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Material Modeling in Additive Manufacturing

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WHILE PHYSICAL EXPERIMENTATION is a necessary aspect of characterizing the life cycle of additively manufactured components—from feedstock material to eventual retirement or failure of the built components—physical experiments, on their own, are insufficient in tackling this challenge. Due to the expansive design space for additive manufacturing (AM) and the cost and time associated with interrogating both the design space and resulting mechanical behavior of parts produced by AM, models of varying degrees of fidelity can be used to provide virtual observations that serve to complement physical experimentation. Such models not only help to populate process-structure-property test matrices but can offer valuable scientific insight into the physics governing various aspects of the process-structure-property relationships for AM.

This article focuses specifically on material modeling applied to structure-property predictions. In this context, structure is intended to represent intrinsic material attributes of the solidified part, as opposed to the structural geometry of the designed part. Process modeling and process-structure predictions, including predictions of part-scale distortion and residual stresses, are described elsewhere in this Volume, including "Process-Structure Relationships in Fusion Metals Additive Manufacturing," "Structure-Properties Relationships in Metal Additive Manufacturing," and "Part-Scale Process Modeling for Metal Additive Manufacturing." Rather than provide an exhaustive review of structure-property modeling for all AM processes, this article provides general guidelines and considerations in terms of modeling the salient material features that ultimately impact the mechanical performance of parts produced by AM.

Microstructure Modeling

Microstructural features of additively manufactured materials can vary dramatically in comparison to those of conventionally manufactured materials. Such microstructural features include grain and subgrain structures as well as pore or void defects. The degree to which each type of feature influences the mechanical behavior of additively manufactured materials depends on the mechanical property of interest and the prominence of the features relative to one another. For example, certain mechanical properties, such as fracture and fatigue, tend to be more sensitive than other properties, such as elastic modulus and yield strength, to pore or void defects. At the same time, the relative influence of such defects may depend on the amount of residual stress in a built part, which can manifest in the development of complex subgrain structures. In terms of modeling the impact of such microstructural attributes on the mechanical behavior of additively manufactured materials, it is important to strike a balance between representing the relevant microstructural features with sufficient fidelity to capture the physics or mechanics at hand and maintaining computational tractability.

Two of the primary ingredients needed to predict structure-property relationships via material modeling include a geometrical representation of the microstructural features of interest (e.g., grain structure and void defects) and a suitable constitutive model describing the material behavior, both of which can be scale and resource dependent.

Effect of Grain and Subgrain Structure on Mechanical Properties

The manner in which material solidifies during any manufacturing process significantly impacts the resulting intrinsic microstructure, including grain and subgrain structures (e.g., twins, dislocations, and second-phase precipitates). For AM processes, the characteristics of intrinsic material microstructures can deviate significantly from those formed during conventional manufacturing processes. This deviation is largely attributed to steep thermal gradients and unique thermal cycles that occur during AM processing. As with any material (including non-additively manufactured materials), the grain and subgrain structures can have a significant impact on the mechanical behavior of the material.

There are two common approaches to model the effect of grain or subgrain structures on the mechanical behavior of additively manufactured materials. In one approach, the simulation domain is treated as a homogeneous material, and the process-induced microstructural features that contribute to the overall material response are accounted for implicitly within a phenomenological constitutive model. Typically, the phenomenological constitutive model comprises an anisotropic yield criterion, associated flow rule, and hardening rule. All of the rules embedded within the constitutive model contain parameters that must be calibrated. The process-induced microstructural features (e.g., crystallographic texture with respect to the AM build coordinate directions) enter into the model implicitly via calibration of the constitutive parameters. The Johnson-Cook model (Ref 1), or modifications thereof, is one common example of a phenomenological constitutive model that has been used to estimate the mechanical or thermomechanical response of AM metals. See Ref 2 to 4 for details and further comparisons among phenomenological constitutive models applied to AM.

A second approach is to resolve the grain or subgrain features explicitly within the geometry of the model and to invoke a constitutive model that represents their deformation mechanisms. The microstructure in such models can be instantiated in several ways. For example, a microstructure model can be instantiated using results from physics-based simulations of microstructure evolution during AM processing (Ref 5, 6), as shown in Fig. 1. Alternatively, synthetic microstructures can be instantiated using algorithms that generate realistic-looking grain structures but do not actually incorporate the physics of process-driven grain evolution (Fig. 2).

A third approach is to instantiate a model directly from experimental measurements of

AM grain structure, a recent demonstration of which was carried out as part of the Air Force Research Laboratory (AFRL) AM Modeling Challenge Series (Ref 8–10) (Fig. 3). Once the simulation domain is instantiated with the microstructural geometry of interest, a constitutive model that accounts for the fundamental deformation mechanisms of the additively manufactured material can be invoked. One common choice is to use a crystal-plasticity model that computes evolution of plastic strain as a function of crystal orientation for each grain in the microstructure.

There are advantages and disadvantages to both the homogenized-microstructure and explicit-microstructure modeling approaches. The former approach tends to be much more computationally efficient than the latter approach, requires fewer fitting parameters, and has been demonstrated over the decades to be tunable to many different materials and manufacturing processes. On the other hand, models in which microstructural features are explicitly resolved and fundamental deformation mechanisms are represented can produce heterogeneous micromechanical fields (Fig. 3) that cannot be produced using the homogenized-microstructure modeling approach. While explicit-microstructure models can offer valuable scientific insight into relationships between grain (or subgrain) structures and mechanical behavior of additively manufactured materials, they often are not used at the engineering-component scale due to their computational expense.

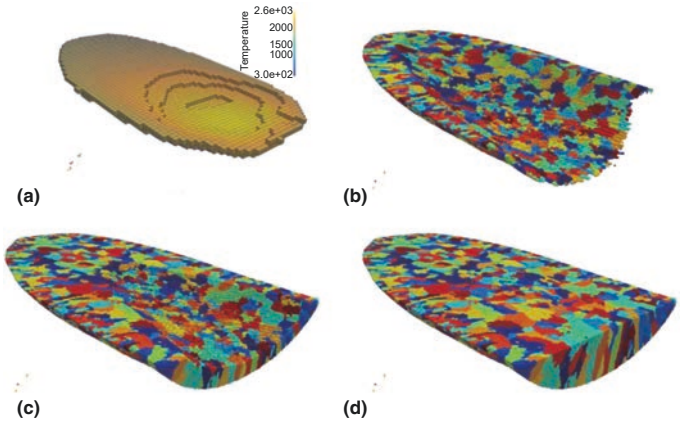

Fig. 1 Physics-based simulation of grain structure used to instantiate a micromechanical crystal-plasticity model. (a) Simulated molten pool temperature profile for selective electron beam melting of Ti-6Al-4V. (b–d) Subsequent solidification grain structure at three sequential time steps. Source: Ref 5

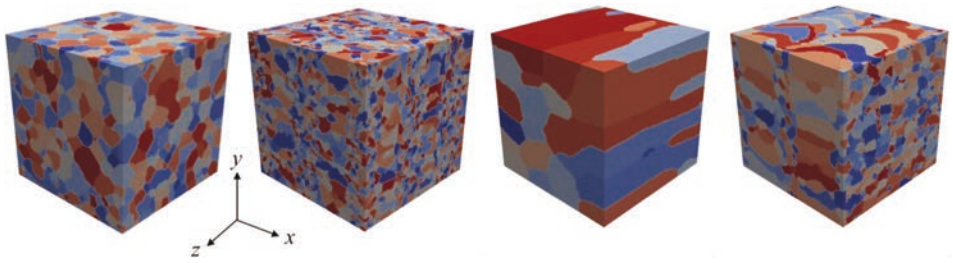

Fig. 2 Synthetic additive manufacturing grain structures instantiated using the Stochastic Parallel PARticle Kinetic Simulator (SPPARKS). Source: Ref 7

Effect of Pore or Void Defects on Mechanical Properties

Microstructural pores or voids are generally regarded as defect structures because they are formed unintentionally and can have a deleterious effect on certain mechanical properties. Technically, pores and voids that are formed during the AM process are distinguished based on the shape of the empty space they comprise within an otherwise fully dense part; pores are spherical and voids are nonspherical and irregular (although, as pointed out by Sola and Nouri in Ref 12, the distinction is rarely made in the literature). The following is a summary of sources of pore or void defects in AM (Ref 12): feedstock-related pores (including pores entrapped in feedstock material), pores from powder compaction, metallurgical pores, and processing-related pores/voids (including those caused by lack of fusion and keyholing). Further details regarding processing defects, including pore or void formation, are covered in "Process Defects in Metal Additive Manufacturing" in this Volume.

The influence of pore or void defects on mechanical properties depends on the specific mechanical property of interest, the characteristics of the pore or void defects, and the relative impact of other features at play, for example, surface roughness and residual stress. A recent survey of the literature by du Plessis et al. (Ref 13) concluded that, in general, pores below a certain size or porosity below a certain limit has negligible influence on properties such as strength and ductility for static loading conditions; however, they note that the pore size that is considered small can be material dependent and that exceptions to this trend can exist depending on the distribution of pores (e.g., small pores distributed in a cluster or in locations where their effect could be critical). However, with increasing pore size and

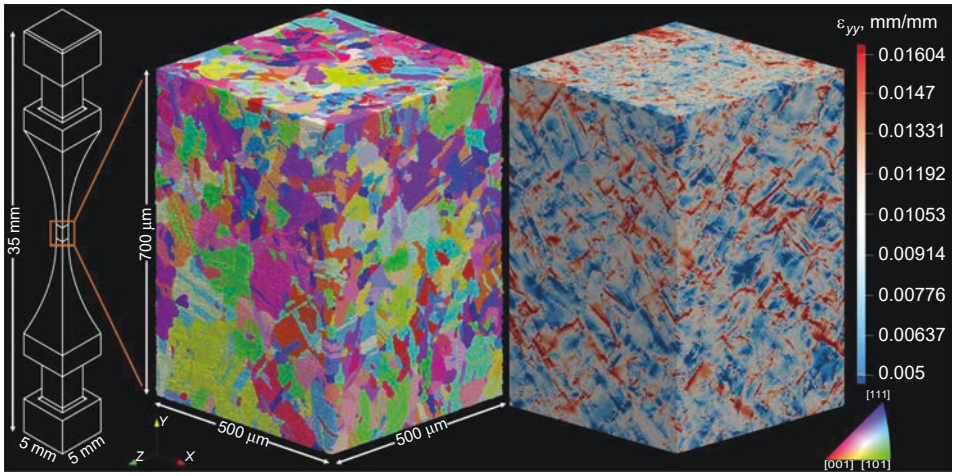

Fig. 3 Experimentally measured grain structure of additively manufactured Inconel 625 and simulated strain fields from crystal-plasticity modeling. Source: Ref 11

porosity content, both strength and ductility are reduced. Additionally, irregularly shaped voids resulting from lack of fusion, for example, can have a more significant and detrimental impact on mechanical properties than spherical pores. In general, fatigue-related properties are shown to be more sensitive than static mechanical properties to pore and void defects. Given the propensity of pores and voids to form during AM processes and the impact that such defect structures can have on mechanical behavior of parts produced by AM, incorporating pore and void defects into structure-property models is critical in many cases to achieve accurate predictions of mechanical behavior of additively manufactured materials.

Two common approaches to account for the presence of pore or void structures in computational models is by implicitly representing the effects of porosity via porous constitutive models or by explicitly representing void space within the geometry of the simulated solid domain (or a combination of the two). In the former approach, phenomenological models are embedded within a material constitutive formulation to represent damage evolution based on nucleation and/or evolution of voids via internal state variables.

As an example, Johnson et al. (Ref 14) used finite-element analysis to predict failure in an additively manufactured stainless steel part using a constitutive model that incorporated a damage formulation that implicitly accounted for growth of existing voids and nucleation of new voids in the simulation domain. Preexisting voids (i.e., process induced) and newly nucleated voids (i.e., mechanically induced) were represented by an element-wise void-volume fraction, where preexisting voids were input to the constitutive model to initialize the damage internal-state variables. The initial void-volume fraction was assigned to each element in the finite-element mesh by sampling from a probability distribution function describing pore size based on x-ray microcomputed tomography (micro-CT) measurements. The predictions were made in the context of the Third Sandia Fracture Challenge, which is discussed later in this article.

In the latter approach, explicit pore or void structures are instantiated within the model geometry via a number of different methods, including direct replication from x-ray micro-CT measurements or by synthetic generation of random or strategically placed pores/voids. Recently, Erickson et al. (Ref 15) used experimental data from 17-4 PH stainless steel tensile specimens manufactured by laser powder-bed fusion (L-PBF) (Ref 16) to generate probability distribution functions of pore count and pore diameter (Fig. 4). Drawing from the probability distributions, 120 idealized tensile specimen geometries were instantiated with geometrically explicit pore structures statistically similar to those from experiment. The pore-instantiated geometries

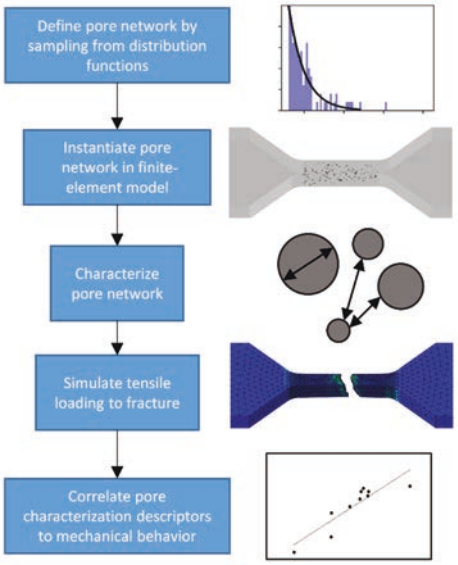

Fig. 4 Example of workflow to represent pores explicitly within the geometry of an additively manufactured part. In this case, pores were instantiated by drawing from probability distribution functions fit to experimental test data of additively manufactured 17-4 PH stainless steel. Source: Ref 15

were then discretized with a finite-element mesh for numerical analysis. As with any modeling approach, model discretization increases as the size of the smallest geometrical feature of interest decreases. To balance computational tractability with feature resolution, modelers must decide the smallest feature size of interest for a given simulation domain. In the work by Erickson et al. (Ref 15), the smallest pore diameter considered for explicitly modeling a pore network was 30 μm (0.00118 in.). This threshold exponentially reduced the number of elements needed to represent a pore network in a given finite-element model in comparison to including all pores below this threshold, while retaining the majority of pores resolvable by most lab-scale x-ray micro-CT systems.

Subsequently, an element-deletion approach was employed, whereby fracture was simulated using a ductile-damage constitutive model (Ref 17) analogous to that used by Johnson et al. (Ref 14). Based on the simulation results and geometrically explicit representation of pore structures, Erickson et al. (Ref 15) derived a void descriptor function to uniquely characterize pore networks, which has since been evaluated against additively manufactured mesoscale tensile specimens of L-PBF Inconel 718 (Ref 18).

Effect of Surface Roughness on Mechanical Properties

Similar to internal pore and void structures, surface roughness, which is generally intended to include all micronotches and protrusions present on the component surface(s), is considered a defect because it occurs unintentionally and can have a deleterious effect on mechanical properties of the built component. The primary length scale of surface roughness depends on the specific AM process used. Sources of surface roughness in AM include balling, partially melted powder particles, partial wicking of melt pools into the powder bed, melt pool instabilities, gravity-driven variations (i.e., surface variations between so-called upskin and downskin surfaces), inconsistent powder feed rates, variation in powder size, and variation in cooling rates, among others. Although there are certain postbuild procedures that can be performed to reduce the surface roughness of the built part (e.g., mechanical or electrochemical polishing), there are occasions when it is either too costly or intractable to perform such procedures. Depending on the severity of the surface roughness and its actual or anticipated impact on mechanical properties of interest, it may be of interest to account for surface roughness in computational models of additively manufactured parts.

Considering surface roughness as a geometrical defect rather than an intrinsic material defect of a built part, the most common approach for modeling surface roughness is by explicitly representing the surface topography within the geometry of the simulation domain. As an illustrative example, Kantzos et al. (Ref 19) instantiated three-dimensional (3D) models of L-PBF Ti-6Al-4V with explicitly resolved surface topography based on x-ray micro-CT measurements with an approximate minimum feature resolution of 1.5 μm (5.9×10^{-5} in.). Micromechanical fields were calculated using a massively parallelized fast Fourier transform (FFT) code with an elasto-viscoplastic constitutive model. The FFT solver required a 3D rectilinear array (grid) as input. Thus, voxelized data from the x-ray micro-CT reconstructions could be input directly upon binarizing the reconstructed volume to distinguish solid material from void space. Voxels within the rectilinear array corresponding to void space were assigned as so-called buffer regions with zero stress in the FFT model. The solid domain was treated as an isotropic homogeneous material. To assess the formation of stress concentrations due to surface topography, the von Mises stress fields were computed under simulated tensile loading for two samples having different powder particle sizes (Fig. 5). Results from the simulations showed that unmelted particles that adhered to the surface contributed to the overall surface roughness but had negligible effect on the development of stress concentrations, whereas surface notches were more significant than powder particle protrusions in terms of developing stress concentrations. Further, the adhered powder particles tended to obscure some of the surface notches, suggesting that 3D experimental imaging techniques that allow seeing beneath the adhered particles are important in resolving the relevant surface features that could lead to crack nucleation.

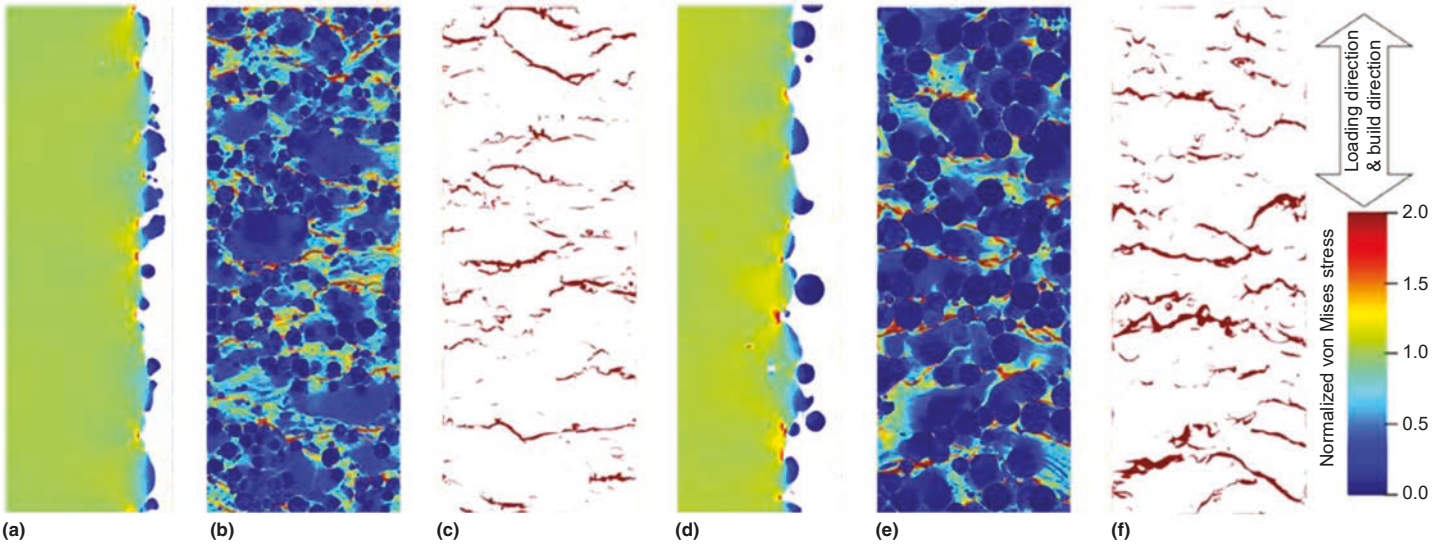

Fig. 5 Representative two-dimensional slices from three-dimensional micromechanical simulations showing the effect of surface roughness on stress distribution near free surfaces. The models were instantiated directly from x-ray microcomputed tomography measurements of laser powder-bed fusion Ti-6Al-4V. Source: Ref 19

In a similar example, Vayssette et al. (Ref 20) assessed the effect of surface roughness on fatigue behavior of additively manufactured Ti-6Al-4V using 3D finite-element models in which surface topography was explicitly represented in the model geometry. The surface topography was instantiated from experimental measurements using two different imaging techniques: 3D optical profilometry of the surface and x-ray micro-CT of the entire volume (Fig. 6). The solid domain of the model was treated as an isotropic homogeneous material. Cyclic loading for a limited number of loading cycles was simulated using finite-element analysis, and a nonlocal fatigue indicator parameter (FIP) was computed. Similar to the findings from Kantzos et al. (Ref 19), Vayssette et al. (Ref 20) found that the 3D imaging technique (x-ray CT) does a better job of characterizing the surface notches than the surface profilometry technique. Based on extreme value statistics of the nonlocal FIP, Vayssette et al. (Ref 20) proposed a methodology to account for the effect of surface roughness on the high-cycle fatigue life of the AM material.

While these examples investigated the effect of surface roughness using 3D image data, the studies treated the solid domain as a homogeneous isotropic material and thus did not explicitly resolve the grain features. Recently, Stopka et al. (Ref 21) studied the effect of surface roughness profiles and various notch geometries in synthetic microstructures representing aluminum 7075-T6 (Fig. 7). Each synthetic microstructure was subjected to simulated cyclic loading using finite-element analysis and a crystal-plasticity constitutive model, and an averaged grain-sensitive FIP was computed. In their numerical experiments, the authors found that for a single notch, the notch depth had a greater effect on the maximum volume-averaged FIP compared to the notch radius. Furthermore, the authors found that for both

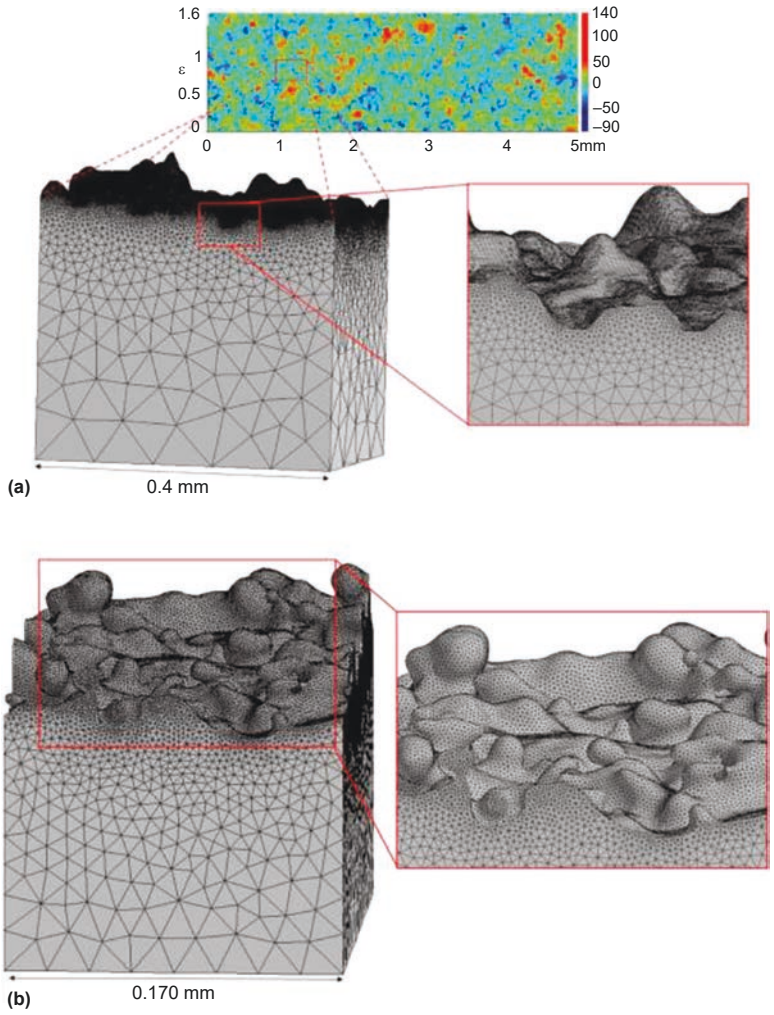

Fig. 6 Meshed volume of additively manufactured Ti-6Al-4V from two types of experimental measurements. (a) Surface profilometry scan. (b) Tomographic volume scan. Source: Ref 20

their synthetic and single-notch models, the effect of surface roughness on the extreme-value FIPs is felt for multiple layers of grains. However, Stopka et al. (Ref 21) postulated that the effect of surface roughness is not primarily influenced by the number of grains but by the distance from the notch surface.

Blind Modeling Challenges

Since approximately 2016, formal modeling challenges have been designed and released broadly to the international modeling community to test the ability of both models and modelers to predict various aspects of (process-) structure-property relationships in AM. In such challenges, a limited set of experimental data is provided to the participants, who are then asked to submit blind predictions of specific metrics of interest. The challenges are conducted on a relatively short timeline (typically 8 to 12 weeks), requiring that modelers make judicious assumptions and idealizations to meet the challenge deadline while leveraging the available experimental data. The challenge hosts then assess the blind predictions against the known experimental results and typically release the results to participants shortly thereafter.

Examples of such modeling challenges include the National Institute for Standards and Technology (NIST) Additive Manufacturing Benchmark Test Series (AM-Bench) (Ref 22, 23), the Third Sandia Fracture Challenge (Ref 24), and the AFRL AM Modeling Challenge hosted jointly with America Makes (Ref 8). Technical publications stemming from the different challenges highlight the state of the art in AM modeling capabilities at the time that the challenges took place. Some key takeaways from these modeling challenges include:

- In the absence of complete experimental data, modelers must make assumptions and idealizations that can influence their predictions.
- There is often a wide range of predictions submitted, highlighting which modeling approaches and modeling assumptions are most effective for a given AM process.
- Regardless of the type of model used for a given challenge, careful model parameter calibration is perhaps the most critical aspect of achieving successful predictions.
- Modelers should identify and, to the extent possible, account for various sources of uncertainty in their models.
- Access to experimental benchmark data is critical to continue advancing the state of materials modeling for AM.

Physics-Driven versus Data-Driven Models

In the context of physics-driven versus data-driven modeling, all of the modeling approaches previously described can be classified as the former. However, in the pursuit of optimizing structure-property relationships for AM, there is an obvious need for data-driven modeling. This need is motivated simultaneously by the expansive AM design spaces and high computational costs of physics-driven models. At the highest level and in the context of structure-property predictions, both physics-driven and data-driven models share a similar aim, which is to predict the mechanical behavior of interest given (micro)structure information for a given set of AM build conditions. However, the manner in which each type of model achieves that aim is fundamentally different.

As described in a recent review article by Kouraytem et al. (Ref 25), physics-driven modeling approaches (including the ones discussed in this article) require a set of governing constitutive equations that represent the physical phenomena underpinning structure-property relationships. The governing equations are then solved over some finite domain using numerical solvers. Such computations can be cost-prohibitive in terms of exploring a high-dimensional AM design space.

Alternatively, data-driven models, which include machine learning models, incorporate training algorithms that are designed to handle problems for which the governing equations relating inputs to outputs need not be known a priori. Often, such governing equations are inferred through correlative relationships between the control (input) variables and the response (output) variables. More recently, there have been efforts to develop physics-informed machine learning models that incorporate governing physics equations into fitness functions evaluated during training to ensure that predictions from the machine learning models are consistent with the relevant physics (Ref 26). Whether physics-based or not, data-driven models that are properly trained with a sufficient amount of training data can make structure-property predictions in orders of magnitude less time than that required for physics-driven models. Figure 8 provides an illustrative example of the difference (and similarity) between physics-driven and data-driven modeling in the context of structure-property predictions for AM. Some of the key advantages and disadvantages of physics-driven and data-driven models are provided in Table 1. More information about data-driven modeling and its applications can be found in Ref 25 and 28 to 30.

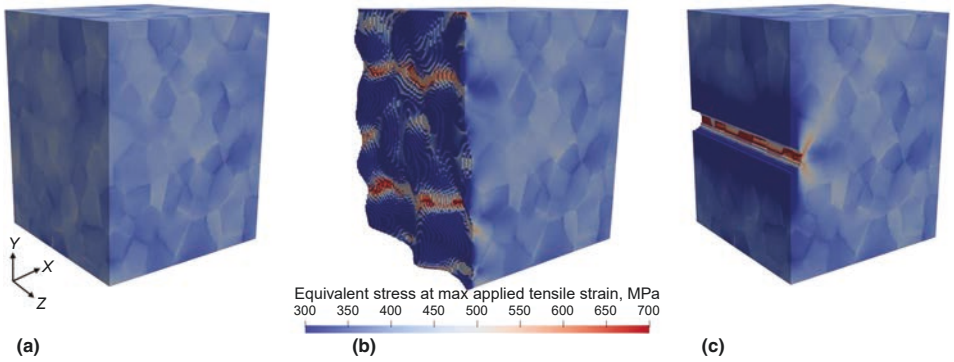

Fig. 7 Synthetic microstructure representing (a) aluminum 7075-T6 investigated with (b) an overlayed surface roughness profile and (c) ideal notch geometries. Source: Ref 21

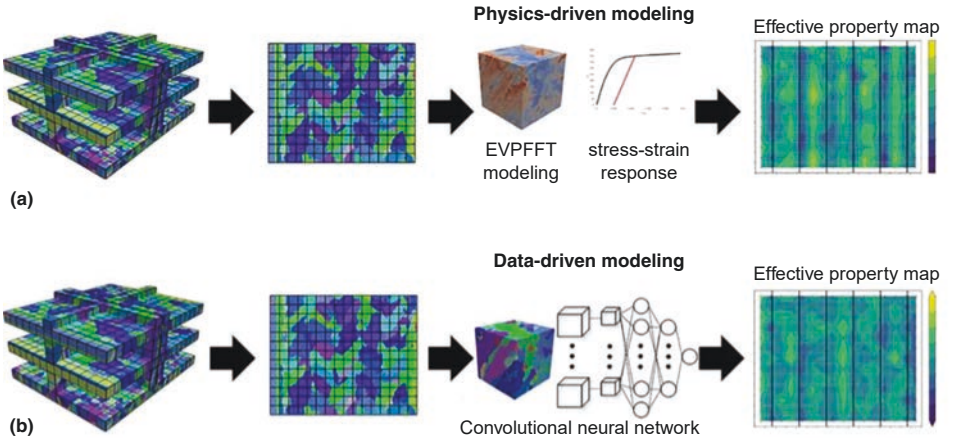

Fig. 8 Example illustrating the difference between (a) physics-driven modeling using an elasto-viscoplastic fast Fourier transform (EVPFFT) model and (b) data-driven modeling using a convolutional neural network to predict maps of effective mechanical properties given grain structure for an additively manufactured type 316L stainless steel. Source: Ref 27

Table 1 Advantages and disadvantages of physics-driven and data-driven approaches in the prediction of process-structure-property relationships in additive manufacturing

	Physics-driven models	Data-driven models
Advantages	• Simulate complex multiphase phenomena • High-fidelity representation of the underlying physics • Results are generally interpretable	• Low computational cost enables the exploration of high-dimensional design space • Predictions of complex phenomena when physics are implicitly embedded within training data • Formalized calibration via model training
Disadvantages	• Need for input parameter calibration • Need for simplifications • High computational cost precludes exploration of the complete design space • Valid within the limitations and context of their original formulations	• Lack of interpretability • Complicated validation • Potential for model bias and brittleness (easy to fool) • Required amount of training data • Valid within the limitations and context of their original formulations

Adapted from Ref 25

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