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CRITICAL REVIEW

Physics-based modeling of metal additive manufacturing processes: a review

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Abstract
In the modern world, the ubiquity and critical importance of metallic materials are evident in everything from infrastructure and transportation to electronics and aerospace. Additive manufacturing (AM) of metals has revolutionized traditional production methods by enabling the creation of high-value components with topologically optimized complex geometries and functionalities. This review addresses the critical need for sophisticated physics-based models to investigate and optimize the AM processes of metals. We explore both melt-based and solid-state AM techniques, highlighting the current state-of-the-art modeling approaches. The purpose of this review is to evaluate existing models, identify their strengths and limitations, and suggest areas for future research to enhance the predictability and optimization of AM processes. By summarizing and comparing various modeling techniques, this review aims to provide a comprehensive understanding of the current research landscape. We focus on the pros and cons of different models, including their applicability to key elements and processes common to both melt-based and solid-state AM methods. Where multiple models exist for a single technique, a comparison is drawn to highlight their relative pros and cons. Concluding this review, we contemplate prospective advancements in sophisticated physics-based process modeling and strategies for their integration with models for structure-properties relations.

Keywords Additive manufacturing · Physics-based modeling · Metallic materials

1 Introduction

The evolution of metallic materials has been a cornerstone of societal progress, marking significant leaps from the Bronze Age to today's high-tech alloys, each transition underpinning advancements in technology and industry [1]. Achieving the urgent societal goals of reduced emissions and increasing energy efficiency is driving the development of novel metals with unprecedented performance [2]. One path is lightweight metals (e.g., Al and Mg) for room-temperature applications such as infrastructure and transportation [3]. A second path is ductile metals at low or cryogenic temperatures (e.g., stainless steels and Ti alloys) for high-latitude vessels and Arctic pipelines [4]. The third path is high-temperature damage-tolerant metals (e.g., superalloys and metallic glasses) for aircraft engines and nuclear reactors where the thermal efficiency generally increases with the operating temperature [5]. Many of these metals can be produced by additive manufacturing (AM), which makes objects from 3D model data, usually layer upon layer, as opposed to subtractive methodologies where objects are formed by removing materials through cutting, drilling, milling, or grinding [6]. AM is advantageous over subtractive manufacturing in that high-value component with topologically optimized complex geometries and functionalities become achievable [7]. Therefore, metal AM (MAM) has the potential to improve the sustainability of key industrial sectors, eliminate several energy-intensive fabrication steps, and reduce raw material requirements [8]. In the meantime, it can produce parts with mechanical properties that are comparable or superior to the traditionally manufactured ones [9].

There are two main types of MAM: melt-based and solid-state [10]. MAM has many advantages, including the freedom to create complex geometries, the ability to process hard-to-machine materials, and the ability to manufacture functional prototypes directly for use. Despite this, there

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are several challenges associated with the melt-based MAM, including high residual stresses, significant thermal gradients, and defects such as porosity and hot cracking caused by melting and rapid solidification [11, 12]. It is possible that these issues can adversely affect the mechanical properties and dimensions of the fabricated parts. In the meantime, solid-state AM processes do not melt the material, thereby reducing residual stresses and defects resulting from phase changes [13]. However, solid-state AM is not without its own challenges, which include limited material choices and difficulty achieving high-density parts. As a general rule, while solid-state AM reduces thermal problems, melt-based AM offers greater versatility when it comes to materials and part complexity [14].

Given the challenges and high costs of preparing feed materials and operating MAM machines [15], utilizing physics-based models to study the MAM process has become increasingly popular [16]. Several reviews have focused on the physics-based modeling of melt-based MAM techniques [17–22], while much fewer have addressed solid-state methods [23]. As a result, we provide here a short review to summarize mainstream physics-based models in most, if not all, MAM processes. This review is unique because it focuses on the pros and cons of different models for important elements or processes, some of which are common between the melt-based and solid-state approaches. A list of open-source software packages is also provided for each model.

2 Classification

There are two types of melt-based MAM methods: powder bed fusion (PBF) and directed energy deposition (DED) [24]. PBF uses a laser or electron beam to selectively melt and fuse powder materials layer by layer within a confined bed area [25]. On the other hand, DED involves no bed but instead feeds powders or wires directly into a focused energy source, such as a laser beam, an electron beam, or an arc, which melts the metal as it is deposited on the build surface or an existing part [26]. Between the two types of feed materials, wires have a higher deposition efficiency with less waste, while powders have greater material variety and are better for complex geometries [27]. PBF is renowned for its high precision and the ability to create complex internal shapes, while DED stands out for its rapid material deposition capabilities and its proficiency in repairing or adding to existing parts [28]. In both approaches, compared with the laser beam, the electron beam offers deeper material penetration and faster build rates but requires operation under vacuum conditions and may not be optimal for metals that are prone to adverse effects from electron scattering [29]. A summary of different types of melt-based MAM techniques is provided in Fig. 1.

There are four types of solid-state AM methods: cold spray, field-assisted AM, friction-based AM, and binder jetting [30]. The cold spray uses a high-velocity gas jet to accelerate metal particles onto a substrate, creating a coating or part without significant heating [31]. Working at room temperature, it preserves the original material properties and avoids thermal distortion. Field-assisted AM employs electric, magnetic, acoustic, shear, and/or thermal fields to facilitate the bonding of powders, foils, plates, or wires [32]. It can process a wide range of metals, including difficult-to-sinter ones. Friction-based AM, such as friction welding, generates heat through mechanical friction to join metals [33]. Because the metal is refined, the produced parts can have excellent mechanical properties. Binder jetting deposits a liquid binding agent onto layers of powder metal, bonding these layers together to form a part [34]. It is material-efficient and suitable for complex geometries without support structures. An overview of the various solid-state AM techniques is offered in Fig. 2.

3 Feedstock models

3.1 Powder

One of the most popular types of feedstock in either melt-based or solid-state AMs is the powder. For example, in PBF and powder-based DED, respectively, powder spreading and powder feeding are the first step and significantly influence

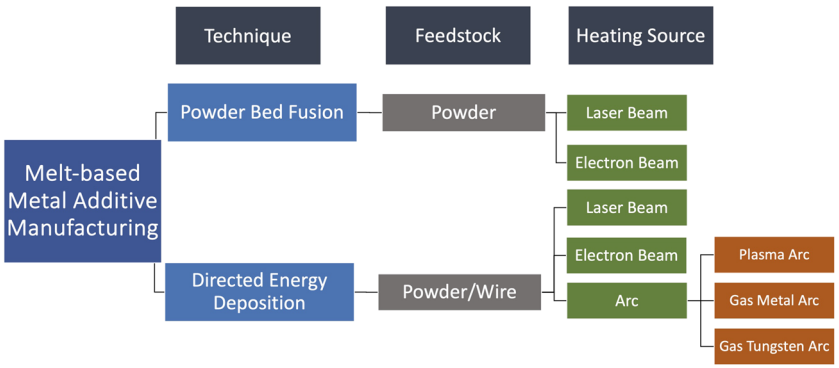

Fig. 1 Different types of melt-based MAM methods

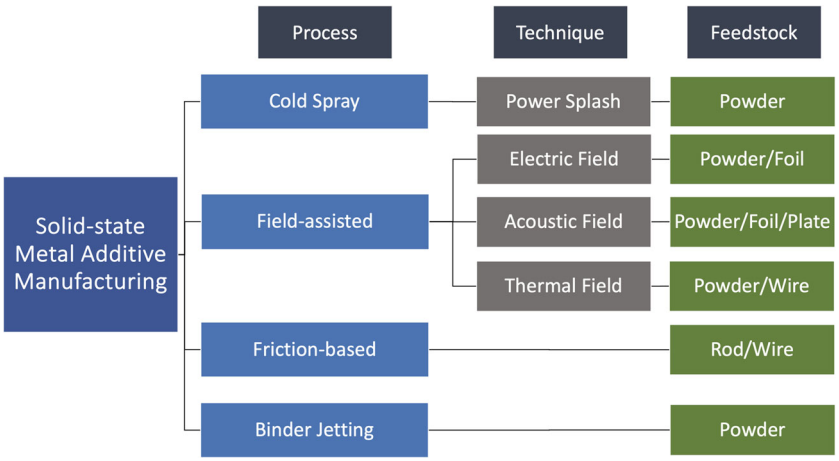

Fig. 2 Different types of solid-state MAM methods

the subsequent melting process [35]. Powder dynamics also play an important role in cold spray [36], field-assisted AM [37], and binder jetting [38], as long as the feedstock is powder. For a given metal, factors relevant to powder dynamics include but are not limited to powder shape, powder size, powder layer thickness, powder feeding rate, rake shape, and rake speed. There are mainly two views of the powders: discrete and continuum, as shown in Fig. 3. In the discrete view, cubic arrangements [39] and particle deposition [40] have been employed to simplify the powder bed. However, the most popular method is the discrete element method (DEM) [41], because it accurately simulates individual par-

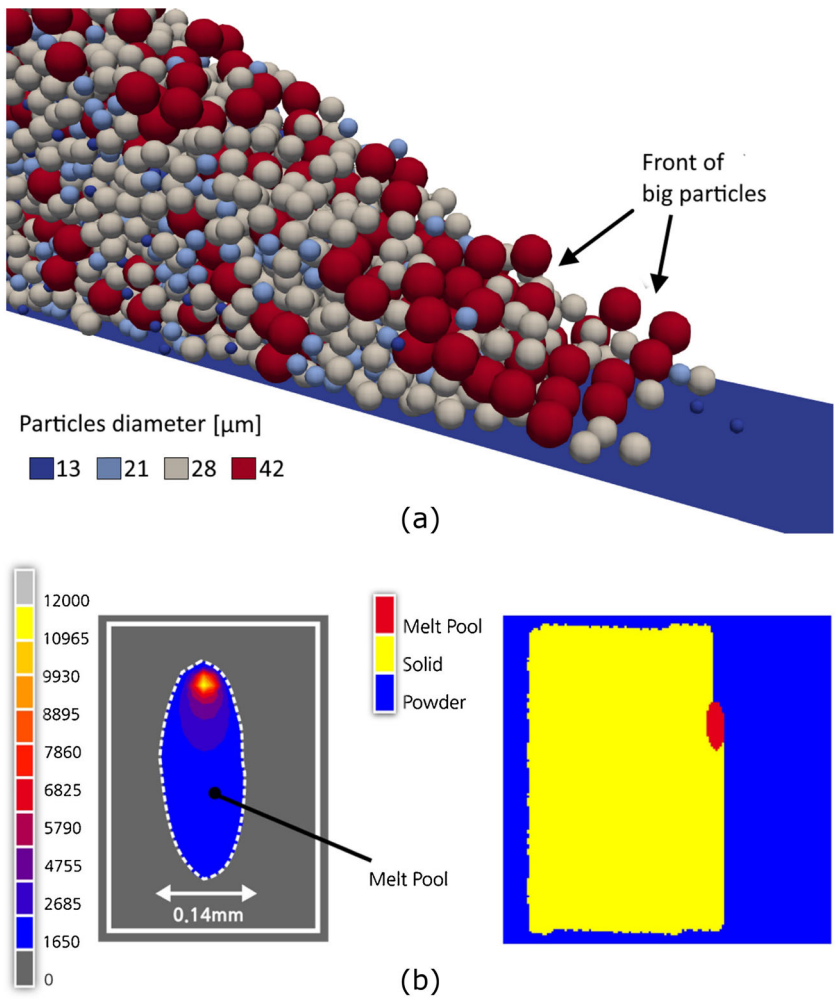

Fig. 3 **a** Discrete and **b** continuum treatments, respectively, of the powder bed. In **b**, temperature is in units of °C. **a** is reproduced from Ref. [47], which is under CC BY. **b** is reproduced with permission from Ref. [48]

ticle interactions, including contact mechanics, cohesion, and adhesion. DEM's ability to handle non-spherical particles and dynamically track their behavior allows for realistic simulations of powder flow, crucial for optimizing machine design and process parameters [42]. In the continuum view, the powder is treated as a granular flow. As such, common fluid models such as the computational fluid dynamics (CFD) method [43], the lattice Boltzmann method (LBM) [44], and the smoothed particle hydrodynamics (SPH) method [45] can be applied. However, one shortcoming of approximating the powders as a continuous fluid is that it fails to accurately capture collision, friction, and interlocking between particles, which are critical in determining the realistic behavior of powder deposition and spreading in MAM processes [46].

A powder model can be calibrated by adjusting the physical properties of particles such as shape, size, cohesion, friction, and inter-particle forces, to align the model's predictions of powder behavior and flow characteristics with experimental observations [49].

Nine open-source DEM software packages were recently reviewed by Dosta et al. [50]. It was found that while each can handle selected case studies with similar initial setups yielding comparable results, variations are mostly due to differences in the implementation of contact models, particularly the treatment of tangential forces in particle-wall interactions, and the sensitivity of results in penetration tests. As of July 2024, DEM software packages that are being actively developed include GranOO [51], Kratos Multiphysics [52], MercuryDPM [53], MUSEN [54], and Yade [55].

3.2 Other feedstocks

In addition to powders, other feedstocks in MAM include wires, rods, plates, sheets, and foils. In melt-based methods, the only non-powder feedstock is wire which is used in some DED processes, e.g., wire arc AM (WAAM). When simulating the WAAM process, the wire itself is usually not explicitly modeled [56]; instead, only results of the heat/wire interactions, e.g., thermal energy or melt, are considered. In solid-state AMs, deformation of the non-powder feedstocks is mainly described by continuum models such as SPH or finite element method (FEM) due to their ability to simulate complex structural behaviors and mechanical interactions under various loading conditions especially severe plastic deformation. For example, a rod in additive friction stir-deposition (AFS-D) processes has been modeled using SPH [57, 58]. Overall, there are much fewer modeling studies of non-powder feedstocks compared with powders in the literature.

4 Melting

Once the feedstocks are in place, they are selectively melted by a heat source in melt-based MAM. Therefore, modeling melting is relevant only in melt-based MAM, not in solid-state one. The melt pool behavior in MAM is complicated because the interaction between the beam and the metallic powder or wire introduces variables such as the Marangoni effect, evaporation, and denudation zones [59]. The processing parameters can significantly influence the melt pool behavior [60]. Take the PBF as an example. When the laser or electron beam power is too high, deep penetration is created in the melt pool resembling a keyhole shape [61]; when the heat power is too low, the powder particles are insufficiently melted, leading to poor bonding between particles and layers, known as lack of fusion [62]. In addition, thermal gradients within the melt pool result in various solidification rates, residual stresses, and potential defects like porosity or microcracks, making precise control challenging [63].

In the literature, different CFD techniques such as FEM [64], LBM [65], and SPH [66], the finite volume method (FVM) [67], and the level set method [68], have been employed for melting. Two examples are shown in Fig. 4. Each of these methods brings distinct advantages when applied to the melting process of MAM. For example, LBM is good at handling complex boundary interactions, making it efficient for modeling the rapid dynamics [69]; as a mesh-free method, SPH can well handle the free-surface flows and large deformations occurring in the melt pool [70]. However, they may face specific challenges too. For instance, FVM may struggle with capturing sharp interfaces such as those between solid and liquid metals without adequate mesh refinement [71]; LBM may fail to capture the phase change phenomena due to the inherent simplifications in its collision model.

Two phenomena that are closely intertwined with melting are heat transfer and evaporation. The former is related to one unique characteristic of melt-based MAM — high thermal gradient [74]; the latter affects the size, shape, and stability of the melt pool while altering the heat and chemical composition in the molten metal [75]. Thus, melting, heat transfer, and evaporation are strongly coupled, necessitating their simultaneous resolution. All five CFD techniques mentioned earlier can be coupled with additional equations to model heat transfer and evaporation [76]. However, their efficacy in capturing key physical phenomena varies. For instance, FVM is perhaps the best-suited because it conserves mass, momentum, and energy effectively, making it ideal for addressing the interactions among fluid flow, thermodynamics, and mass loss [77]. Meanwhile, typical implementations of SPH struggle to accurately simulate mass transfer and sharp interfaces, rendering it less ideal for modeling evapo-

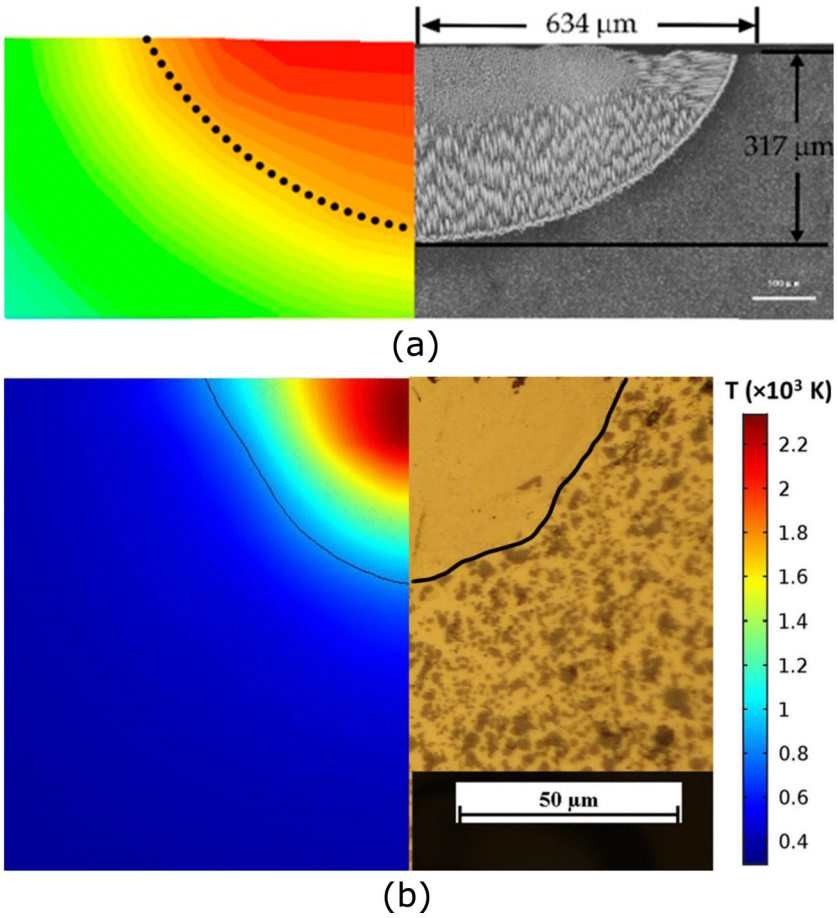

Fig. 4 Laser-induced melt pool modeled by **a** FVM and **b** FEM, respectively, compared with experiments. **a** is reproduced from Ref. [72], which is under CC BY. **b** is reproduced with permission from Ref. [73]

ration without significant modifications to the code [78]. On another note, regardless of the chosen CFD technique, the melting model should be integrated with the powder dynamics model (e.g., DEM) [79] to simulate related phenomena such as powder spattering [80].

A melting model can be calibrated by modifying thermal properties, energy input parameters, and phase change characteristics to ensure its predictions of melt pool geometry match experimental observations [81].

There are many CFD software packages that, when combined with appropriate heat transfer and evaporation models, can be applied to the melting process in MAM. Some open-source, general-purpose CFD software packages have been customized specifically for MAM. For example, additiveFOAM [82], developed at the Oak Ridge National Laboratory, is based on OpenFOAM [83] and utilizes FVM. Similarly, researchers at the Los Alamos National Laboratory developed TruchasPBF [84], which is based on Truchas [85] and also employs FVM. In other cases, software was applied to MAM without significant modification, for example, FEniCS [86] (which uses FEM), Palabos [87] (which uses LBM), and DualSPHysics [88] (which uses SPH).

5 Solidification

As the heat source moves away, the molten metal solidifies. Thus, like melting, modeling solidification is not relevant in solid-state MAM, but only in melt-based one. During the solidification, key microstructural characteristics such as grain boundaries and cracks emerge. Hence, solidification directly influences the microstructure of the printed metals [89], which in turn dictates their mechanical properties such as strength, toughness, and fatigue resistances [90]. The rapid cooling rates typical of MAM can lead to non-equilibrium microstructures, such as fine grains and metastable phases, which may enhance material properties but also introduce anisotropy and residual stresses [91]. Accurately modeling solidification is thus essential for predicting and controlling these microstructural features and ensuring the structural integrity and performance consistency of the final product [92]. Moreover, understanding solidification patterns allows for the optimization of process parameters to minimize defects such as unwanted porosity and cracking, thereby enhancing the reliability and efficiency of the MAM process [93].

The initial and boundary conditions, e.g., thermal gradients and cooling rates, for solidification modeling are usually provided by the melting simulation. Simple solidification models, such as those based on the volume-of-fluid (VOF) method [96], can distinguish between fluid and solid phases. However, these models do not account for the microstructure of the solid phase. Three numerical methods most commonly applied to microstructure modeling during solidification in MAM, in order of decreasing computational complexity, are: the phase-field (PF) method, kinetic Monte Carlo (kMC), and cellular automata (CA) [89]. Examples based on the PF and CA methods are shown in Fig. 5. PF is adept at handling the diffuse interface between phases and capturing the complex morphologies of solid-liquid interfaces without the need for tracking or remeshing [97]. Nonetheless, the accuracy of PF simulations is highly dependent on the choice of input parameters, which can be difficult to determine and requires extensive calibration against experimental or higher-fidelity simulations. kMC can effectively handle complex reaction mechanisms and is adaptable to varying conditions, making it useful for exploring different solidification scenarios [98]. However, due to its stochastic nature, kMC can introduce statistical noise into the results, requiring multiple simulations or larger sample sizes to achieve reliable outcomes. The last method, CA, is particularly effective at modeling the microstructures of materials, allowing detailed visualization and analysis of grain growth and orientation during solidification [99]. Nevertheless, CA often simplifies complex physical phenomena into discrete states, which can limit its accuracy in predicting continuous physical changes and interactions. All three methods require thermodynamic data as inputs to accurately simulate the microstructural evolution during solidification. For pure metals, simple data such as melting point and latent heat of fusion are sufficient [100]. For binary alloys, the solidification path can be pre-determined from the phase diagram [101]. For multi-component alloys, however, the use of thermodynamic software becomes necessary because the complexity of interactions among multiple elements requires detailed calculations of phase equilibria and thermodynamic properties across a range of temperatures and compositions [102].

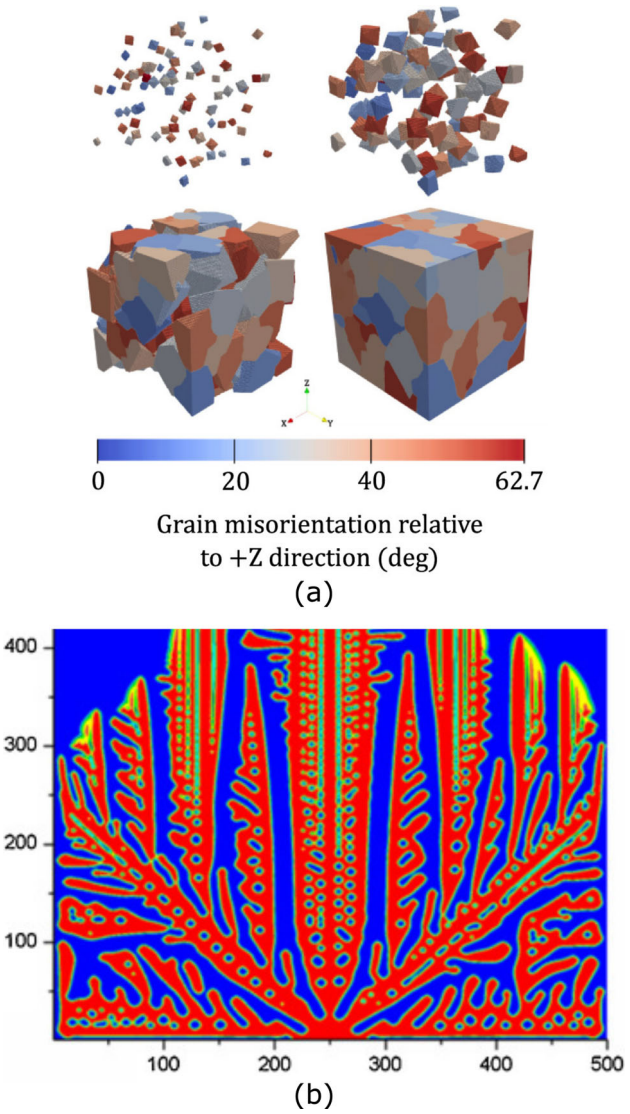

Fig. 5 Solidification modeled by **a** CA and **b** PF methods, respectively. In **b**, the edge lengths are in units of 0.2μm. Reproduced with permission from Refs. [94, 95]

A solidification model can be tuned by altering material properties and processing conditions to ensure its predictions of microstructural evolution and the final structure conform to experimental observations [103].

Many open-source software packages based on PF, kMC, or CA can be directly employed or adapted to simulate microstructural evolution in MAM. For example, Tusas [104] and AMPE [105], both of which are based on the PF method, have been employed for the subgrain scale solidification. SPPARKS [106], which was originally designed for atomic-scale kMC simulations, has been extended to micro-scale solidification. Based on the CA method, ExaCA [94] was developed for CA simulations on exascale supercomputers.

6 Late-time microstructural evolution

In melt-based MAM and some solid-state MAM processes that involve heat (e.g., AFS-D), solid-solid phase transformations occur during cooling or heating [107]. For example, in PBF, the previously solidified grains may experience re-growth as they are re-heated when powders above are being scanned [108]. The same phenomena can also manifest during post-build heat treatments, which are frequently

required when the "as-built" microstructure through melt-based MAM does not satisfy the targeted property specifications [109]. For instance, in precipitation-hardened alloys, the rapid cooling rates associated with laser PBF typically preclude the possibility of diffusion-based precipitation reactions [110]. Consequently, a post-build heat treatment, such as annealing or aging, is essential to facilitate the precipitation of strengthening phases. An example is displayed in Fig. 6. Both *in situ* and post-build solid-solid phase transformations are collectively called "late-time" microstructural evolution. Since the physics at this stage is similar to the microstructural evolution in solidification, all three methods — PF, kMC, and CA — are theoretically applicable. For example, the PF method, using MEUMAPPS-SS [111], has been applied to describe the heat-treatment process for alloys made by laser PBF. As another example, kMC has been adopted to simulate the grain growth in friction-based solid-state MAM processes [112, 113]. Generally, inputs to late-time models are the as-built microstructures generated from the solidification models.

7 Processes unique to solid-state AM

As mentioned earlier, there are four solid-state AM techniques: cold spray, friction-based AM, field-assisted AM, and binder jetting.

In cold spray, powdered metals are accelerated at high velocities onto substrates without melting. SPH has been employed to simulate the cold spray AM process involving multi-layer multi-track powders [115]. This mesh-free approach, enhanced by kernel gradient correction, adaptive smoothing length, and a constitutive model, adeptly handles large deformations and moving interfaces typical in cold spray processes. The use of SPH, inherently suited for capturing discontinuities such as voids during high-velocity impacts, provides a robust framework for modeling complex physical phenomena, including phase changes and jet formations at the substrate-powder interfaces. The experimental and simulation results are compared in Fig. 7.

There are three stand-alone field-assisted MAM processes, based on electric field, acoustic field, and thermal field, respectively [116]. To our best knowledge, no physics models have been developed or applied to any of them. However, physics models have been employed to simulate these fields when they were used as auxiliary fields to aid in melt-based AM processes [117]. For example, in DED, acoustic and thermal fields, respectively, have been simulated using VOF [118, 119] and FEM [120, 121]. We emphasize that those AM processes are melt-based instead of solid-state.

In friction-based AM processes, metals are joined and built up by using frictional heat generated through mechanical rubbing, which softens the materials without fully melting them. The AFS-D process has been simulated using SPH [57, 58]. This approach employs a fully coupled thermo-

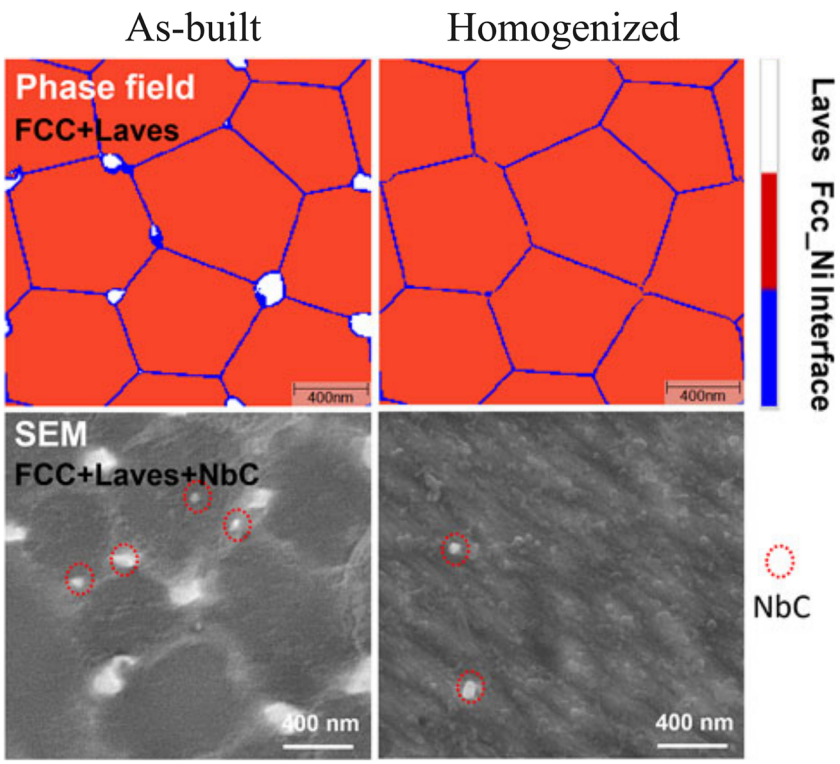

Fig. 6 PF simulations and experimental images of AMed Inconel 718 before and after homogenization at a temperature of 1080°C. Reproduced from Ref. [114], which is under CC BY

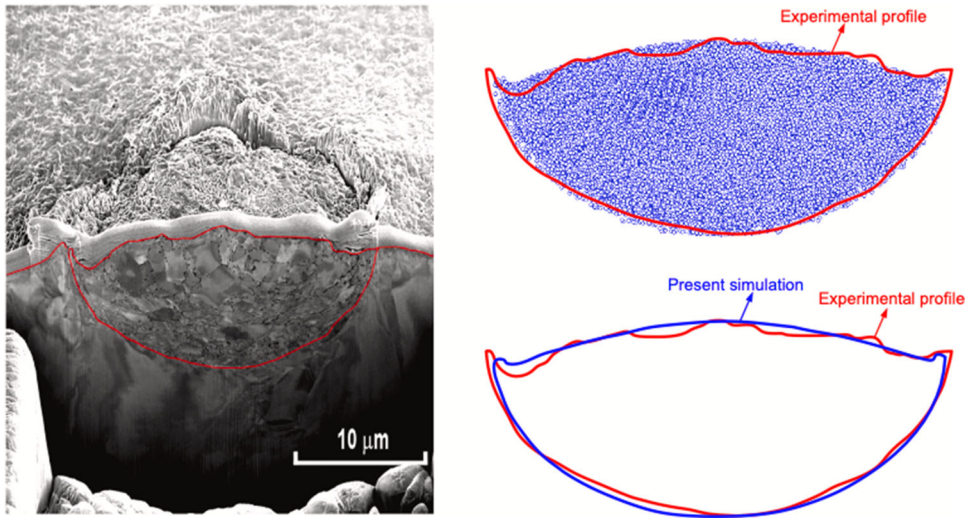

Fig. 7 Comparisons between experimental observation and simulation for the spraying of a Cu powder. Reproduced with permission from Ref. [115]

mechanical model to handle the substantial plastic deformation and thermal gradients due to frictional heat. As shown in Fig. 8, different actuator feed rates lead to different temperature contours.

In binder jetting, a liquid binding agent is selectively deposited onto a powder bed layer by layer to bond the powder particles and form a solid part. Tan [122] employed a Cartesian grid-based VOF method to study the impact of penetration of micrometer-sized droplets on a powder bed. The physics-based model accurately tracks the interface between the liquid and air during the impact, by integrating a contact angle model to account for the wetting effects on the powder particles.

Once a material is made by binder jetting, it is usually sintered to fuse particles together, thereby increasing the material's density and mechanical strength by reducing porosity and creating solid, interconnected bonds between the powder particles. The densification process in sintering has been simulated by FEM [123], which incorporates material properties such as viscosity, creep parameters, and thermal-mechanical properties dependent on relative density and temperature. Predictions based on the FEM model aligned well with experimental observations [124, 125].

8 Conclusions and perspectives

Melt-based and solid-state MAM processes underscore the transformative potential of these technologies in shaping the future of industrial manufacturing. While both MAM techniques offer distinct advantages — melt-based MAM for its precision in creating complex geometries and solid-state MAM for its superior mechanical properties and reduced residual stress — the choice between them depends largely on the specific application requirements and the inherent material characteristics. As MAM continues to evolve, the employment of advanced computational models is crucial

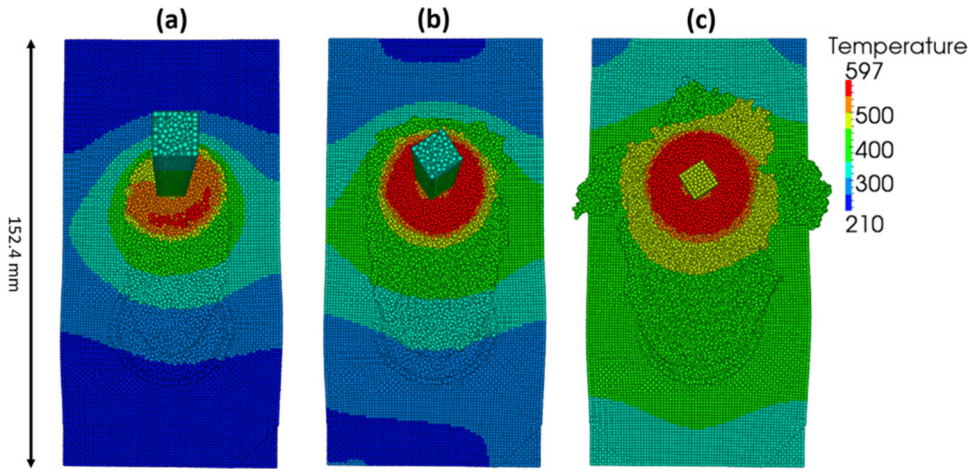

Fig. 8 Temperature (in °C) contours in AFS-D corresponding to different actuator feed rates: **a** 63.5 mm/min, **b** 127 mm/min, and **c** 254 mm/min. Reproduced with permission from Ref. [58]

for enhancing the predictability and reliability of these processes. The present review of those models not only helps in understanding the intricate microstructural evolution during and post-manufacturing but also aids in optimizing process parameters to mitigate defects and enhance material properties.

Looking forward, the ongoing development and refinement of these computational tools will play a pivotal role in overcoming current limitations related to material properties, process stability, and cost-effectiveness. Moreover, as industry and academia push the boundaries of what's possible with MAM, continued collaboration and knowledge exchange will be vital. Open-source software and community-driven innovations will likely lead to more accessible and versatile MAM solutions, broadening the scope of applications across sectors such as aerospace, automotive, and biomedical. Ultimately, the future of MAM is not only about refining the processes and materials but also about integrating these advancements into a sustainable manufacturing paradigm that aligns with global economic and environmental goals.

Integrating physics-based process models with models that elucidate the structure–property relation is essential for comprehending the entire process-structure–property continuum in MAM. This integration enables a holistic understanding of how variations in manufacturing parameters influence microstructural features, and subsequently, how these microstructures determine the mechanical properties of the final product. Such models help in predicting and optimizing the properties of manufactured parts by enabling simulations that adjust processing conditions to achieve desired outcomes. For example, adjusting heat power and scan speed in melt-based MAM can be simulated to predict changes in grain size and orientation, which directly impact the metal's strength and fatigue resistance. Ultimately, this comprehensive modeling approach is fundamental for advancing MAM technologies, allowing for the precise tailoring of materials to meet specific performance criteria, and facilitating the development of next-generation alloys with optimized properties.

Author contribution SX and YS conceptualized the review article. SX and MYA wrote the first draft of the manuscript. All authors revised the manuscript and approved the final manuscript.

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Declarations

Conflict of interest The authors declare no competing interests.

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