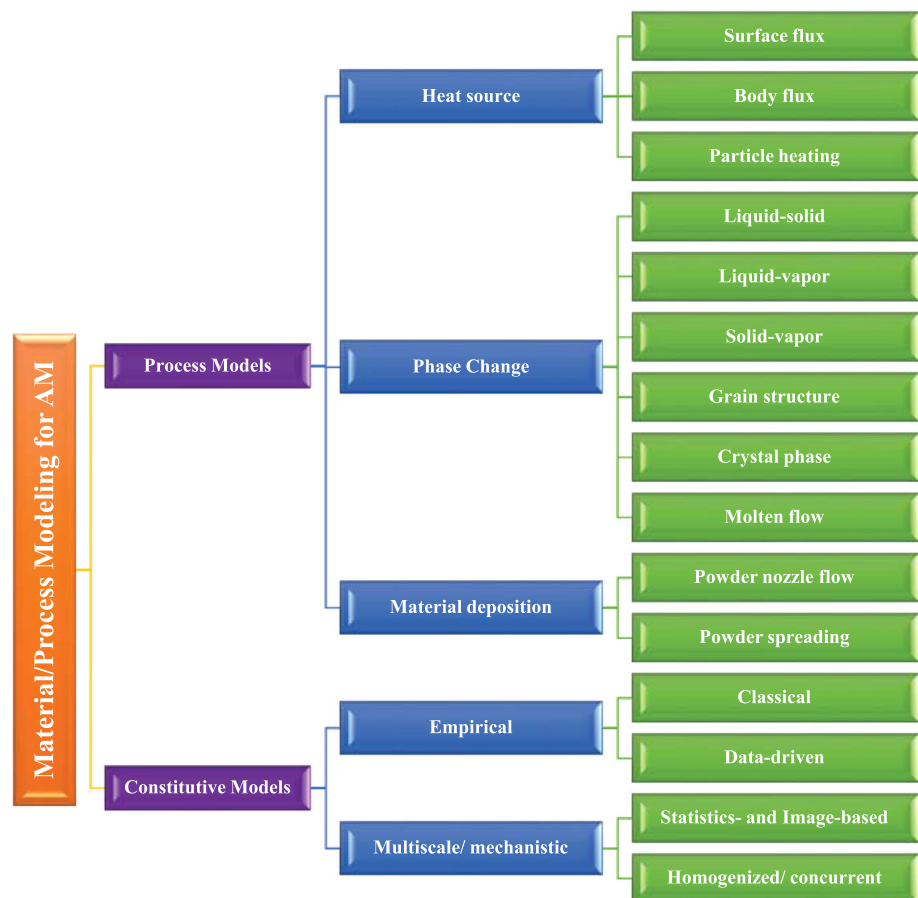
4 Computational challenges and current approaches in AM

The primary purpose of this section is to discuss and spark interest in the many computational challenges that have been presented in AM research. In particular, the need for high-fidelity physics-based models for AM applications and the necessary hardware, software, and theoretical developments needed to facilitate AM processing as effectively as possible. Additionally, current approaches taken by the authors, as well as others, are discussed in order to benchmark the state-of-the-art in computational analysis of AM methods. This section will focus on the key computational areas that most urgently need to be addressed, as observed from the perspective of the authors.

4.1 Process modeling challenges

As schematically shown in Fig. 9, AM processes are extremely complex, involving multiple physical phenomena at multiple scales; the strongly non-equilibrium processes

Fig. 9 Multiscale multiphysics phenomena in AM processes and materials



stemming from molten pool flow, energy deposition, and phase transformations are of particular importance. The heat source model on the macroscale represents the energy absorption and interactions between electrons/photons and powders. Since the individual powders get varied amounts of thermal energy from the interactions, a variety of heat transfer takes place, including thermal conduction inside the powder particles and heat transfer between them through surface radiation, conduction at the contact regions and convection (if not in a vacuum environment). Meanwhile, the phase of the material is changing along with the temperature, from solid to liquid when the temperature is higher than the melting point, even from liquid to gas with the temperature higher than the boiling point. The latent heat associated with the phase transformations has an enormous effect on the temperature distribution, which makes the heat transfer analysis highly nonlinear. Moreover, it should be noted that the individual powders may get partially or entirely melted, which makes the solid-liquid interface very complex. The molten liquid flow is driven by a variety of forces, e.g., gravity, capillary forces, Marangoni forces caused by temperature gradients, and recoil pressure if evaporation occurs. The highly complex flow also strongly influences the heat transfer. Finally, when the heat is transferred away and the temperature falls below

the melting point, the molten liquid solidifies, re-forming portions of the previously solidified structures, which is the basic principle of AM. In addition to the complex behavior taking place during the manufacturing process, the powder bed formation or the powder feed properties are also of significance in terms of process modeling. The powder formation process consists of elastic and/or inelastic frictional collisions of a large number of powder particles, while the powder feed by high-pressure gas is a multiphase flow problem.

The first process modeling challenge is related to developing models that include all of the complex physical phenomena into strongly coupled multiphysics analysis procedures. As mentioned in Sect. 4.2, current computational approaches often simplify the interactive influences between different physical phenomena and build models separately; this approach is not able to provide a thorough enough understanding of the many complex processes observed in AM. Again, most of the current thermal models do not consider the effect of the molten pool flow. Current molten pool flow models ignore the evaporation and the recoil pressure is applied according to empirical equations, which is not convincing in terms of the physics. The evaporation is a major concern, especially for manufacturing within a vacuum chamber, resulting in obvious changes in the chemical compositions

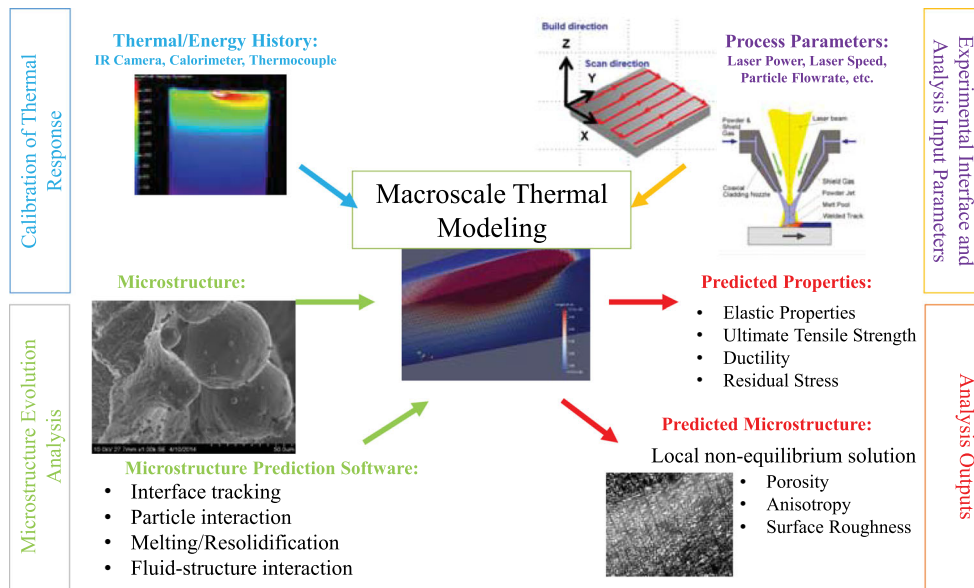


Fig. 10 Integrated computational toolset approach for understanding process–structure–property relations for AM processes

and physical properties of the final products. The evaporation of lightweight elements, e.g., aluminum alloys, has been experimentally observed to be serious enough to influence the microstructures and properties [20]. Thermal simulations have also been used to demonstrate the importance of evaporation [75]. Therefore, a successful multiphysics model should consist of heat transfer, phase transformations including melting, evaporation and solidification, molten liquid flow, and should consider the strong interactive effects.

Developing an understanding of how to obtain valuable information at multiple spatial and temporal scales is another challenge. As previously illustrated, the mesoscopic models tracing individual powders changing in very short time periods (milliseconds) during heating, melting, and subsequent flow to solidification will be valuable in understanding the underlying physical mechanisms of AM processes. However, the actual components are mostly in complex shapes with dimensions of centimeters or even meters, and the actual manufacturing processes could last as long as hours or even days. Therefore, determining how to link the scales in time and space is critical to simulation of the fabrication process of AM products. To be more specific, for a given set of process parameters there are both mesoscopic and macroscopic characteristics that require prediction. At the mesoscale, it is desirable to understand mechanisms such as the flow of the molten liquid and the heat in the powder bed along with the evaporation behavior in order to predict the development of microvoids and material loss. At the macroscale, the thermal stress and distortions, which will influence the service life and dimensional accuracy of the final product, must be accurately predicted for part qualification.

It is also challenging to integrate models pertaining to individual phenomena into one framework that is accessible to researchers and engineers in the area of manufacturing (see Fig. 10). The widely used finite element method (FEM) has certainly been established as a primary contributor to simulation and analysis of AM processes but does not seem to be enough to handle such complex problems alone. Some other methods like Reproducing Kernel Particle Method (RKPM), Lattice Boltzmann Method (LBM), Discrete Element Method (DEM), phase-field methods and level set methods will act as useful tools with some unique advantages in modeling complicated interfaces, contact, and large deformations. Aside from selecting and incorporating the advantages of specific methods on particular aspects, how to effectively integrate the different models together without reduction of the efficiency and accuracy is a key challenge. More importantly, it is unlikely that the integrated frameworks will play useful roles in practical applications of AM unless they are easily obtained and can be used in a manner similar to commercially available FEM software.

4.2 Heat source modeling

The heat source model is the most fundamental aspect of computationally analyzing AM processes. Moreover, the heat source model is the primary factor driving the prediction of the temperature field for a given AM process, with accompanying process parameters. The inherent physics of interest in AM are directly dependent on the temperature field, e.g., the activation forces for the molten pool flow including the Marangoni convection force due to the temperature gradient

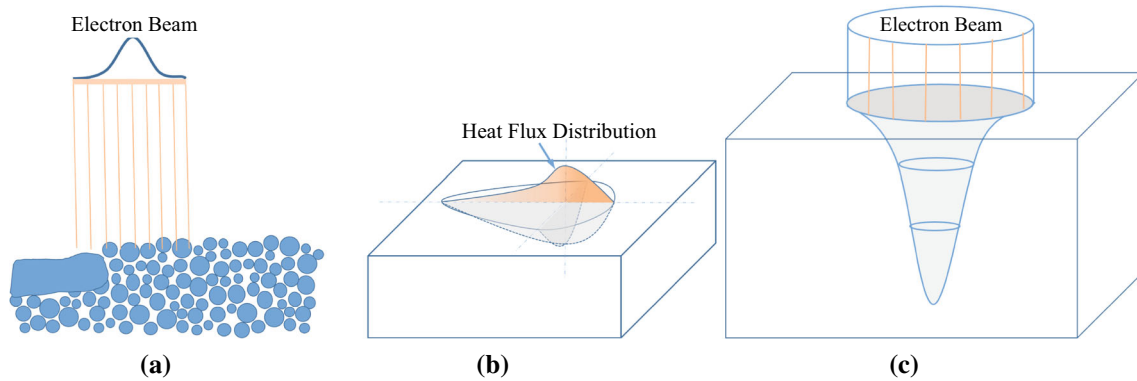


Fig. 11 Traditional heat source models. **a** Surface Gaussian model [37]. **b** Double ellipsoidal model [22]. **c** Rotatory Gaussian body model [46]

and the recoil pressure caused by the evaporations when the local temperature reaches the boiling point.

Most of the current heat source models (see Fig. 11) originate from welding simulations because the fundamental physics of the welding process are very similar to those seen in AM processes for a single pass. More specifically, aside from the point or line heat source models for analytical analysis [61], the Gaussian-distributed surface flux model [55] and the volumetric flux model [54] remain the most popular to date in the thermal analysis of welding [46] and AM [37] processes. Another popular volumetric flux model takes on the double ellipsoidal shape proposed by Goldak [22]. The Gaussian-distributed and double ellipsoidal models were established based on the experimentally observed shape of the solidification zone. For instance, in keyhole-mode melting, which has been observed both in welding [11] and AM [34], the depth of melting is increasingly large because of the recoil pressure caused by evaporation and the established volumetric flux model has an extremely large penetration depth [62]. In other words, the traditional heat source models are effective combinations of many influencing factors such as convection and evaporation, rather than the actual input energy from the laser/electron beam. The traditional models are simple and efficient but are not able to capture some of the more detailed information related to the complex physical processes [84] observed in AM.

As explained in Sect. 2.2, the two primary heat sources used in AM applications are lasers and electron beams, which are characterized by different physical phenomena. It is intuitive that different input energy types that incorporate differing governing physics should have unique heat source models. Therefore, new heat source models should be developed according to the actual physical mechanisms rather than based on the experimentally observed solidification zone in previous studies. It should be noted that the powder bed used in many AM processes has significant effects on the absorbed input energy distribution and the thermal conduction. The interaction between the laser/electron beam and the metal

powder results in energy distributions that differ greatly from that observed in welding. For laser-based processing, the heat source model should be selected based on the type and state of the material being processed. Because the material is in a powder state for the SLM process, photons emitted by the laser penetrate through the material and repeatedly reflect between the powder particles, thus volumetric heat source models with a penetration depth should be used. In contrast, the material in laser welding is well-represented by a continuum state and most of the photons get reflected by the surface, rather than penetrating into the continuum, so the surface heat source model is more appropriate. Some studies [27] analytically approximated the deposited energy profile in the powder bed under strong simplifications and assumptions.

4.3 Modeling phase change during the powder–beam interaction

The material phases in AM processes evolve over space and time as the process continues. Material close to the location of the laser/electron beam interaction can be in a liquid phase while the near-field surrounding material is in a mixture of liquid and solid phase, and interacts with the solid far-field phase. The liquid phase incorporates complex liquid flow behavior including Marangoni convection and melt pool hydrodynamics. When the energy of the laser/electron beam is high enough, as it often is to ensure sufficient melting, an additional gas phase due to vaporization may be important. Gas formation from vaporization can cause recoil pressure and capillary forces to drive liquid transport, further increasing complexity to modeling the process. Modeling the multiphysics nature of AM processes requires the ability to model the fluid–solid interaction while tracking the interfaces between the multiple phases existing near the local interaction region. While detailed mesoscale calculations capturing these interactions are computationally expensive, they can certainly be useful in understanding the

microstructure conformation that results from AM processes. The material porosity, microstructure anisotropy, and surface roughness are a few examples of the outputs that can be obtained from modeling the fluid-solid interaction taking place at the mesoscale.

Using pore formation as an example, Vilaro et al. [71] hypothesize that material evaporates during melting and the subsequent gas becomes entrapped in the build due to rapid solidification, developing a more porous component. Qiu et al. [58] argued that insufficient re-melting between the liquid and solid phase at localized sites could lead to discontinuous tracks, developing more pores at the top surface. Qiu et al. [59] theorized that instability in the melt pool induced “splashing” of the molten material, which in turn causes pore formation. These are just the few examples where prior investigations have shown that interaction between liquid, solid and gas phases play a crucial role in the quality of the final part. Being able to simulate these complex interactions will enhance our understanding of the governing physics occurring at the powder-scale. Unfortunately, this information will only give insight into the local microstructure due to limitations of the current state of high-performance computing (HPC) (see Sect. 4.7).

There are a number of methods for implicit tracking of the phase interfaces. Such methods include the level set method (LSM), volume of fluid (VOF) method, and phase field methods. These methods are able to implicitly track the interface by solving an additional partial differential equation for an auxiliary function, which acts to describe the phase of a material. Although implicit tracking of the interface involves an additional equation to solve for the auxiliary variable, they are still more computationally efficient than explicit tracking and maintain a reasonable accuracy.

A number of investigations into numerically modeling laser-material interaction have created a foundation for modeling the AM process. For example, Zhang et al. [85] implemented a modified level set method to track the liquid-gas interface evolution. By accounting for effects such as recoil pressure, surface tension and the Marangoni effect, molten ejection effects seen in experiments can be captured computationally. Ki et al. [33] developed a level set based model to analyze the liquid vapor interface produced by the high-energy density laser beam-material interaction process. Through incorporation of complex physical effects, e.g., Knudsen layer, thermo-capillary effects and recoil pressure, phenomena such as fluid ejection and evaporation of material, and thus loss of mass during the process, can be simulated. Current modeling methods for AM processes have been directed at establishing the underlying physics of the laser-material interaction at the powder-scale. Klassen et al. [36] utilized a lattice Boltzmann method (LBM) for hydrodynamics coupled with VOF to track the evolution of the free surface between the gas-liquid phase during EBM. They

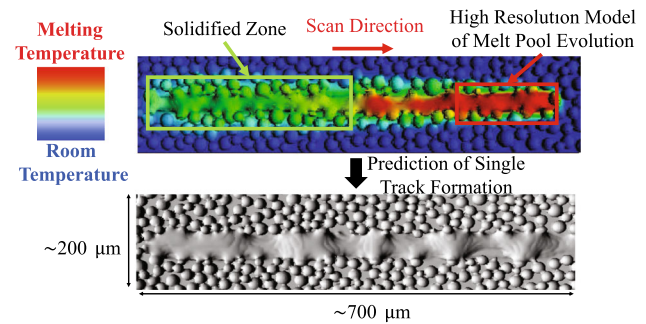


Fig. 12 Particle scale phase transformation analysis for a single track in the SLM process [32]

found that the penetration depth of the beam plays a significant role in evaporation effects. Khairallah et al. [32] developed a 3D powder-scale hybrid finite element finite volume model, which couples hydrodynamic and thermal interactions throughout the process. Their model accounts for temperature-dependent material properties, surface tension and particle distribution, all of which play a crucial role in driving the outcome of the process in terms of microstructure and properties. By modeling at such a high resolution, the hydrodynamic and stochastic effects, which homogeneous or effective models do not capture, can be accounted for. Figure 12 provides an example of the particle-scale phase transformation model utilized by Khairallah et al. Much of the applications of interface tracking methods to the AM process demonstrate that the complex physical interaction among phases at the powder-scale can have a profound impact on the outcome of the process. Developing methods to model such complex interactions are necessary to establish a fundamental understanding of AM processes.

4.4 Computational materials characterization

Computational materials characterization is perhaps the most intricate and yet critical area of study that will dictate the future of AM processes. The reason that this particular area is of such great importance is because of the effects of the process on local microstructure and properties. The local microstructure and properties will be controlled by both local process parameters as well as powder composition. The microstructural features that are of particular interest encompass phase fraction, grain size and structure, dendrite formation/structure, porosity, inclusions, and surface roughness. While there are many computational methods and models that can be used to predict these microstructural features, there are few methods that can predict the evolution of the microstructure over the course of the entire manufacturing cycle.

4.4.1 CALPHAD-informed AM process modeling

The CALculation of PHase Diagrams (CALPHAD) approach is widely accepted in the materials research community as a powerful engineering method in predicting material thermodynamics and kinetics of materials [7,31,52]. It was originally developed for computational modeling of alloy thermodynamics based on experimental phase equilibria and thermodynamic properties. A further development made in the CALPHAD research community enabled this approach to be applicable for diffusion kinetic modeling of inorganic systems [6]. Therefore, the state-of-the-art CALPHAD method and its developed database is considered as one of the most important methodologies for constructing materials genomic databases. The primary advantage of the CALPHAD approach is the fidelity of model prediction for multicomponent alloys. For example, Saunders [63] demonstrated the good agreements in phase equilibria and thermodynamic properties between the CALPHAD method predictions and experimental results on multicomponent commercial alloys.

Fundamentally, the CALPHAD model is based on the thermodynamic description of the pure elements composing the material, which is expressed as heat capacity starting from room temperature to temperatures well-above the melting point. The standard CALPHAD database of pure elements, made by SGTE (Scientific Group Thermodata Europe) in 1991 [16], allows the CALPHAD community to perform CALPHAD-type thermodynamic modeling for binary, ternary and multicomponent alloy systems.

In the CALPHAD approach, the Gibbs free energy of phase ϕ in a multicomponent alloy system G_m^ϕ can be defined as:

$$G_m^\phi = \sum_i x_i^0 G_i^\phi + R\theta \left[\sum_i x_i \ln(x_i) \right] + {}^{Ex} G_m^\phi + {}^{Magn} G_m^\phi \quad (1)$$

in which, R is the gas constant, θ is temperature, and x_i is the composition of element i in the multicomponent system. The third term on the right hand side (RHS) stands for excess energy in the system, and the last term on the RHS evaluates the magnetic contribution to the Gibbs energy of the system [80]. Different types of thermodynamic models have been developed for different crystalline and liquid phases, and the model parameters are optimized according to phase diagrams and/or thermodynamic property data, which can be obtained by experiments or sometimes atomistic modeling, e.g., quantum mechanical calculations.

Several comprehensive software packages have been developed for CALPHAD-based research, e.g., Thermo-Calc, which is generally considered as the pioneering

software package in computational thermodynamics and kinetics. Thermo-Calc was developed in 1981 by research groups at KTH Royal Institute of Technology in Sweden. Prediction of phase equilibria, phase stability, and thermodynamic properties are considered basic features of the CALPHAD approach, which serves as a basis of performing diffusion kinetic simulations and non-equilibrium studies during the solidification process. For example, the Scheil–Gulliver model has been adopted in the Thermo-Calc software package for estimating thermodynamic properties during solidification [9,64], which is demonstrated briefly in the current work.

In simulation of the solidification process of alloys, the behavior of the solidifying alloy under local equilibrium conditions can be simulated based on the thermodynamic and kinetic properties, which is readily obtainable using the CALPHAD approach. Analogous to the phase equilibrium case, alloys solidifying under rapid cooling conditions require predictions based on a non-equilibrium solution, which can be described using the Scheil–Gulliver model [24,65] as a good approximation. This model provides a qualitative analysis of the solute redistribution during solidification processes. It assumes that no diffusion takes place in the solid phases and that solute redistribution in the liquid is infinitely fast. In the Thermo-Calc software, the Scheil–Gulliver simulation is available as a built-in module that generates thermodynamic properties, e.g., latent heat and phase fraction, during rapid cooling under the Scheil–Gulliver condition. Further descriptions of these models can be found in [9].

One methodology that is currently under development by the authors is a CALPHAD to 3D FEM coupling [68]. The benefits of such an approach are: (1) the material composition is used as an input, (2) the non-equilibrium solution incorporating supercooling effects in AM can be simulated, and (3) high-resolution material properties with nonlinear temperature-dependence can be obtained. The EBM model described in Sect. 3.2 was used to showcase the developed method (see Fig. 13). The material composition used as inputs for the CALPHAD-derived properties are shown below in Table 3, whereas the predicted liquidus and solidus temperatures are shown Table 4. As can be seen in Fig. 14, the impact of (1)–(3) is that the thermal history in terms of the heating and cooling rate, which has a dramatic impact on the microstructural evolution of stainless steel 316L, is noticeably effected. While the specific heat capacity and latent heat are readily available in common engineering handbooks and look-up tables, these experimentally detected values are only rough approximations to the real values for known materials.

A comparison of the CALPHAD and handbook derived properties can be seen in Fig. 15. The noticeably different temperature histories (Fig. 14a) and heating/cooling rates (Fig. 14b) observed between the handbook-based properties and CALPHAD-derived properties imply that the predicted

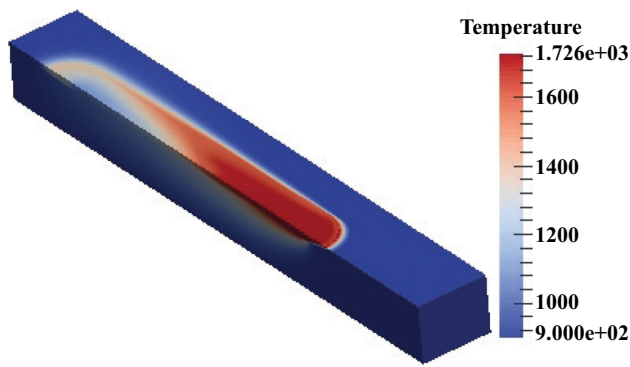


Fig. 13 Single track EBM model using CALPHAD-derived thermodynamic properties (Note max temperature shown is liquidus)

Table 3 CALPHAD material composition inputs for stainless steel 316L (wt%)

	Cr	Ni	Mo	Mn
Fe	16.3	10.3	2.09	1.31
Balance				
Si	C	P	S	
0.49	0.026	0.026	0.006	

Table 4 CALPHAD-derived solidus and liquidus temperatures for stainless steel 316L

T_S (K)	T_L (K)
1607.15	1726.15

microstructure can be significantly influenced by the input thermodynamic properties. More specifically, the handbook properties do not take into account the impact of the supercooling in AM processes and are also extremely simplified (see Fig. 15a, b) in the temperature ranges that are most important for understanding as-built AM materials, i.e., between the solidus and liquidus temperatures. The difference in the prediction of the secondary dendrite arm spacing, which can be obtained from the simulated cooling rate [1, 63], is one example of a prediction that could be strongly influenced by poor material property assumptions.

4.4.2 Multiscale microstructure evolution analysis

Although the tools utilized in additively manufacturing a part are conceptually simple, the processes are rather complex in that there are multiple physical phenomena involved. Included in these phenomena are defect formation, dendrite formation, and cyclic melting/solidification during the build process, all of which contribute to the quality of the finished part. These behaviors are largely affected by the input process parameters, e.g., laser power, speed, scan direction, layer depth, and hatch spacing. Figure 17a illustrates how process parameters can dictate the complex physics and behavior seen from the global part scale to the powder scale,

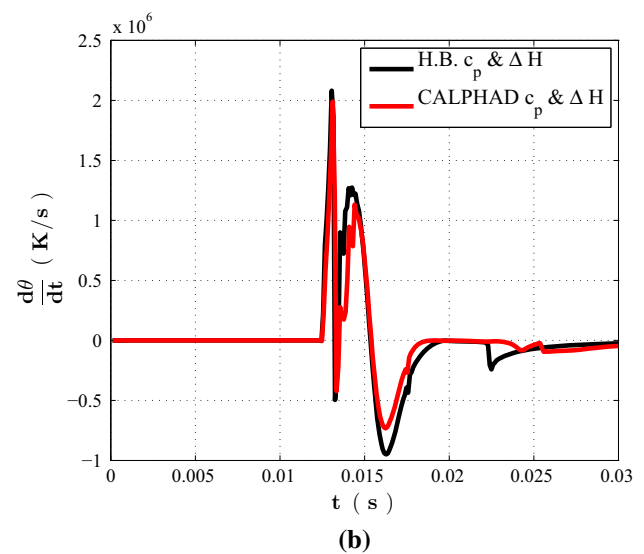
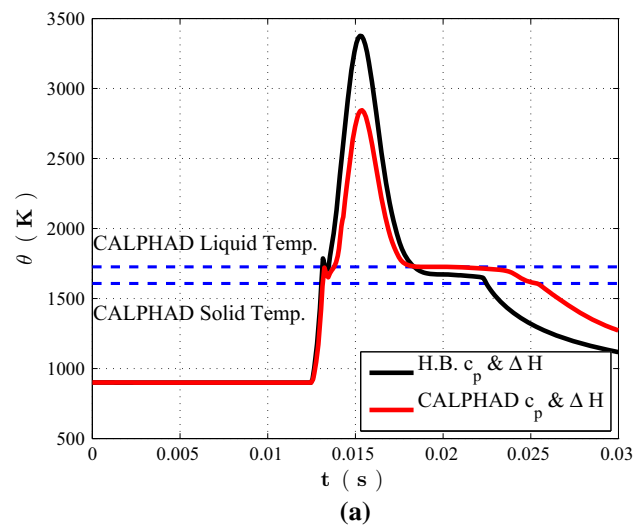
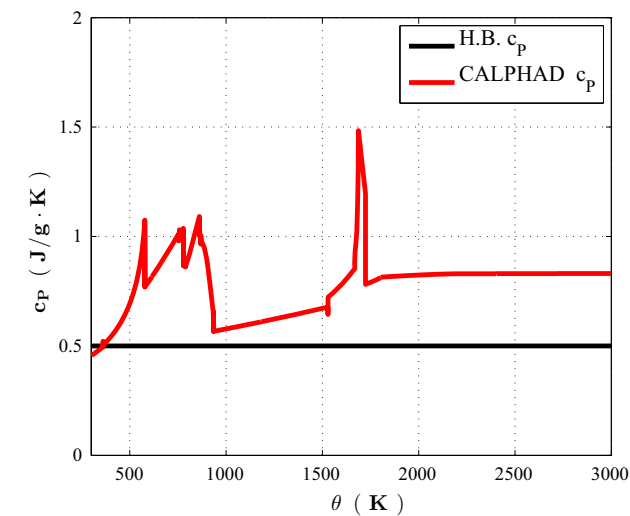


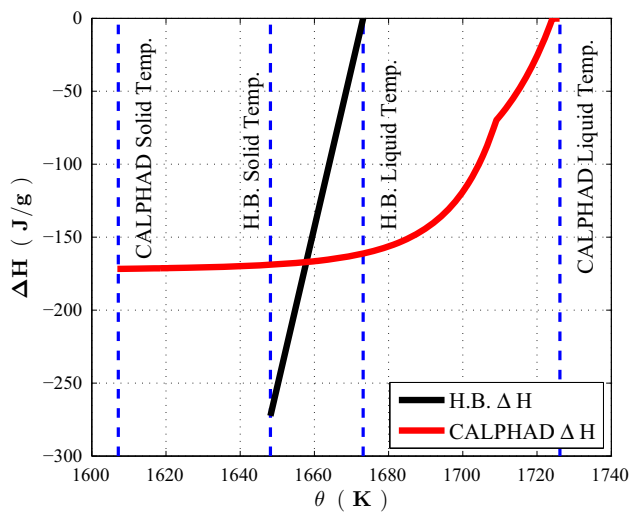
Fig. 14 Comparison of the predicted response of a selected node calculated using handbook-based specific heat and change in enthalpy due to phase change and CALPHAD-derived specific heat and change in enthalpy due to phase change for stainless steel 316L. **a** Thermal history for selected node. **b** Temperature rate history for selected node

establishing AM as a multiscale and multiphysics problem. Qualification of the produced part is established as a significant challenge stemming from the fact that there is still a degree of uncertainty associated with the understanding of the influence of process parameters on the observed physical phenomena.

Numerous experimental investigations have been carried out to develop an understanding of the physics driving AM processes. The underlying goal of these experiments is to create a relation between the process parameters and the resulting response of the material to the manufacturing process. Although much progress has been made in this area of research, there still remains enough uncertainty to



(a)



(b)

Fig. 15 Comparison of handbook and CALPHAD-derived temperature-dependent specific heat and change in enthalpy due to phase evolution for stainless steel 316L. **a** Specific heat as a function of temperature. **b** Change in enthalpy as a function of temperature

prevent ubiquitous commercialization of AM. Furthermore, performing these experiments is costly and time consuming. The inefficiency of experimentally linking AM processes to final part quality implies that a combined experimental-computational approach has a higher potential for success. With the ever-increasing power and affordability of fast parallel computers, computational modeling has become a major tool in providing a physical explanation for complex physical phenomena. As a result, researchers have resorted to computational modeling and simulation to provide a physical understanding of AM processes.

Numerically modeling the AM process is further complicated by the fact that the complex physical phenomena

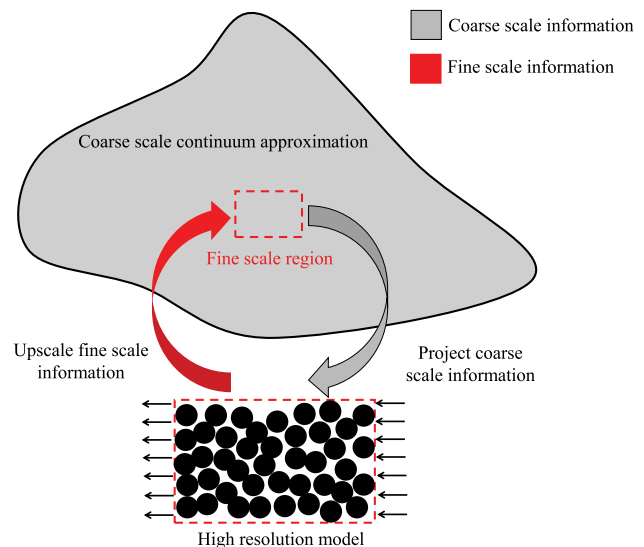
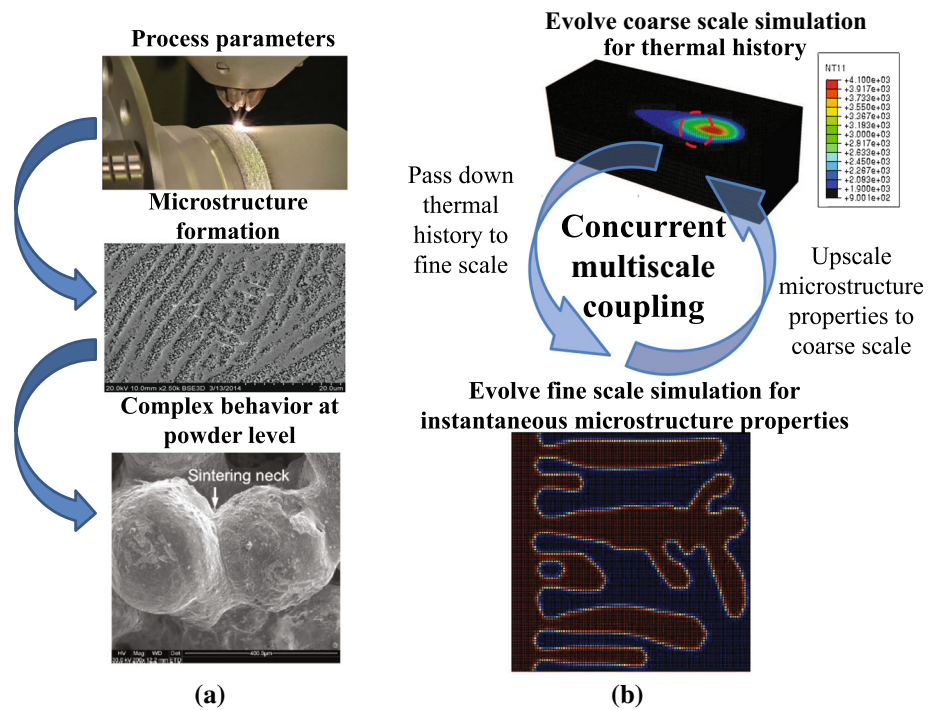


Fig. 16 Schematic of concurrent multiscale coupling

occur over a broad range of length and time scales. Zohdi [90] utilized a discrete element method (DEM) to capture the powder scale behavior during the laser sintering process. Furthermore, Bauereiß et al. [5] developed a mesoscopic Lattice Boltzmann model to capture the melting behavior at the powder scale during the EBM process. Yan et al. [84] developed a new heat source model to capture the thermal profile on the part scale. Despite the progress made in computational modeling, AM is an inherently multiscale problem. Figure 17a demonstrates how multiple length scales can evolve to control the quality of the finished part. Being able to accurately represent the complex physical evolution of an additively manufactured part requires a computational tool to couple the various scales of interest. Such a tool can then connect process, structure and properties to the final part quality and performance. Initial work has been done by King et al. [35] in developing a methodology to couple multiple models on various time and length scales. Through their effective medium and powder models, they are able to reproduce results that are observed in experiments. Their work demonstrates that a multiscale model is necessary to develop a true understanding of the governing physics of AM processes, and is part of a strategy aimed at qualification of AM parts.

It is evident that a multiscale method is necessary in order to accurately depict the evolution of the powder scale during the AM process. There is still no conclusive understanding of how the rapid and complex phase evolution occurring at the powder scale affects the product scale behavior after AM processing. Concurrent multiscale methods may offer valuable insight into the instantaneous behavior and interaction among disparate spatial and temporal scales. There has been recent efforts devoted to developing concurrent methods capable of performing this intricate analysis. Chu et

Fig. 17 Experimental and (concurrently coupled) computational framework for characterizing process–structure–property relationships in as-built AM materials. **a** Experimental characterization of as-built AM microstructure. **b** Schematic of concurrent multiscale coupling technique



al. [14] proposed a concurrent multiscale method through coupling conservation laws for mass. Similar concurrent methods [8, 10] have been developed by coupling macro- and micro-pressure equations through boundary conditions and iterating until the resulting pressures between disparate scales match. Gu et al. [23] coupled a coarse scale meshfree analysis to a fine scale molecular dynamics (MD) simulation. They utilized transition particles to couple the two domains while implementing a penalty method to ensure compatibility of displacements. Wagner et al. [76] established a bridging scale decomposition that couples fine scale MD to a continuum scale finite element model into a single multiple-scale simulation. This was done through a projection of boundary conditions and MD displacement degrees of freedom between the two models. These aforementioned concurrent methods rely on some form of immediate exchange of information among scales, as depicted in Fig. 16. Choosing the information being transferred among these scales is an integral part of designing concurrent methods, as the fidelity of this transfer determines the accuracy and effectiveness of the method.

The authors are in the process of developing a multiscale method to concurrently couple and evolve disparate spatial and temporal scales. This method passes thermodynamic information between scales to calculate boundary conditions ensuring conservation of the total energy of the system. Such boundary conditions result in microstructural evolutions at each individual scale that are energetically consistent. Figure 17b presents a simple concept of how the method currently operates. At the coarse or global part scale, the thermal his-

tory is passed down to a finer (microstructure) scale. Using the thermal history, the fine scale is evolved to the same temporal state of the coarse scale, tracking microstructure formation through solution of a coupled temperature-phase field model. The solution at the fine scale gives information related to the properties of the evolved microstructure, which can be homogenized back to the coarse scale to give an effective capacitance, conductivity and phase composition. By performing concurrent simulations, instantaneous information can be passed between scales to provide an accurate representation of the real time process. This method can be advantageous for AM applications as it is able to provide a rapid depiction of the resulting microstructure evolution at specific points of the part given a set of process parameters. Future implementations of this method will also incorporate the powder scale. Concurrently evolving this scale allows for prediction of the complex phase history of the powders, offering insight into the cyclic melting/solidification and its effects on track distortion. Results from these multiscale models can then strengthen our understanding of the complex physics governing the process, which in turn can accelerate the qualification process of additively manufactured parts.

4.5 Computational characterization of mechanical behavior

The experimental characterization of additively manufactured components drives the development of the computational material models used for analysis of final product performance. Purely phenomenological models for analyzing

these materials are enticing but will ultimately be limited in predictive capabilities; while useful, these models are unlikely to be robust outside of the training data used to develop them. Instead, it is more desirable to focus on mechanics-based models such that a correlation can be made between the material properties and the material microstructure. The microstructure of additively manufactured materials is of course dependent on local process parameters, and thus a mechanics-based constitutive law has a higher probability of alluding to the process–structure–property relations that are so important for design of processes, products, and materials.

4.5.1 Microstructure-informed plasticity and damage

As indicated in Sect. 3.2, there are many different aspects of the microstructure which can be taken into account in a mechanics-based constitutive law. The primary question that must be answered is, what microstructural components have the highest contribution to material behavior, and can any be eliminated from consideration? For example, there are a number of void/inclusion-based constitutive models available that could potentially account for the voids and inclusions experimentally observed in the additively manufactured microstructure. However, most of these models would require the assumption that the phase fraction, grain size, dendrite spacing, etc., will not explicitly have a tremendous impact on the overall behavior of the material. Many models would also require the assumption that the microstructure is uniform, which is known to be a falsity in additively manufactured components. An ideal solution would be to combine microstructurally-informed models as basic building blocks of advanced material laws, e.g., anisotropic void growth caused by local grain orientation, which is the primary goal of a recently developed generalized anisotropic plasticity framework [67].

One example of a void/inclusion-based constitutive law which can address the complex microstructure and mechanical behavior of additively manufactured materials is the Gurson–Tvergaard–Needleman (GTN) model [13,25,73,74]. As indicated by Fig. 18, the microstructure of additively manufactured materials has a relatively high density of voids and oxide inclusions that are spherical in geometry, which fits within the assumptions made during theoretical development of the GTN model. However, the GTN model cannot by itself reflect the heterogeneity in the void and inclusion distributions within the microstructure. The alternative is to reconsider the homogeneity assumptions in the original GTN model as local homogeneities such that the initialization of the void and inclusion parameters can now be a function of spatial coordinates. In this sense, the spatial coordinates of interest could either be dictated by image-based microstructural reconstruction or perhaps the process

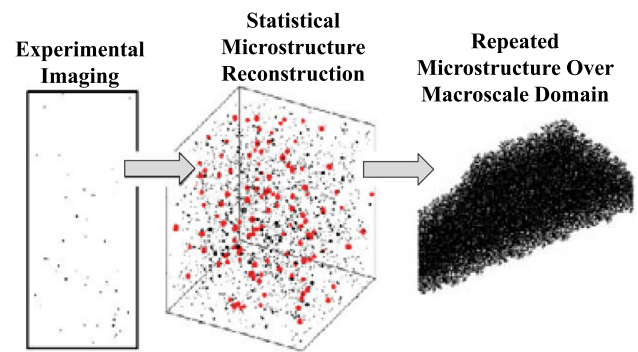


Fig. 18 Schematic showing the process of experimental imaging, 3D statistical reconstruction, and placement of defects in a macroscale FEA model

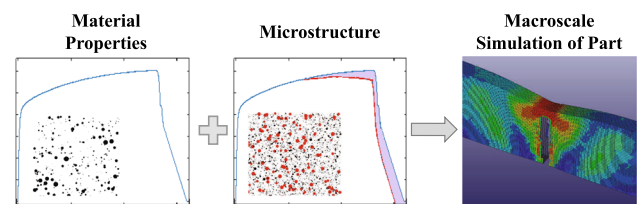


Fig. 19 Depiction of macroscale sensitivity to microstructural defects using the locally homogeneous modeling approach throughout a mesh geometry. The underlying bulk material properties can be extracted from specimens containing a relatively low density of defects and can be later used to analyze the impact of higher defect densities

parameters, the latter of which could potentially be used to predict the microstructure through development of accurate process–structure relations. Conceptually, the idea behind this approach is to incorporate experimentally consistent microstructural information into the modeling approach in order to analyze the sensitivity of the material to defects, as depicted in Fig. 19.

4.5.2 Computational fatigue life prediction based on mechanics and microstructure

The previously discussed mechanical models provide critical information about the material response. However, many current applications of interest for AM involve cyclic load conditions, which require experimental and computational approaches differing from those already mentioned. Fatigue performance is linked with four primary factors: (1) defects such as voids (micro-pores) and microcracks, (2) high residual stresses, (3) poor surface finish, and (4) microstructure [17,30,41,60,66,69,77]. However, few computational studies of fatigue life for AM materials has been conducted, whereas current experimental results indicate that fatigue performance is poor to fair. There have been attempts to apply or adapt current phenomenological models to AM, e.g., [42,43,79], that met moderate success. As with monotonic

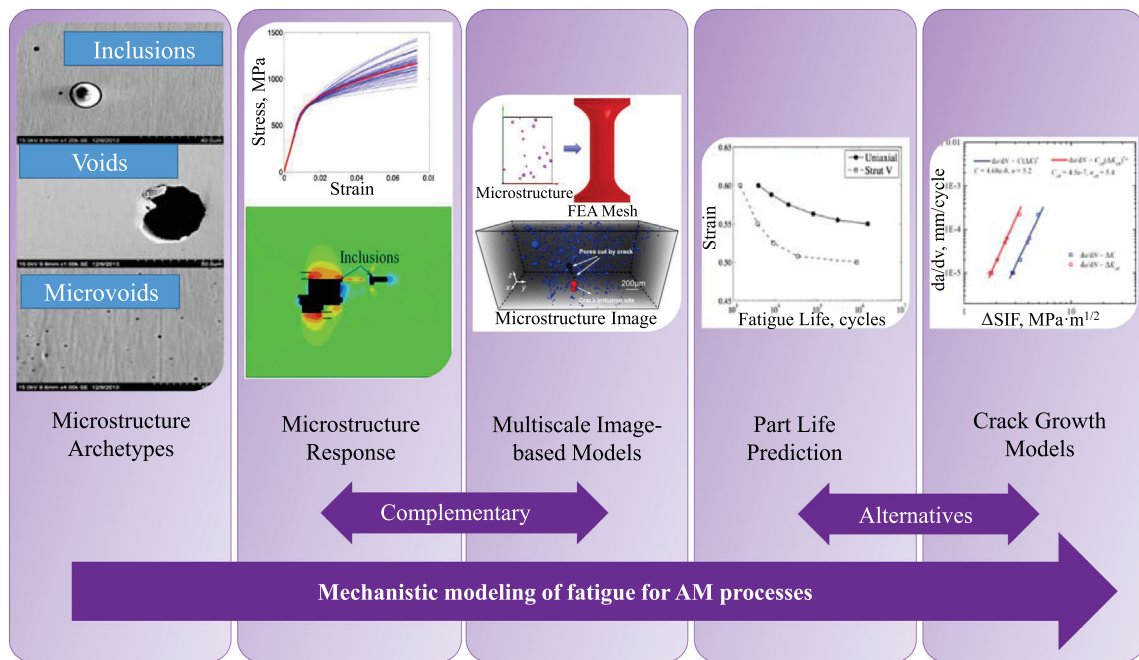


Fig. 20 Mechanics-based and microstructure-informed fatigue life prediction

simulations, such models are unsatisfactory for developing a deeper understanding of the system.

There are ongoing efforts to apply mechanistic models to AM, though no such model is currently available to our knowledge. Approaches to mechanistic simulation of high cycle fatigue (HCF) include micromechanics models to capture microstructures that influence fatigue, discrete dislocation models, and localized plasticity methods. Most HCF methods use pre-fracture or microstructurally small cracks considered at the grain scale (e.g., Christ et al. [12]). Such features are common in AM products meaning that perhaps current models are adaptable to the AM setting. Application of multiscale methods are required to extend micro-scale models often used to understand fatigue processes to scales of practical interest for the engineer. Such techniques often use image-based or statistical reconstructions (see Fig. 18) to generate a relatively large spatial volume of data with relative ease. Once implemented, these methods can be used to determine fatigue life with relatively high accuracy. Fatigue crack growth can often be predicted directly, e.g., using finite element analysis, for lower cycle count applications. A schematic diagram to represent this is shown in Fig. 20.

4.6 Data-driven analysis

An important and rapidly developing field of interest in engineering simulation that extends to AM is data-driven analysis. The use of advanced data mining techniques can help expose the complex correlations between processing

conditions and the resultant material structure. It is appropriate to separate the many modeling methods for AM into two categories: (1) those intended to capture processing and (2) those intended to capture mechanical response. As discussed on a number of occasions in this document (e.g., Section 4.4.2), there are current efforts to use CALPHAD-based modeling techniques, which relies on materials genomic databases, in order to determine phase evolution during AM processing. However, other opportunities exist that can also be characterized as data-driven analysis, as will be elucidated by the following selection of example cases. Given sufficiently rich datasets, database-driven methods are shown to effectively optimize processing conditions for desired build properties, e.g., Krol et al. [39] used a Full Factorial Experimental Design approach to prioritize processing parameters. Lu et al. [45] predicted the effects of changing primary build parameters on the precision of the build based on least square support vector machine networks, a type of learning algorithm. Similarly, Fathi and Mozaffari [18] developed a fully data-driven process prediction and optimization scheme: the mutable smart bee algorithm and fuzzy inference system models are used to relate process parameters to layer thickness and melt pool depth, then the non-dominated sorting genetic algorithm is used to optimize the build process. The ability to predict the total process time of complex parts is important in commercial applications, where the cost of manufacturing depends on machine time required. Zhang et al. [86] used Grey Modeling, a development of fuzzy logic, to predict process time based on statistics from large datasets.

Within the mechanics community, data-driven analysis often refers to the use of large datasets paired with data-mining or machine-learning algorithms to predict mechanical behavior without the expense of an entirely new physics-based computation at each material point. The specifics of how this is achieved vary depending upon the goals of the simulation and the type of data to be used. The predictions of such models are purely phenomenological, but the goal of these analyses is to identify and characterize complex, nonlinear, multivariate interactions, just as was shown possible for process modeling. Currently, the use of data-driven mechanical analysis for AM products is scarce in the literature. In one of the few examples, Garg and Tai [19] use genetic programming and artificial neural networks to predict strength of parts created using fused deposition. The lack of examples in this area is the result of two primary factors: (1) these methods have only recently arrived, although are growing rapidly, to mechanical engineering fields and (2) high quality, sufficiently large databases are difficult to develop and are not easily accessible to date. The success of this kind of approach depends upon the quantity and quality of the training data provided to the analysis algorithm—a statistically sufficient amount of data is required for accurate prediction.

Data compression is extremely important for both storage of large datasets and also for efficiency in data mining approaches. One data compression technique that can be applied to both processing and materials characterization is to save only a statistical representation of important information. Reduced-order modeling approaches, for example, can be used to incorporate the stochastic nature of AM processes and materials. By coupling experimental characterization methods, e.g., SEM imaging, with statistical modeling approaches, reduced-order models incorporating statistical microstructure descriptors can be utilized to produce fast computational frameworks for prediction of structure–property relations.

Another emerging approach is reduced-order modeling using data analytics. By identifying similarities between the current (deformed) configuration and initial configuration, these methods can be used to rapidly compute mechanical responses. An example of this, which is currently under investigation by the authors [44], uses a clustering method to group material regions with similar mechanical responses under elastic loading. Once this grouping is achieved, larger and more complex deformations can be analyzed using a reduced set of degrees of freedom corresponding to the previously identified regions. Similar clustering techniques are standard in fields such image processing and finger-print scanning, but have only recently appeared in mechanics. Applications in AM include reduced-order modeling for mechanical response, e.g., fully detailed models could be

seeded with complex microstructures and used to train the reduced-order models.

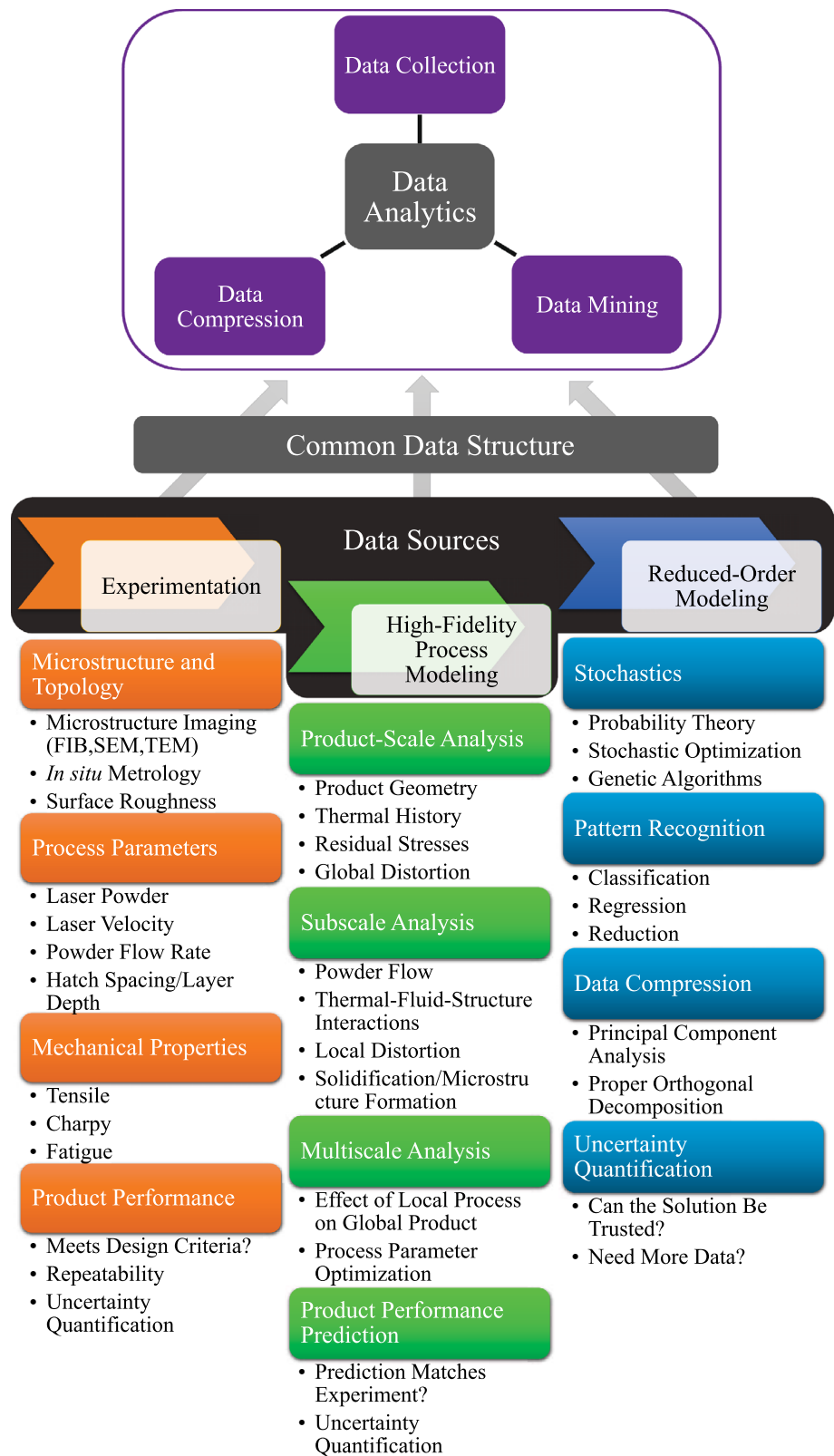
Each area presented above, all of which are related to data-driven analysis, motivates the development and dissemination of accurate, accessible, and extensive databases for AM processes, products, and materials (Fig. 21 shows the impact areas of data analytics in AM processes). However, there are many challenges associated with such an effort. Proprietary rights, widely varying AM technologies, variations in novel and existing powder compositions, and limited standardization of the industry are a few examples of the key detriments that prohibit the construction and management of comprehensive databases. One initiative that could be adopted by the research community that can simplify this task is the development of, and adherence to, standardized data collection procedures across the industry. Additionally, approaches developed for the MGI could be adopted with modification to support development of large-scale databases to enhance the capacities of data-driven analysis in AM-related endeavors. AM supports the MGI by allowing rapid alloy development and application of novel alloys through powder metallurgy and powder mixture. Database driven methods, such as the CALPHAD approach, facilitate the computational design of materials. This philosophy can be deployed in powder-based AM methods to process new materials at an accelerated rate. Application of powerful MGI-derived approaches could even couple material and topological design in the development of functionally graded components.

4.7 High-performance computing challenges

Perhaps the highest impact in computationally solving AM problems is in the area of HPC. The localized nature of the process requires any predictive simulation to have sufficiently small time steps in order to generate useful and accurate information. However, as the global size of the manufactured component increases, the number of time steps necessary to complete the analysis will also increase. Figure 22 describes the primary competing limitations of simulating AM processes. Another underlying issue that arises in this case is that the impact of successive passes on previous passes will depend largely on the part geometry, initial conditions, and process parameters and therefore is history dependent. Unfortunately, it may not be initially obvious how much information will be required in order to simulate the process and it may not be possible to predict the correct boundary conditions accurately enough to use simplified or reduced-order models.

The next issue is related to the characteristic length scales used in simulation. The coarsest possible full-scale model could perhaps make the assumption that a single element

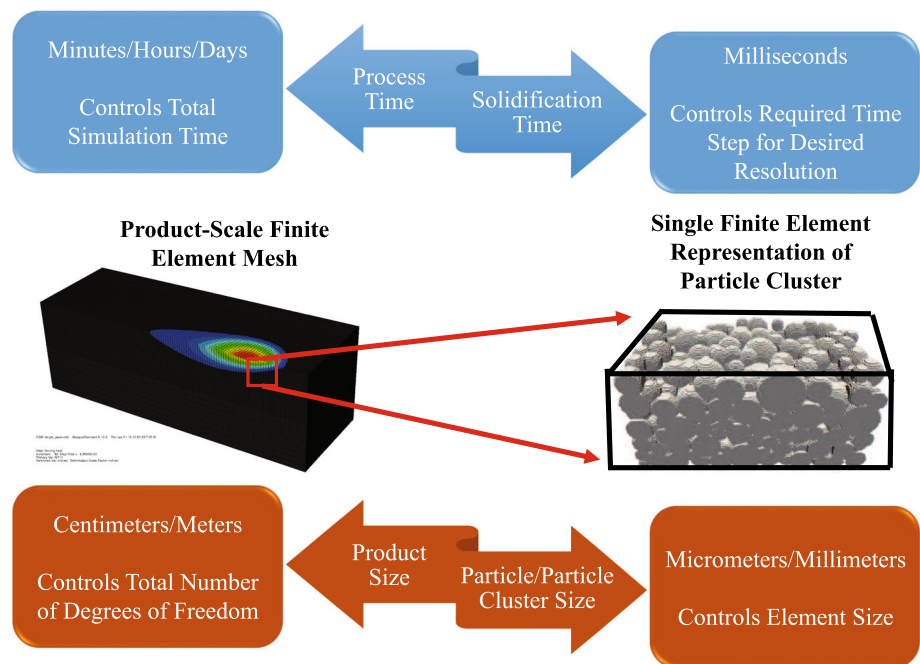
Fig. 21 Data analytics for AM applications



in a finite element mesh represents a particle cluster. The maximum particle cluster size will have dimensions dictated by the toolpath, i.e., the hatch spacing in the in-plane direction

and the layer depth in the out-of-plane direction. The particle cluster length-scale can be on the order of μm to mm while the length-scale of the global part shape might be cm or even

Fig. 22 HPC considerations for process modeling of AM applications (particle model obtained from Ammer et al. [2])



m. Therefore, the number of degrees of freedom in the model will be dictated by the global part shape.

The numerical scheme used to compute the solution will have tremendous impact on the analysis completion time. Not only are AM processes highly localized, but the heating and cooling rates are extremely rapid with high gradients in the thermal solution. In order to obtain accurate predictions, the time step must be selected to capture the heating and cooling with substantial resolution. This time step limitation will require implicit schemes to iteratively solve the nonlinear thermal problem over thousands of steps (although it will likely be tens or hundreds of thousands of steps for many practical applications). Combining this fact with the poor scalability of implicit schemes as additional degrees of freedom are added, and the additional memory requirements to the simulation, yields the conclusion that implicit schemes may not be appropriate for AM applications in predicting the complete description of the process history.

Efficient utilization of HPC capabilities is critical for the success of data-driven approaches. In particular, large numbers of operations are generally required in order to conduct computations on big datasets. The speed of the initial computations, which typically require solution of multiple case studies to obtain training data for subsequent simplified/reduced-order models, can be dramatically improved using the latest HPC technology, e.g., massively parallel computer clusters and Graphical Processing Unit (GPU) computing, and algorithms. The primary benefits of the reduced-order models developed from the training data is the improved speed of computation and the reduction in necessary data, which often leads to simulations capable of

being conducted using generic desktop workstation computers. Application of data-driven methods to create simplified models can enhance the speed at which the research community can develop an understanding of the impact of process parameters on the structure of AM materials. A successful example of this is the already discussed (see Sect. 4.4.2) CALPHAD method, which utilizes a materials database for calculations of the material property and microstructure evolution during the solidification process. Thus, development of well-scaled routines for HPC on large datasets is of interest to the AM community.

5 Future goals of computational modeling for AM applications

It is of ample value to give structure and direction for future goals in computational research for AM applications. In particular, short-term and long-term goals should be highlighted to ensure that research efforts align to contribute to high impact goals requiring urgent attention while preparing for extensibility and portability of methods for long-term goals. Since the process–structure–property paradigm can be considered as a general research guideline in AM, both short-term and long-term goals are given with the purpose of strengthening the linkage of process–structure and structure–property relationships, which can be summarized in Fig. 23. Particularly, corresponding experiments are considered as indispensable support to validate and/or calibrate theoretical modeling, which also require significant improvements for AM applications.

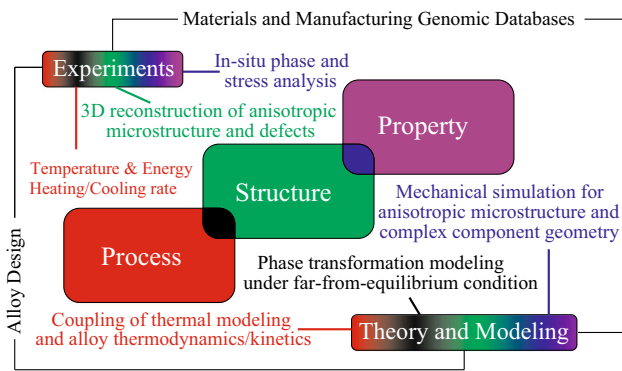


Fig. 23 Highlights of short-term and long-term goals for predictive-science based computational modeling supported by experiments

5.1 Short-term goals

As discussed previously, traditional thermal modeling techniques without considering reasonable material thermodynamics will potentially neglect valuable information, and therefore, cannot accurately model the full process–structure relationships. Alloy thermodynamics have been relatively well-understood for years; reliable information regarding latent heat can be easily obtained from established thermodynamic databases, which are usually constructed using the CALPHAD method. However, in order to comprehensively model process–structure interactions, alloy diffusion kinetics must also be considered. Therefore, material phase and microstructure simulations will require the integration of thermal modeling, alloy thermodynamics and alloy diffusion kinetics; computational prediction methods based on alloy thermodynamics and diffusion kinetics require further advancement for more depth and breadth. Existing modeling techniques used in welding processes [87] may be considered as a starting point. However, it should be noted that most often the cooling and heating rates observed in AM processes are much faster than those observed in traditional welding processes. Therefore, more challenges are expected in simulating the microstructural evolution during AM processes.

Reliable simulation often requires experimental verification or calibration, which also applies to the AM process simulation. As a short-term focus, experiments on monitoring the thermal process to determine in situ temperature gradient profiles in the as-fabricated alloys are of prime importance. One of the current constraints for high reliability thermal modeling is the lack of experimental evidence. Although the ex situ cooling rate can be estimated as a compromise [87], this cannot be a remedy for performing high quality thermal modeling. Moreover, the microstructure features of some alloys, e.g., Ti-based alloys, can be complex and without dendrite formation; estimation of ex situ cooling rates for these alloys is thus quite difficult. Accurate methodologies for in situ measurement of the heating and cooling

rates should be developed and adopted for calibrating thermal modeling approaches. Due to the rapid heating/cooling rates in AM processes, ultrafast response and high sensitivity thermocouples are currently required for precise measurement. However, such thermocouples [4, 15] are mostly only available for low temperature applications, e.g., lower than 400 °C, which is not remotely suitable for alloy studies because of the high melting point of most alloys.

Aside from experimental support to thermal modeling, another urgent need constituting a short-term goal is to develop effective microstructural characterization toolkits for 3D reconstruction of defects, which include internal cracks, inclusions, micro-voids and submicron voids. Two development thrusts should be highlighted. Firstly, a complete 3D reconstruction of multiscale defects should be established. Due to limitations of individual microstructural characterization methods, as of yet there is no single effective method of representing a complete 3D reconstruction of defects in a 1 cm³ volume. As a rapid solution, one should consider a statistical algorithm to combine the results by different characterization methods, and thus generate a complete 3D reconstruction of defects. Synchrotron tomography is often used for 3D tomography and has the potential for further development for such purposes. It should be noted that the synchrotron X-ray diffraction approach is a promising method for performing in situ phase and stress analysis [38]. Similar methods should be employed to inform strain-hardening models based on crystallographic properties, e.g., crystal plasticity.

In order to directly link defect properties with mechanical properties, it is essential to emphasize the modeling efforts of performing simulations based on anisotropic microstructural properties of the as-fabricated alloys. Based on the above discussion about the microstructure of as-fabricated alloys, the anisotropic grain features directly cause anisotropic mechanical properties. Therefore, more effort is required in studying the influence of anisotropic microstructure on mechanical properties in characterizing microstructure–property relationships. In addition, one should also realize the importance of surface roughness and its impact on fatigue resistance of the AM as-fabricated alloys. Microstructure-based mechanical simulations should be further developed and performed under the support of experiments. Geometric factors should be included in finite element simulation of the mechanical properties, since unique complex geometries are often considered as one of the advantages in AM.

Multiscale approaches for AM processes that can be used for linking the process to not only structure and property but also to product performance should be developed. In particular, uncertainty quantification in design constraint satisfaction should be carefully considered due to sensitivity of the response of microstructural evolution to AM process parameters. This may require development of accurate and efficient

algorithms using stochastic methods or reduced-order modeling in combination with high-resolution direct numerical simulations for obtaining training data. Enhanced concurrent modeling techniques are also of interest for determining the effect of local process–structure–property relations on global product performance. In particular, development of new phase field modeling methods that can account for non-equilibrium microstructure evolution is a key focus area. Methods for modeling melt pool dynamics (i.e., interface tracking methods such as Volume of Fluid (VOF) and level set) are also a key interest for understanding process–structure relations and surface morphology characterization, which strongly affects product qualification and fatigue life, in AM-developed components. Without these methods available, process modeling of AM methods is unlikely to be successful in contributing to the advancement of these processes.

Last but not least, materials design engineers should focus efforts on design of alloys that are adaptive to the AM processes. Design of materials for specific processes are not uncommon in materials design practice. For example, in the casting process, alloys are designed with a smaller freezing range to avoid hot tearing effects, which provides accommodation for specific casting techniques. Such alloy design efforts for the short-term goals of AM can provide circumvention of some of the technical challenges in thermal process control for AM processes.

5.2 Long-term goals

Although some of the long-term goals are further extensions of the above short-term goals, there are several key points that should be highlighted for special consideration.

Fundamental models in phase transformations of rapid heating and solidification should be further developed. The current materials simulation on phase transformations mainly assume local equilibria, which may have significant deviation from the far-from-equilibria case as observed in AM processing. According to secondary dendrite arm spacing measurements, the cooling rate of AM processes can be more than 1000 K/s [87]. As a compromise, the current simulation based on the Scheil model [24,65] is considered as a good starting point. Compared to rapid cooling, the fast heating can be a more severe challenge in the process–structure simulation in terms of nucleation and growth. So far, studies have been confined to metallic glass [56]; more rigorous theoretical work should be performed on crystal materials, which is suitable for AM process simulation.

Understanding that many challenges in AM can only be solved through collaboration between experimentalists and theorists, a data repository is highly desired for sharing valuable information, which is also considered a primary goal of the Materials Genome Initiative. Materials and manufacturing informatics should be well-defined for

AM research, which involves not only materials engineers but also mechanical engineers and physicists. Databases with original information of processing, microstructure and mechanical properties will be greatly beneficial to engineers/scientists with common interests. This will accelerate materials and manufacturing innovation in the AM research community. By developing theories and databases for AM, it is expected that an integrated computational manufacturing design framework can be built for AM research. The blueprint of computational material and microstructure design can be realized with predictive-science approaches for AM. Once all the steps of the process–structure–property relationship for an AM process have been well-characterized, it will be possible to control the final material properties by varying parameters in each subsystem.

The primary long-term goal for the computational community should be directed at the collection of the combined knowledge of materials engineers, mechanical engineers, computer scientists, and physicists to development an integrated solution platform that incorporates robust analysis frameworks. While there are many software programs available (and many others are being developed) for solving individual pieces of the AM puzzle, the lack of a common data structure for swift and seamless flow of information between these software packages is prohibitive. A fully-integrated system can enable high-level development of AM applicability, such as the reduction of variance in product performance or increase in computational efficiency of product scale simulations.

6 Conclusions

AM methods have the potential to revolutionize the manufacturing industry and to promote rapid development of novel materials and products. While a multitude of research is currently being conducted in order to establish these methods as viable manufacturing solutions, there are still a number of detriments that are prohibiting ubiquitous use of AM technologies for practical applications. It is becoming ever-increasingly apparent that computational methods can play a key role in understanding the fundamental driving physics that control the properties of as-built AM products. The authors have presented an extensive review of the current computational and experimental challenges that are crucial to the short-term and long-term success of AM to provide key focus areas and structure for the computational and experimental research communities (see Fig. 24). The state-of-the-art in computation as well as experimental motivation for future scientific investigations into the materials and products developed in AM has been provided. Moreover, the authors have discussed their current research initiatives in the area of computational analysis of AM materials, processes and products as potentially acceptable solutions.

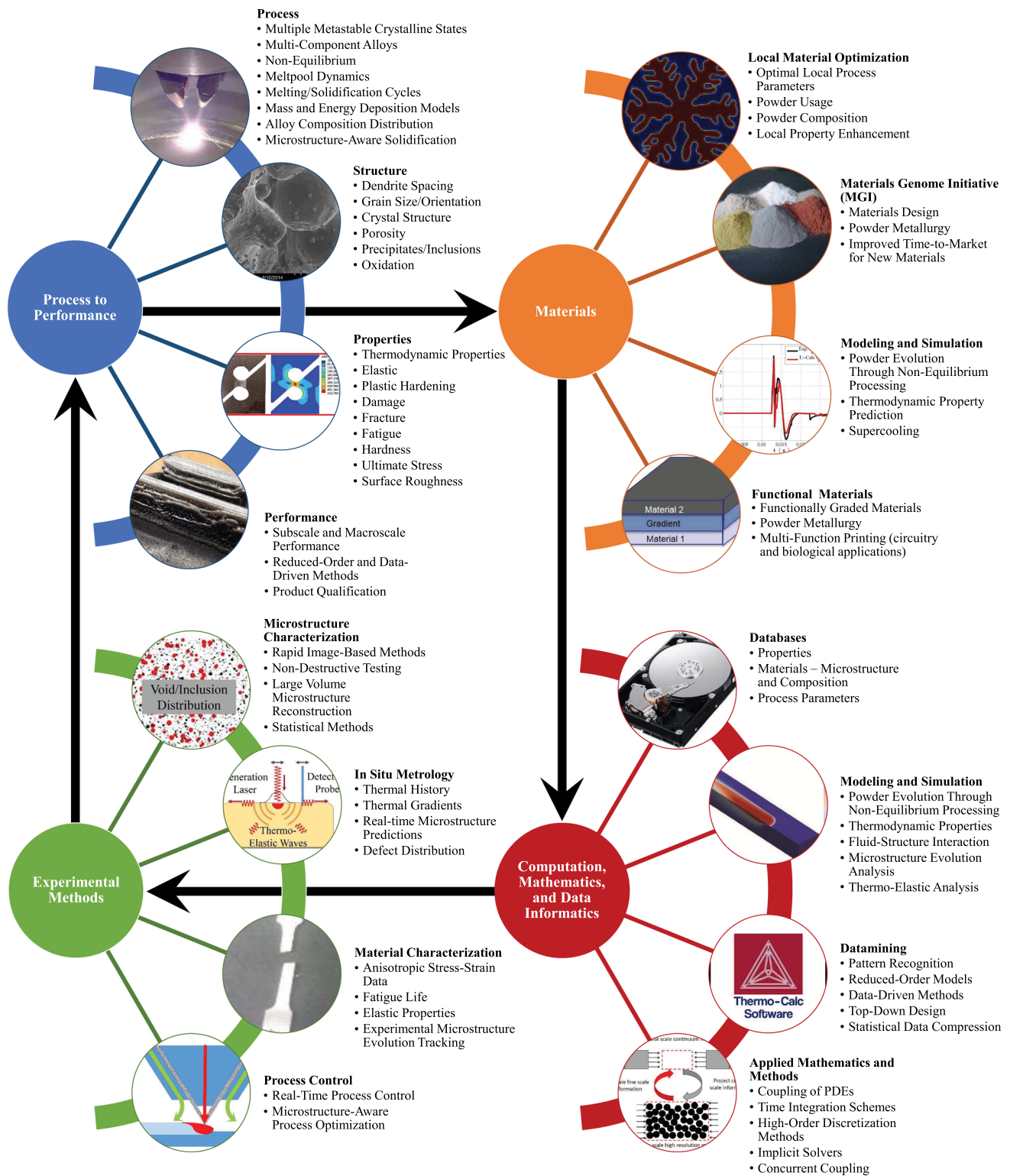


Fig. 24 Key impact areas for future goals in AM processing

Acknowledgments The authors would like to gratefully acknowledge the support for this work provided by National Institute of Standards and Technology (NIST) and Center for Hierarchical Materials Design (CHiMaD) under grant No. 70NANB13HI94 and 70NANB14H012.

Jacob Smith would like to acknowledge the United States Department of Defense for their support through the National Defense Science and Engineering Graduate (NDSEG) fellowship award. Orion L. Kafka would like to thank the United States National Science Foundation

(NSF) for their support through the NSF Graduate Research Fellowship Program (GRFP) under financial award number DGE-1324585. The authors would also like to acknowledge Sarah Wolff and Fuyao Yan, both at Northwestern University, for their intellectual contributions through discussion on experimental characterization of mechanical behavior and microstructure resulting from AM processes.

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