



## Melt-based additive manufacturing of refractory metals and alloys: Experiments and modeling

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### ABSTRACT

Refractory metals and alloys possess unique properties, such as high melting points and excellent mechanical stability at elevated temperatures, making them attractive for aerospace, nuclear, and other demanding industries. However, fabrication of these materials using traditional manufacturing techniques is challenging due to their high melting points and intrinsic brittleness. Additive manufacturing (AM) techniques provide an approach to mitigate some of these challenges, but systematic insights into their process parameters, microstructure control, and mechanical performance remain fragmented in the literature. This paper provides an overview of the challenges and future prospects associated with melt-based AM of refractory metals and alloys from the perspectives of experiments, physics-based models, and data-driven approaches. Our review concludes by summarizing the frontiers in the field and highlighting the future developments necessary to enable efficient AM fabrication of refractory metals and alloys.

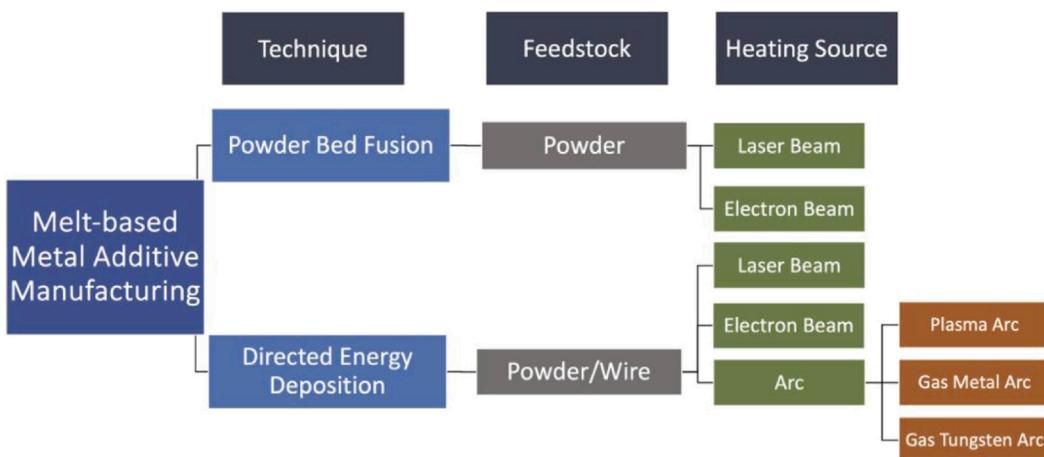
### 1. Introduction

Refractory metals are a class of materials with superior resistance to high temperatures and mechanical wear [1]. Historically, metals with a melting point above 2200 °C are considered refractory metals, including Mo, Nb, Re, Ta, and W [2]. Under a broader definition, elements such as Cr, Hf, Ti, V, and Zr may also be considered refractory metals [3]. Refractory metals face three main challenges for use in industrial settings: room-temperature (RT) brittleness, oxidation susceptibility, and high density [4]. One approach to overcome these issues is the development of refractory dilute alloys, in which one refractory metal serves as the principal element, supplemented by minor additions of other elements to enhance specific properties [5]. An alternative approach involves the development of non-dilute binary alloys comprising two refractory principal elements [6]. Through controlled alloying, these systems can attain an improved balance between strength and ductility [7]. However, both dilute alloys and non-dilute binary alloys typically limit the scope of compositional variations [8]. Since 2010, researchers have developed numerous refractory multi-principal element alloys (RMPEAs) [9], which contain three or more refractory principal elements. The intricate interactions among elements modify their fundamental properties such as diffusivity and elasticity [10,11] and can attain high strength at elevated temperatures [12].

Refractory materials exhibit high potential for industrial, nuclear, and aerospace applications [13–15]. However, they are challenging to fabricate using conventional subtractive manufacturing techniques due to their limited RT ductility [16–18]. Consequently, Additive manufacturing (AM) is increasingly favored for fabricating complex parts due to its layer-by-layer approach, which enables intricate geometries, minimizes waste, and streamlines the manufacturing process, which can simplify the manufacturing workflow [19]. Moreover, AM offers opportunities for *in-situ* compositional and microstructural control, allowing tailoring of properties in real time [20]. Melt-based AM methods—such as powder bed fusion (PBF) and directed energy deposition (DED)—have enabled the successful fabrication of refractory alloys, including W-based systems [21], TaW binaries [22], MoRe binaries [23], NbTaTi RMPEAs [24], and HfNbTiV RMPEAs [20]. For all these alloys, elemental powders were mixed according to the specific composition. Nevertheless, AM of refractory materials still faces significant challenges. For instance, their elevated melting points necessitate high beam power during melt-based AM, resulting in substantial residual stress and a heightened susceptibility to microcracking from rapid solidification [25,26]. Furthermore, the high reflectivity of certain refractory metals impedes efficient laser absorption, complicating laser-based processes by increasing energy losses and necessitating greater

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**Fig. 1.** Different types of melt-based MAM methods [29].

beam power; in contrast, electron beam-based methods are generally less affected by reflectivity due to their different energy transfer mechanism [27]. In addition, incorporating non-refractory elements with substantially lower melting points can lead to unintended local compositional gradients during solidification, posing further obstacles to process control [28]. Consequently, optimizing powder feedstocks and refining processing parameters remain critical for achieving consistent and reproducible part quality in the AM of refractory metals and alloys.

Due to the complexities associated with preparing feedstock materials and operating AM machines, direct experimentation is infeasible for optimizing AM processes. Therefore, multiscale modeling approaches have been employed to understand and optimize them [30]. At the smallest length scales, molecular dynamics (MD) simulations capture atomic-level interactions during melting and solidification, providing critical insights into laser-powder interactions [31]. At the microscale, continuum-based physics models simulate coupled thermal, fluid flow, and phase-change phenomena within the melt pool [32,33]. However, as component size and geometric complexity increase, these physics-based models often become computationally prohibitive for large-scale AM parts [34]. While some investigations report the effects of process parameters on near-fully dense refractory metals at small scales (e.g., Ta [35]), large-scale validation remains scarce. Furthermore, physics-based models cannot adequately capture phenomena that are not yet fully understood or theoretically established [33]. To overcome these limitations, data-driven strategies — such as surrogate models — offer dramatically lower computational costs to enable rapid process-property predictions [36]. Nonetheless, purely data-driven approaches require extensive high-quality datasets to avoid overfitting and lack transparency [37]. In response, there is a growing interest in frameworks that integrate physics-knowledge into data-driven models [38, 39] for advancing the design and development of refractory materials and alloys under extreme conditions [18].

In the literature, several review articles have discussed the AM fabrication of refractory materials and alloys. However, they primarily focus on a single refractory metal (e.g., W) [21], multiple refractory metals [40], or RMPEAs [41–43]. In contrast, this review considers AM fabrication of both refractory metals and alloys, discusses advances in process–microstructure–property modeling, and overall AM process feasibility. We focus on melt and powder-based AM techniques including LPBF and DED since other AM technologies are yet to be successfully applied for fabrication of refractory metals and alloys.

The remainder of this paper is organized as follows. In Section 2, we provide an overview of experimental efforts aimed on AM of refractory metals and alloys. In Section 3, we discuss the development of physics-based modeling approaches for predicting thermal histories and defect formation observed during AM fabrication. In Section 4, we examine

recent progress in machine learning (ML) techniques applied to these physical phenomena. Section 5 discusses the open problems for the optimization of AM processes for refractory alloys fabrication and design.

## 2. Experiments

The majority of metal AM (MAM) processes are melt-based, including PBF and DED, as summarized in Fig. 1. PBF excels in creating highly detailed and intricate geometries with exceptional precision, making it ideal for applications that demand complex designs [44, 45]. However, the process can introduce residual stresses and distortions due to rapid cooling, potentially compromising the mechanical properties and dimensional accuracy of the final product [46–48]. In contrast, DED enables the rapid buildup and repair of materials by melting them as they are deposited, which is advantageous for large-scale or repair applications [49]. However, DED can result in larger slag inclusions and requires precise parameter control to maintain quality and consistency in the build [50]. Recent advancements in melt-based AM of refractory materials have enabled the development of next-generation refractory alloys with tailored microstructures and improved mechanical performance. Table 1 provides an overview of the materials and corresponding AM techniques to be discussed in this section. The subsequent discussion examines findings from various studies on PBF and DED, highlighting experimental approaches and addressing challenges to improve manufacturing outcomes.

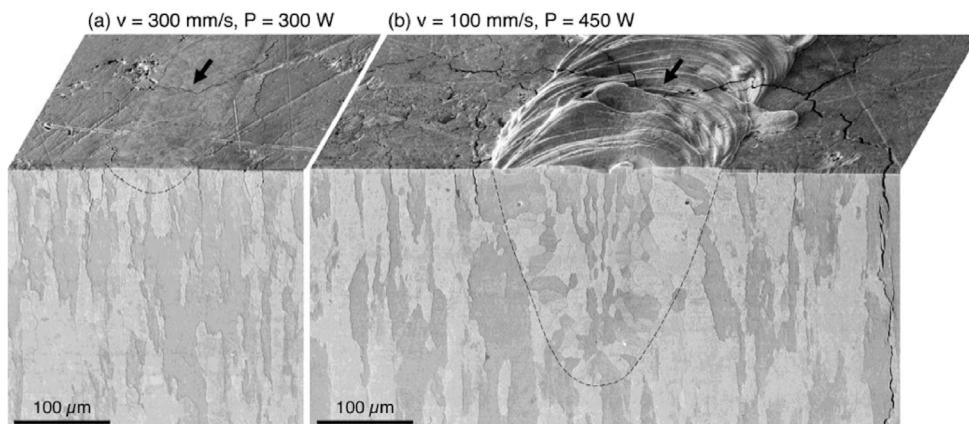
### *2.1. Powder bed fusion*

The power source in PBF is primarily a laser, and secondarily an electron beam. Compared with electron beam PBF (EBPBF), laser PBF (LPBF) offers high precision, but has issues such as cracking, residual stress, and thermal distortion [45,68]. The use of LPBF to manufacture RMPEAs like MoTaTiW has demonstrated high relative densities and good mechanical properties [55]. In the meantime, cracking has been one of the most challenging aspects of LPBF. This aspect is especially important in refractory materials whose high melting points mandate excessive heat which then leads to high thermal gradients and significant residual stresses. Therefore, recent studies have focused on understanding cracking mechanisms during LPBF processes [69]. Vrancken et al. [64] analyzed laser-induced microcracking in pure W during AM, finding that microcracking occurs within a narrow temperature range and is influenced by strain rate and local stress orientations. They also found that a higher laser power results in deeper melt pools and more cracks due to increased vaporization and melt pool instability (Fig. 2). Liu et al. [57] conducted a study on

**Table 1**

Refractory materials and corresponding AM techniques discussed in Section 2.

Material	Article	AM process	Variables
HfNbTiV	[20]	Laser DED	Material properties, mechanical properties
Mo	[51]	EBPBF	Material properties, beam Current, scan Speed, hatch spacing, preheat temperature
Mo-Re alloy	[23]	LPBF	Re Content, scan speed
MoAlCrNbTa	[52]	EBPBF	Powder parameters, phase formation
MoNbTaTiW	[53]	EBPBF	Material properties, scan speed
MoNbTi	[54]	Laser DED	Material properties, scan speed
MoTaTiW	[55]	LPBF	Powder parameters, beam power, scan speed, hatch spacing
Nb	[56]	EBM	Powder morphology, beam focus, speed, and current
Nb	[57]	LPBF	Powder morphology, beam energy, oxygen content
NbTaTiZr	[58]	LPBF	Laser power, material properties
NbZr1 dilute alloy	[59]	Arc DED	Grain texture, morphology, slip plane
Ni-Nb alloy	[60]	LPBF	Laser power, scan speed
Ta	[61]	LPBF	Scan speed, particle size distribution
TaTi	[62]	Laser DED	Scan speed, beam diameter, powder absorptivity
Trabecular Ta	[63]	LPBF	Trabecular structures, porosity, strain levels
W	[64]	LPBF	Laser power, scan speed, beam diameter
W	[64]	LPBF	Laser power, scan speed, hatching space
W	[65]	LPBF	Scan speed, beam diameter, powder particle size
W-5Re alloy	[66]	LPBF	Laser power, scan speed
W-5Re alloy	[67]	LPBF	Laser power, layer thickness, scan speed, hatch spacing

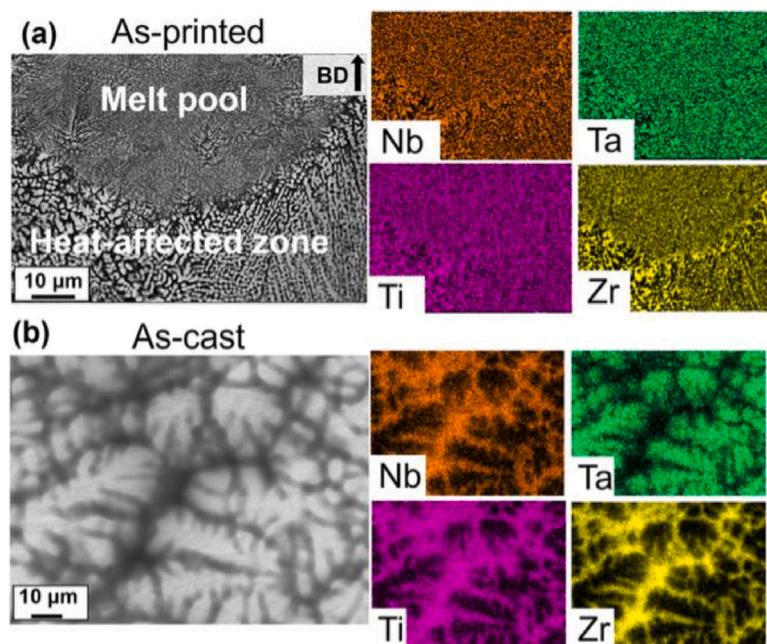
**Fig. 2.** Melt pool of top surface for different laser powers and scanning speeds in LPBF of W. The black arrows indicate transversal cracks [64].

LPBF of pure Nb, a material with a melting point of 2468 °C, high corrosion resistance, and high biocompatibility [70–73]. The focus of the study was on how energy density and oxygen content affect Nb densification, microstructure, and mechanical properties due to its high sensitivity to oxygen [74–77]. The authors found that an optimal energy density of  $146 \text{ J mm}^{-3}$  achieved a high density of 99.7%, while increased oxygen content enhanced strength but drastically reduced plasticity due to dislocation blocking by interstitial oxygen. Similarly, the existence of defects such as cracks, undissolved particles, lack of fusion, and unmelted powders after the manufacturing of RMPEAs are reported by other researchers in the literature [17,78–80]. Mooraj et al. [58] used LPBF to fabricate NbTaTiZr RMPEA with minimal defects, achieving enhanced elastic isotropy and slightly higher yield strength compared to as-cast samples, due to finer microstructures and reduced chemical segregation [81]. The as-printed sample showed a more uniform elemental distribution than the as-cast sample, which exhibited significant segregation (Fig. 3).

EBPBF mitigates oxidation by operating in a vacuum and preheating the powder bed, yet often leaves residual porosity and risks element vaporization under high beam currents. Using EBPBF, Popov et al. [52] explored the possibility of producing an AlCrMoNbTa RMPEA by blending elements of different metals. Because all elemental powders have low flow rates, they used a modified powder delivery system with vertical containers [82–84]. Microstructural characterization revealed that the as-manufactured samples consisted of two phases, one being a CrMoNbTa-based solid solution with low Al content and the other

an Al-rich solid solution. The two phases in an as-manufactured sample are shown in Fig. 4 (a,b). Additionally, samples that are further heat-treated at 1000 °C and 1300 °C, respectively, produced slight homogenization, but left significant residual porosity, as shown in Fig. 4(c–f). This work demonstrated the difficulty of achieving fully dense and uniform microstructures using EBPBF, even with the help of heat treatment.

To evaluate the effects of different scanning speeds on the alloy's properties, Xiao et al. [53] used EBPBF to fabricate an MoNbTaTiW RMPEA. They found that the as-deposited RMPEA based on various scanning speeds maintained a stable body-centered cubic phase, despite a significant vaporization of Nb and Ti, which is a common phenomenon when using an electron beam [85]. The microstructural analysis of the RMPEA revealed that lower scanning speeds reduced crack susceptibility and improved homogeneity, resulting in a balance between strength and ductility. As illustrated in Fig. 5, the material contains more low-angle grain boundaries than high-angle grain boundaries, which facilitate dislocation movement and improve the RMPEA's ductility and crack resistance, contributing to its improved mechanical properties [86]. Generally, W- and Mo-based RMPEAs show reduced brittleness and achieve up to 99% density under high beam currents using EBPBF with preheated powder beds in vacuum conditions. Nb- and Ta-based RMPEAs exhibit finer microstructures and have the potential for tailored mechanical properties when processed with LPBF [87].



**Fig. 3.** Scanning electron microscopy and energy dispersive X-ray spectroscopy maps show the melt pool and the elemental segregation in (a) as-printed and (b) as-cast NbTaTiZr [58].

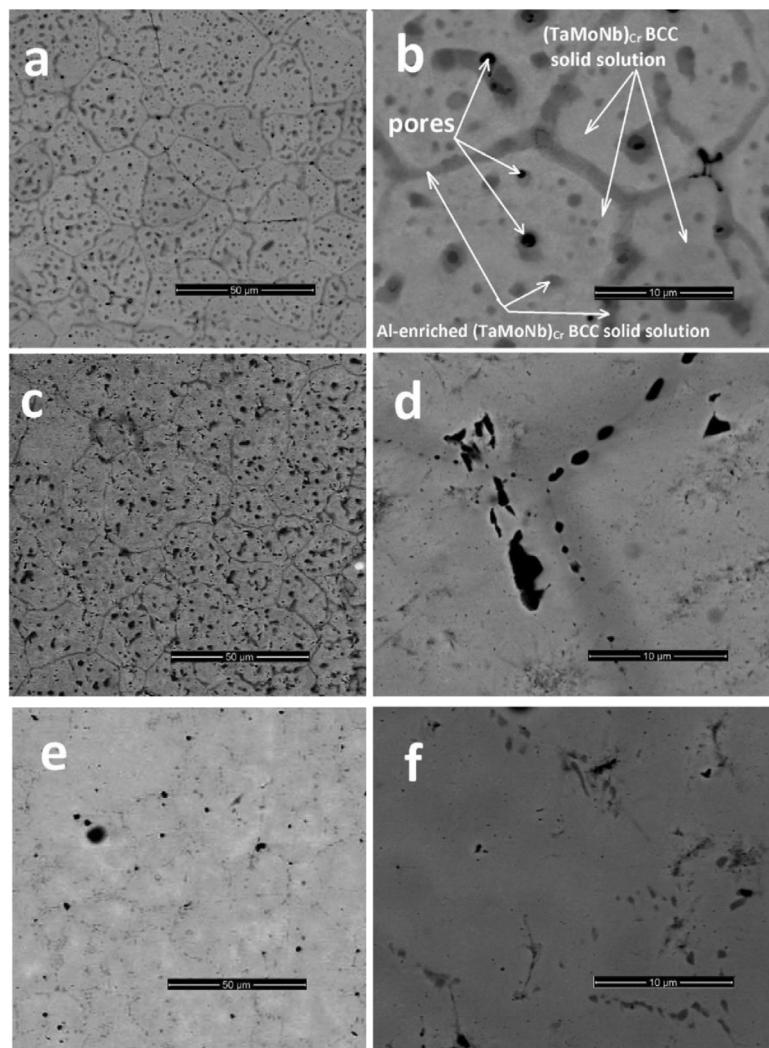
## 2.2. Directed energy deposition

DED involves directly melting materials onto a substrate using a laser, electron beam, or plasma arc in conjunction. This enables the fabrication and repair of complex, high-performance components with superior material efficiency and the ability to produce tailored microstructures. Laser- and arc-based DED methods are the most common techniques for manufacturing refractory metals and alloys, due to their broader availability, established process control, and shorter build times. For example, laser-DED has been explored for the production of many RMPEAs, including MoNbTi using elemental powders [88], with promising results in terms of density and phase composition. Zhang et al. [20] optimized the laser-powered DED process parameters for the HfNbTiV RMPEA, resulting in an equiaxed grain morphology with uniform alloy distribution and minimal macro-segregation. The same result was reported by Jin et al. [89]. Compared with as-cast samples, DED-fabricated samples usually have smaller grain sizes. Fig. 6(a–c) illustrates electron backscatter diffraction (EBSD) inverse pole figure maps of the HfNbTiV RMPEA, revealing equiaxed grains with varying sizes and orientations. DED-fabricated samples had the smallest grain size of 196 μm, while as-cast samples showed larger, randomly oriented grains, demonstrating that DED produces finer grain sizes. Among the three heat sources in DED, arc excels at large-scale builds but requires precise parameter control to avoid inclusions and anisotropic structures. By using wire-arc DED and crystal plasticity modeling, Islam et al. [59] predicted the mechanical response of the NbZr1 dilute alloy. With EBSD, they identified large columnar grains with a strong crystallographic texture aligned along the build direction, as shown in Fig. 6 (d,e). A microstructural analysis showed that the grain structure significantly affected the alloy's anisotropic mechanical properties, with strong texture contributing to variations in mechanical behavior. In comparison, electron beam-DED is less frequently used because it requires more complex equipment, such as vacuum chambers, and presents greater challenges for scalability. While it has been demonstrated with Cu components [90], to the best of our knowledge, it has not yet been utilized for refractory materials.

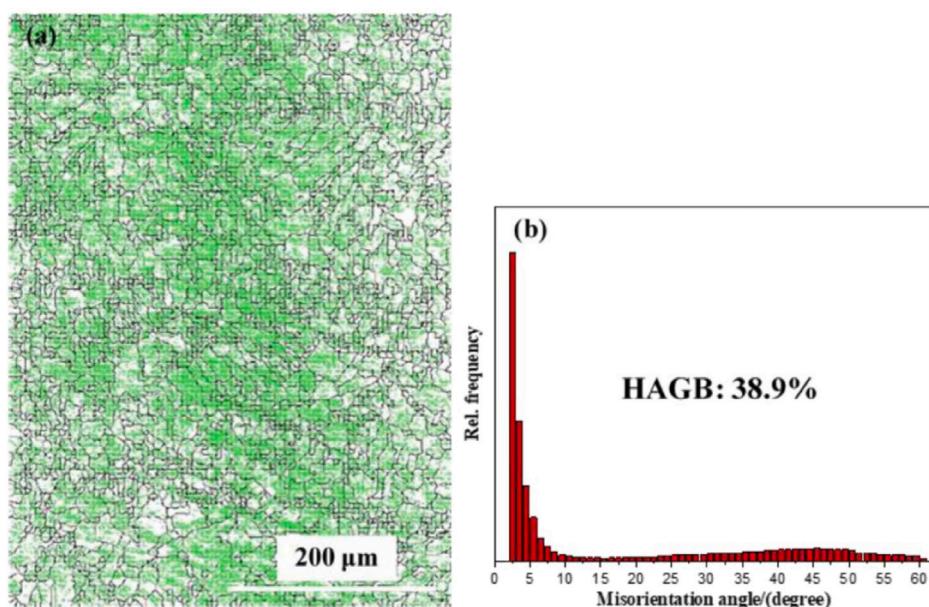
## 2.3. Future research opportunities

Fig. 7 shows a high-level schematic summarizing the state-of-the-art experimental approaches, challenges, and future opportunities needed to achieve reliable and scalable products in melt-based AM of refractory materials. Moving forward, researchers could first focus on improving feedstock purity and uniformity: reducing oxygen and carbon impurities helps minimize embrittlement in metals like Nb and W [57,73, 77], while controlling powder shape and size distributions provides more consistent melt pool formation [55,91]. In parallel, maintaining stable or preheated build environments — especially relevant for DED setups — can reduce vaporization and prevent contamination in sensitive alloys [52,82,84]. Next, enhanced in-situ and post-treatment analyses are key to address the root causes of defects. High-speed cameras or acoustic emission sensors can monitor the melt pool in real-time, allowing quick detection of hot spots where cracks or pores might form [92,93]. Meanwhile, synchrotron-based X-ray tomography and electron microscopy can map the internal distribution of defects, clarifying how process parameters like scanning speed, beam power, or powder feed rate affect overall part integrity [46,94]. Design-of-experiments approaches will help isolate which process parameters most directly influence cracking or phase formation [20,89,95]. Larger build trials are also needed to observe scale-dependent phenomena not captured in smaller coupons [90,96]. Such detailed insight not only helps optimize microstructure — for instance, controlling oxygen content to boost strength without sacrificing ductility — but also guides the development of post-processing treatments (e.g., heat treatments and surface finishing) tailored to each alloy's brittleness or segregation tendencies [81,97]. For instance, accurate post-processing techniques, such as annealing or aging, can produce an optimized microstructure while relieving stress [98].

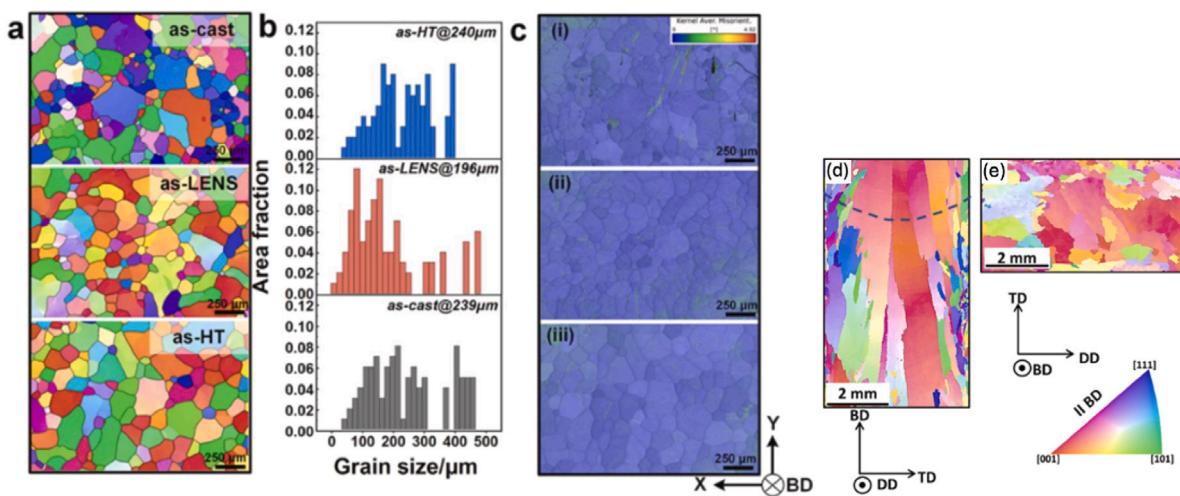
Finally, the field will benefit enormously from collaborative data repositories and standardized test artifacts that allow consistent comparisons across different facilities and material batches [93,99]. For example, ASTM International, through Committee F42, has developed a suite of AM standards addressing terminology, testing, process control, and data reporting. Notably, ASTM F2971 provides guidance on reporting AM data, and ASTM F3303 outlines practices for consistent process



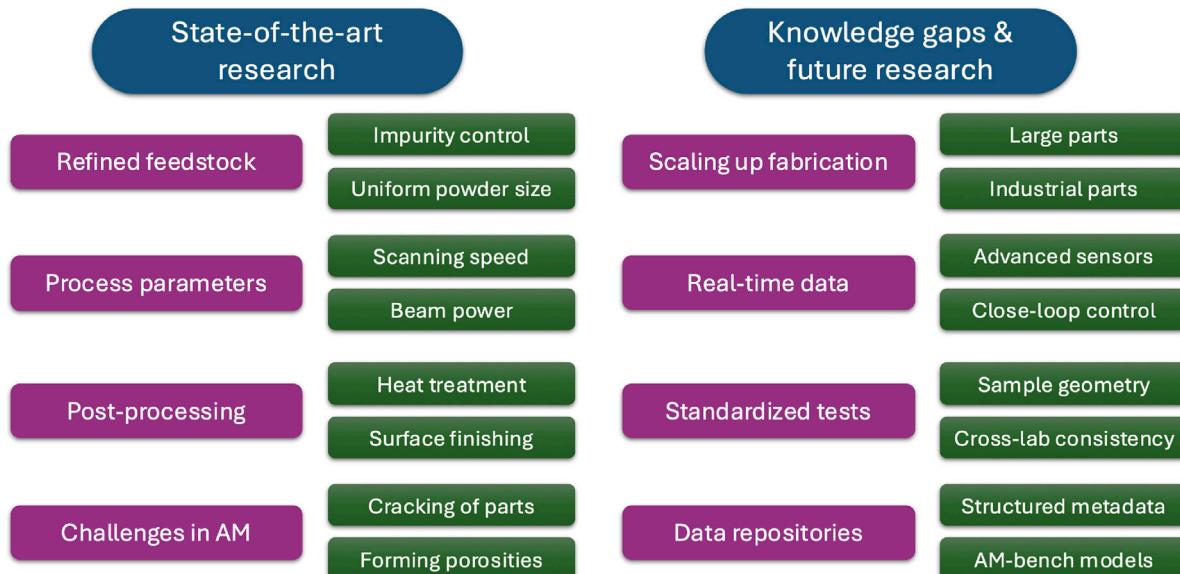
**Fig. 4.** Typical microstructures of AlCrMoNbTa RMPEA samples made by EBPBF: (a,b) as-manufactured and heat-treated samples at (c,d) 1000 °C and (e,f) 1300 °C [52].



**Fig. 5.** (a) Grain boundaries and (b) misorientation angle of the as-deposited MoNbTaTiW RMPEA at a scanning speed of 2.5 m/s [53]. In (b), HAGB stands for “high-angle grain boundaries”.



**Fig. 6.** (a-c) Microstructure characterization of Hf<sub>21</sub>Nb<sub>21</sub>Ti<sub>42</sub>V<sub>16</sub> RMPEAs following casting, DED, and/or heat treatment [20]. (d,e) Inverse pole figure map showing the grains of wire-arc DED-fabricated NbZr1 deposit: (a) TD-BD plane and (b) DD-TD plane [59].



**Fig. 7.** Summary of current and future directions in experimental approaches for melt-based AM of refractory materials.

control [100,101]. Incorporating these standards into data sharing platforms would significantly reduce dataset variability and improve interoperability across research groups working on refractory metal systems. To translate these standardization efforts into an actionable framework for collaborative repositories, we suggest the following steps:

- **Step I:** Standardize build geometries, specimen designs, process parameters, and testing protocols across institutions using ASTM references (e.g., F2971, F3303) to ensure consistent experimental setups and enable direct data comparison.
- **Step II:** Establish a centralized, open-access data repository with metadata tagging, traceability, and version control to ensure transparency, reproducibility, and long-term usability of validated experimental datasets.
- **Step III:** Promote inclusion of simulation-ready inputs and outputs (e.g., thermal gradients, solidification model parameters, dislocation data) alongside experimental results to support model development and cross-institution benchmarking.

Several database models provide strong examples of how to build collaborative data infrastructures for AM. The collaborative AM data management system developed at NIST employs a NoSQL backend (MongoDB) and XML schemas to enable flexible data ingestion, visualization, and querying across research teams [102]. Similarly, the NIST additive manufacturing integration framework outlines how material, process, and machine data can be linked with systems used in manufacturing and quality management to support digital thread workflows, qualification pipelines, and process traceability [103]. An excellent complementary model is the cybersecurity framework-based layered approach [104], which demonstrates how asset management standards (e.g., ID.AM-3) can be tailored for AM environments. Their work emphasizes mapping data flows, prioritizing critical information (e.g., CAD files, G-code, process parameters), and adopting standardized formats such as ISO 14649-17 (STEP-NC Part 17) for structured, interoperable AM data representation. Together, these frameworks and tools provide both the technical foundation and practical guidance to implement secure, reusable, and standardized data repositories that can

**Table 2**

Refractory materials and corresponding simulations/modeling approaches in the Section 3.

Material	Article	Modeling technique	AM Process	Variables
304L stainless steel	[108]	MC	LPBF	Material parameters, microstructure evolution
316L stainless steel	[109]	MC	LPBF	Hatch spacing, layer thickness
AlCoCrFe	[110]	MD	LPBF	Tribological properties
AlTiV	[111]	MC	EBPBF	Grain morphology
AlTiV	[112]	PFM	EBPBF	Beam power, scanning speed
CoCrFeMnNi	[113]	MD	LPBF	Melt pool dynamics, Mn, Co content effects
CoCrFeMnNbNiV	[114]	PFM	LPBF	Microstructure evolution, elemental segregation
HfNbTaTiZr	[115]	MD	LPBF	Grain configuration, mechanical properties
Inconel 625	[116]	MC	LPBF	Mechanical properties
Inconel 718	[117]	MC	EBPBF	Grain structure, hatch spacing
Inconel 718	[118]	CFD	EBPBF	Beam power, melt pool dynamics
Mo	[119]	Thermo-fluid dynamics	LPBF	Powder characteristics, melt pool dynamics
Mo	[51]	FEM	EBPBF	Temperature maps, surface temperature
Mo	[120]	CFD	LPBF	Density, laser power and velocity
Mo	[121]	CFD	EBPBF	Phase formation, melt pool, defects
MoNbTaW	[122]	FEM	LPBF	Thermal stress, microstructure evolution
NbNi	[60]	PFM	EBPBF	Phase formation, melt pool, defects
TaTi	[62]	FEM	Laser DED	Process parameters, microstructure evolution
Ti	[123]	FEM	EBPBF	Beam power, scanning speed
Trabecular Ta	[63]	FEM	LPBF	Porosity, mechanical properties
W	[65]	FEM	LPBF	Powder size, density, process parameters
W	[64]	FEM	LPBF	Melt pool dynamics, defects
WRe	[67]	FEM	LPBF	Process parameters, mechanical and physical properties

support large-scale collaboration, model validation, and accelerated material qualification in AM of refractory metals.

### 3. Physics-based models

Physics-based models are crucial for understanding the thermal and microstructural properties of refractory metals and alloys during melt-based AM. The importance of these models lies in the fact that they predict microstructural evolution [105] as well as mechanical properties, which are crucial factors for optimizing the AM process for refractory materials fabrication [106]. The challenges of applying physics models to AM of refractory materials include the complexity of material behavior, difficulty coupling different scales, high computational costs, limited material data availability, and experimental validation. Rapid and directional solidification plays an important role in shaping the microstructure of metal deposits produced by AM [107], yet they make the modeling of phase transformation and microstructural evolution particularly challenging. Furthermore, inhomogeneous microstructures and defect prediction across scales complicate the modeling. In what follows, we examine various physics-based modeling approaches for AM of refractory metals and alloys, considering multiple scales. Table 2 provides an overview of different refractory metals and alloys, along with the computational strategies and AM processes used to understand their behavior.

#### 3.1. Atomic-scale

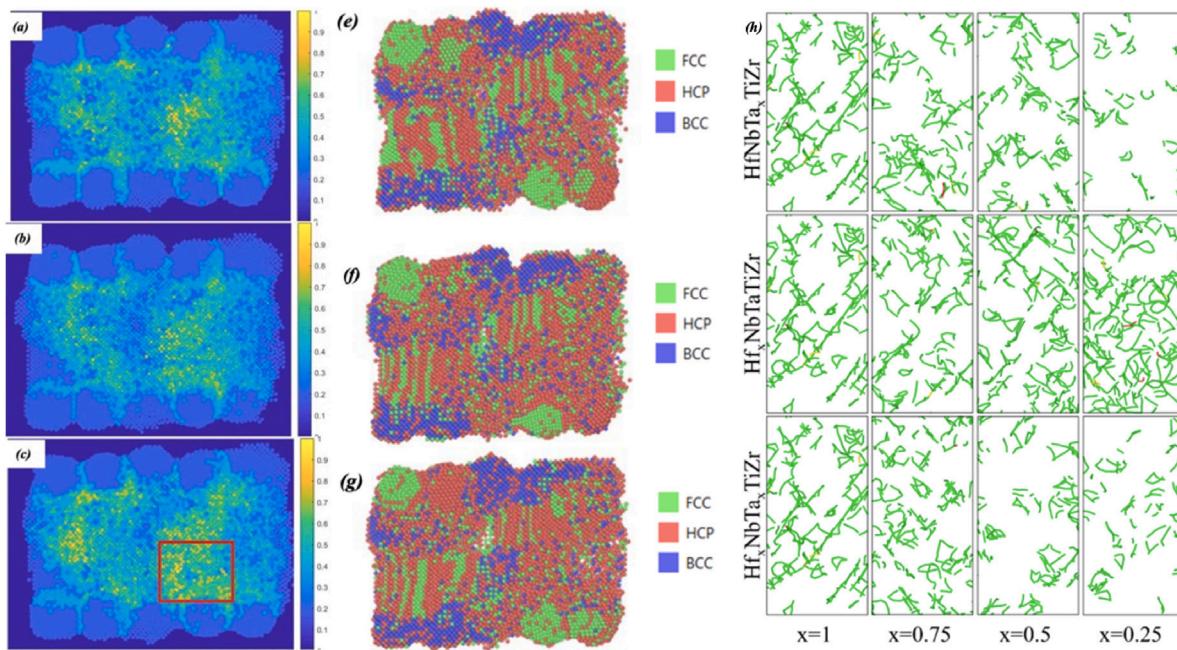
The MD simulation method is the main tool for simulating the AM-related phenomena at the atomic-scale [124]. Through solving Newton's equations of motion on atoms, MD simulations provide a detailed understanding of phenomena (e.g., laser-powder interactions) by predicting the trajectories, interactions, and dynamic behavior of atoms and molecules over time, enabling insights into material properties, phase transitions, and defect dynamics [125–128]. In the context of AM, MD simulations provide insight into the diffusion behavior, mechanical characteristics, and thermal conditions that influence the fabrication process, thereby serving as a key tool for exploring and optimizing AM processes at the smallest scales [129]. Liang et al. [115] utilized MD to explore the effect of the reduction of high-density elements from LPBF-produced HfNbTaTiZr RMPEA on its grain configuration and dislocation density by changing the atomic percentages of Ta and Hf (Fig. 8(h)). Farias et al. [110] utilized MD to simulate

LPBF of AlCoCrFe MPEA coating on Al substrate to improve the latter's mechanical and tribological properties. They compared simulated wear tracks of pure Al and Al with MPEA coating utilizing LPBF, along with experimental results in another work [130]. Their work illustrated the impact of the MPEA coating on reducing wear track depth and width, demonstrating the enhanced tribological properties achieved through the coating. In another study, Farrias et al. [113] conducted research using MD simulations for an LPBF melt pool of CoCrFeMnNi MPEA. Their results revealed that the diffusion rate varied among different elements, with Mn and Co exhibiting higher mean squared displacement values, indicating greater mobility of those atoms. Fig. 8 shows a pixel overlay analysis that visualizes the mixing of different elements in the powder bed at various laser scanning speeds.

#### 3.2. Microscale

##### 3.2.1. Monte Carlo method

Monte Carlo (MC) simulations rely on random sampling to model and analyze systems with inherent randomness or uncertainty, providing insights into phenomena such as phase transitions, statistical thermodynamics, and probabilistic processes in materials and physical systems [131]. For AM processes, MC simulations address the complexities of thermal dynamics and microstructural evolution by capturing uncertainties in thermal dynamics and microstructural evolution [132]. Particularly for refractory metals and alloys, MC methods offer more accurate predictions of final material properties and performance than purely deterministic approaches [108,109,133]. Lozanovski et al. [116] utilized an MC simulation to predict the mechanical properties and reliability of LPBF-fabricate Inconel 625. Their study revealed how variations in the effective diameter of the struts, caused by manufacturing defects, impacted the stiffness and overall mechanical response of the lattice structures. Fig. 9 illustrates the stress distributions and deformed shapes of five strut realizations generated by MC simulations for a 4 mm strut built at a 90-degree angle, highlighting how LPBF defects lead to varying stress concentrations along the strut length. These variations significantly impact the stiffness and mechanical response of the struts, demonstrating the influence of stochastic factors such as powder property distribution and laser power fluctuation. Despite the successful applications of the MC method to the AM process, one limitation is its inability to account for the crystallographic orientations of grains. Additionally, it does not explicitly incorporate physical time or directly link to the temperature changes occurring during AM [134,135].



**Fig. 8.** Pixel overlays analysis of MD simulations of the powder bed of CoCrFeMnNi during LPBF with three different scanning speeds: (a) 0.060 nm/ps, (b) 0.045 nm/ps, and (c) 0.030 nm/ps. (e–g) Polyhedral template matching analysis of solidified powder bed corresponding to different scanning speeds [113]. (h) Schematic diagram of dislocation density obtained from MD simulation of HfNbTaTiZr RMPEA powder via laser-DED by changing the atomic percentages of Ta and Hf [115].



**Fig. 9.** Five stress distributions within deformed 4 mm long strut built of Inconel 625 at a 90-degree angle with respect to the build platform [116]. The AM technique is LPBF while the physics-based model is MC. Stresses are shown in MPa and the deformed shapes are scaled to represent 10% strain.

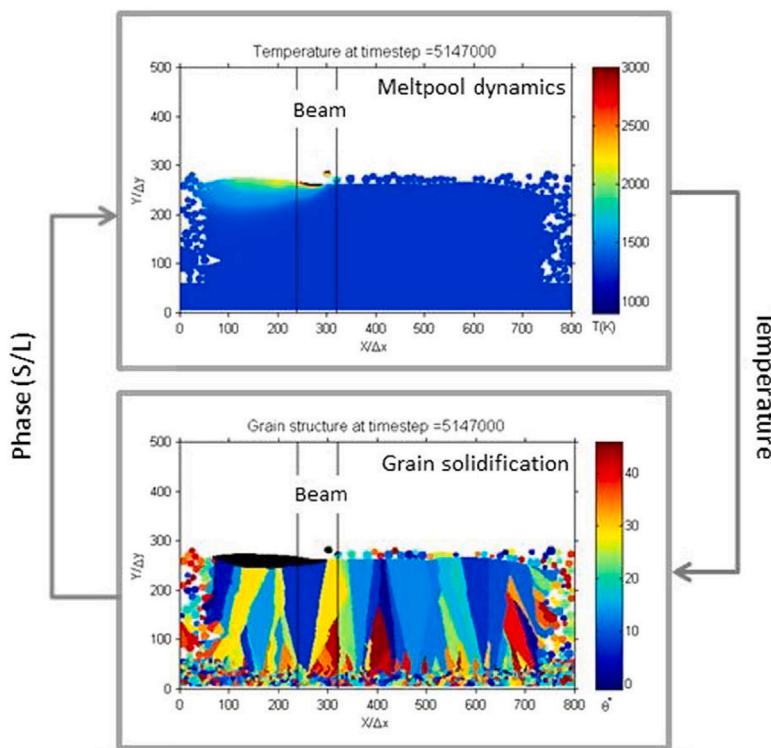
### 3.2.2. Cellular automata

In a cellular automata (CA) simulation, the system evolves over discrete time steps based on local rules applied to cells within a grid, allowing the modeling of complex phenomena such as pattern formation, phase transitions, and microstructure evolution in materials [136]. For AM, CA simulations can model microstructural evolution, thereby integrating thermal histories and processing parameters to improve understanding of process–structure–property (PSP) relationships and predict material properties [137]. To simulate the grain structure evolution during EBPBF, Rai et al. [117] utilized a CA-Lattice Boltzmann (CALB) model. The model integrates various physical phenomena, such as melt pool dynamics, grain growth, and thermal effects, to accurately simulate the microstructure of Inconel 718 using the properties in

Ref. [138]. Fig. 10 shows the temperature field in the melt pool and grain structure during EBPBF. Lian et al. [111] utilized a 3D CA model combined with the finite volume method to predict the grain morphology of AlTiV during the EBPBF process. They found a columnar structure, growing upward and slightly tilted along the direction of the beam scan which is aligned with the temperature gradient. The simulation results are in agreement with experiments [107,139].

### 3.2.3. Phase-field model

The phase field model (PFM) is a key computational tool for predicting microstructural evolution and phase transformations in materials [140]. In melt-based AM, PFM can aid in optimizing processing conditions and improving the mechanical properties of refractory



**Fig. 10.** The temperature field and the resulting grain structure calculated using CALB model for Inconel 718 manufactured by EBPBF [117]. Color bar: (top) temperature in K and (bottom) grain misorientation with respect to the build direction. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

metals and alloys, enabling the design of high-performance materials tailored to specific needs [141–143]. Shah et al. [114] investigated the microstructural evolution of CoCrFeMnNbNiV MPEA during the LPBF process using PFM. They simulated the thermal cycles typical of the LPBF technique to predict how the alloy's microstructure would evolve. PFM revealed the formation of a sigma phase within the primary face-centered cubic phase, with elemental segregation where Cr and V concentrated in the sigma phase while Ni and Nb were depleted. Fig. 11 demonstrates the predicted microstructural changes through composition maps and virtual line scans after multiple thermal cycles. In another study, Sahoo et al. [112] utilized PFM to simulate the microstructure transformation of the AlTiV alloy during EBPBF. They focused on the effects of process parameters, such as beam power and scanning speed, on the formation and growth of dendritic structure. They found that by increasing the scan speed, the concentration of solute in the liquid region near the dendritic tips decreases. This is because higher scanning speeds lead to faster solidification rates, which results in less time for solute redistribution.

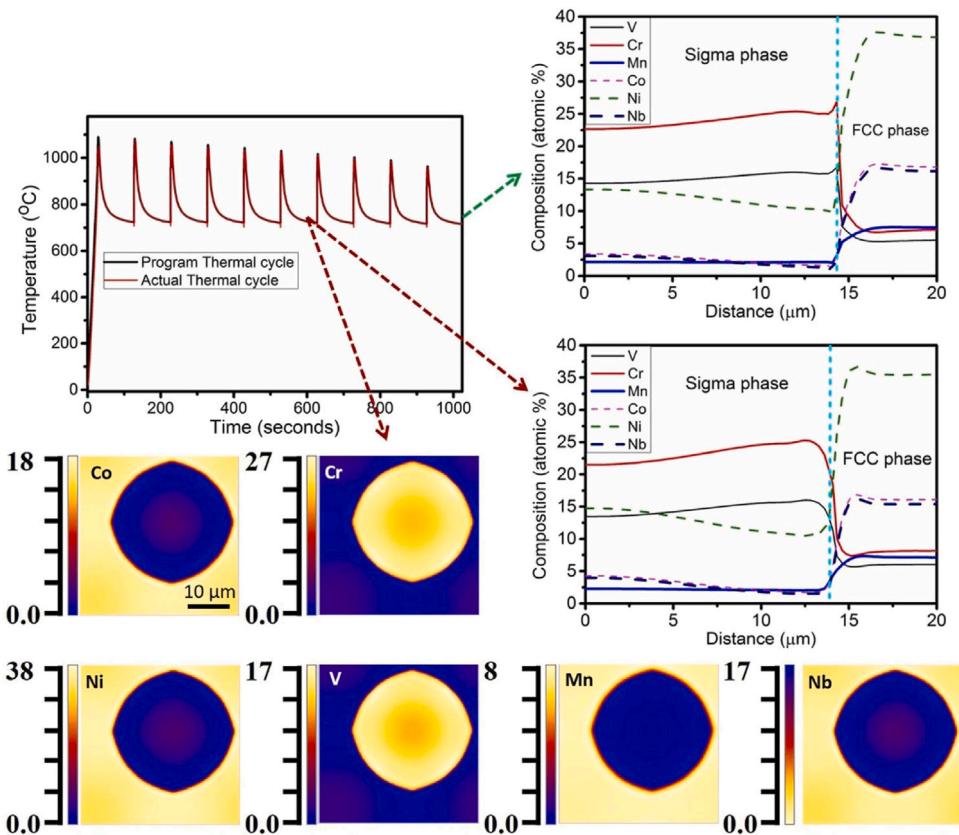
### 3.3. Macroscale

Computational fluid dynamics (CFD) simulations have been used to model melt pool dynamics and heat transfer at the macroscale in refractory metals and alloys. For example, Kaikai et al. [118] used a finite volume method in conjunction with a discrete element method to simulate PBF of Inconel 718. They found that the molten pool dynamics changed from random to uniform flow as the heat source approached, which is critical for optimizing layer deposition and minimizing defects. To investigate LPBF-fabricated MoNbTaW RMPEA's thermal-mechanical behavior, Zhang et al. [122] utilized both experimental methods and numerical simulations to study temperature distribution and thermal stresses. Using the finite element method (FEM), they revealed that the temperature field around the laser spot exhibited a high temperature gradient, reaching up to  $1.86 \times 10^4$  K mm<sup>-1</sup>, which significantly influenced the formation of the melt pool and the resultant microstructure

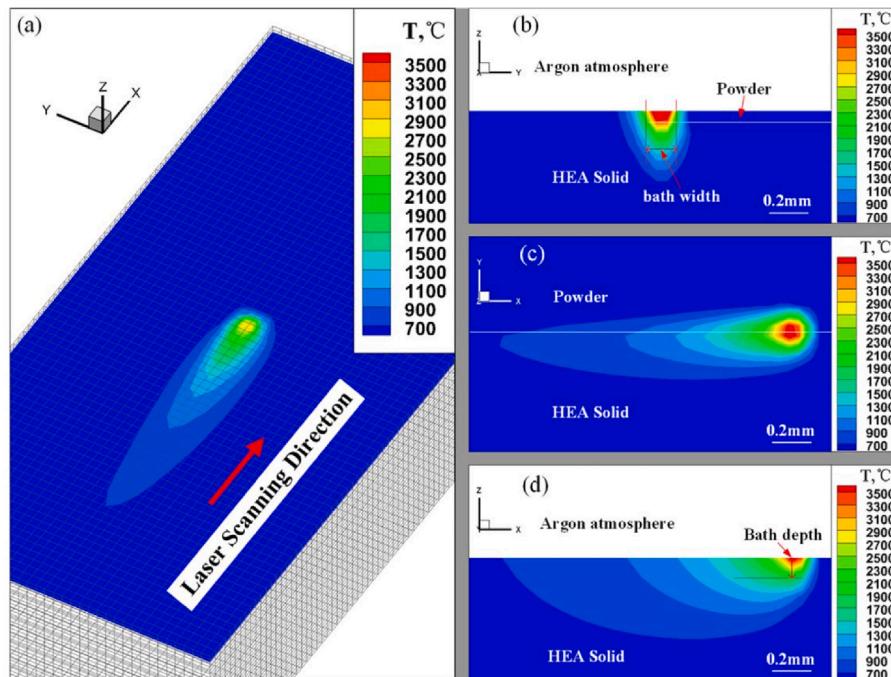
(Fig. 12). Thermal stresses caused by uneven temperature distribution led to cracking in the fabricated part. In another work, Li et al. [123] developed a 3D FEM model for commercial pure Ti powder to study the thermal behavior of EBPBF with different scanning speeds and/or laser powers. They showed that, as the laser beam proceeds along the scan tracks, the maximum temperature within the molten pool increases from 1929 °C to 2057 °C, while the pool size increases from 73.4 μm to 81.9 μm. Additionally, the minimum temperature in the powder bed rises significantly with subsequent laser passes, indicating an accumulation of heat that results in a hotter and larger molten pool.

### 3.4. Future research opportunities

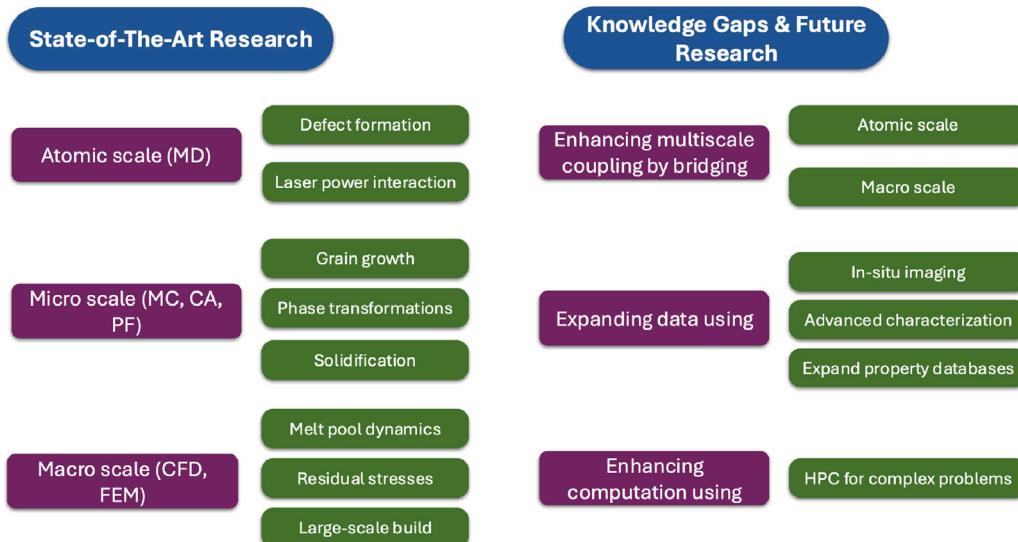
Advances in high-performance computing (HPC) are now making it possible to run more detailed simulations of solidification, defect formation, and residual stresses in MAM, allowing researchers to account for factors like anisotropic strain and complex phase interactions in ways not previously feasible [47,144]. Bridging simulations across atomic, micro, and macroscale levels is equally important, as phenomena at smaller scales can drastically affect the overall structure and properties of these high-temperature (HT) materials [124,126]. Coordinating outputs from MD with microstructural solvers (e.g., phase-field) and then feeding into larger-scale FEM or CFD calculations ensures that critical details — such as rapid cooling rates and directed solidification — should be neither overlooked nor over-simplified [125,129]. For instance, MD simulations can provide key material properties like melting point and diffusion rate, which are then used to inform solidification models at the microscale. These outputs help simulate how grains grow, how interfaces move, or how materials deform under thermal stress. Likewise, MD-derived data such as elastic constants and thermal conductivity can be fed into FEM models to improve predictions of residual stresses or crack formation in larger parts. Just as important is refining the constitutive models used to represent refractory materials. For many of these alloys, basic thermophysical



**Fig. 11.** PFM results of the AlTiV alloy produced by EBPBF: Composition maps and virtual line scan obtained for samples subjected to thermal cycle with a pre-heat temperature of 700 °C [114].



**Fig. 12.** Temperature distribution in microzone (4 mm × 2 mm × 1 mm) around laser spot for MoNbTaW RMPEA, resulting from a 3D FEM model [122]. (a) 3D view. (b) Longitudinal section perpendicular to the x-axis. (c) Top view. (d) Longitudinal section perpendicular to the y-axis.



**Fig. 13.** Summary of current and future directions in physics-based AM modeling for refractory metals and alloys.

data remain scarce, making it difficult to match simulation results with real-world outcomes [110,115,130,145]. Enhanced in-situ characterization and high-speed imaging techniques can provide the missing details, enabling more accurate calibration of models and a tighter feedback loop between theory and experiment [113,130]. Equally vital is establishing broader reproducibility: standardized test builds, inter-laboratory studies, and careful documentation of all processing parameters can help the community validate or refine new modeling approaches [91,99,114]. This consistency ensures that when different teams run the same simulations or experiments, their findings can be meaningfully compared, thereby accelerating the application of physics-based AM simulations for refractory metals and alloys [99, 114]. Finally, expanding property databases for high-melting-point materials is a crucial step for improving model fidelity and bridging experimental gaps [32,112]. By collecting a fuller range of data — covering everything from thermal conductivities to microstructural evolutions — researchers can push these physics-based models further, supporting more comprehensive, high-resolution studies without having to rely on hybrid approaches [32]. Fig. 13 demonstrates the conclusion of physics-driven AM modeling for refractory metals and alloys. It highlights state-of-the-art research in AM, focusing on multi-scale modeling, while identifying future needs like multi-scale coupling, advanced characterization, and expanded data use.

#### 4. Machine learning approaches: Data-driven and physics-informed

The application of the physics-based models discussed in Section 3 is limited to small parts due to their high computational costs and the inherent complexity of the AM process. To overcome these limitations, ML approaches are powerful tools for computationally efficient surrogate modeling of complex physical phenomena [146]. However, purely data-driven ML methods can suffer from overfitting, lack of interpretability, and failure to stick to physical laws [147]. To address these issues, physics-informed ML (PIML) incorporates physics knowledge into ML models, providing new possibilities to understand, predict, and control the complex thermal and microstructural phenomena in AM. The most common PIML approach leverages extensive datasets from both experiments and simulations to approximate partial differential equation (PDE) solutions, capture multi-scale dynamics, and accurately predict future states. These capabilities enhance material design and optimization in AM of refractory metals and alloys. Moreover, such predictive accuracy is crucial for enabling real-time monitoring and control during the AM process, minimizing defects [148,149]. Also,

recent advances in ML for melt-based MAM have been reviewed, particularly in the last five years, as summarized in Table 3. In this section, we explore how physics knowledge is integrated into ML models and discuss data-driven and PIML approaches applied to melt-based AM of refractory metals and alloys for overcoming challenges in thermal and microstructure evolution modeling, as well as process optimization.

##### 4.1. Integration of physics knowledge into ML

The integration of physics into ML models has greatly enhanced their accuracy and reliability in addressing complex physical systems [163]. PIML models achieve this by incorporating physics knowledge through three primary strategies, as Faegh et al. [164] divided: physics-based feature engineering, physics-based architecture shaping, and physics-based loss function modification. These strategies can be explained by the following four key steps that systematically embed physical knowledge into ML workflows [147]. First, physics-based feature engineering involves enriching input data with physical information or features derived from governing equations, empirical data, or hybrid methods [165]. This ensures that the data reflects real-world dynamics, enabling models to learn from a physics-informed dataset. Second, physics-based architecture shaping aligns model components and architectures with physical principles, such as physics-based activation functions or specialized layer structures in NNs [166]. For instance, Oommen et al. [167] utilized a U-Net architecture with temporal conditioning to combine direct numerical simulations with neural operators, efficiently simulating material evolution across spatial and temporal scales. Third, physics-based loss function modification incorporates physics-based constraints during training to penalize model predictions that violate physical laws [168–171]. For example, physics-informed NNs (PINNs) embed penalties for discrepancies in PDEs and boundary conditions into the loss function [162] as illustrated in Fig. 14. Lastly, output analysis is applied to ensure consistency with known physics. This foundation is particularly valuable in advancing PSP relationships and addressing challenges in AM [172].

Following these steps, extensive research has been conducted on HT alloys using PIML and related techniques to it on AM. For Inconel 718, studies have focused on a wide range of critical aspects, including the prediction of grain structure characteristics [173], defect reduction [174], optimal process design to minimize porosity [175], determination of optimal process parameters [176], prediction of density and defects [177], and comprehensive analysis of the PSP relationships for this material [178]. Similarly, research on Inconel 625 has

**Table 3**

A review of papers on ML in melt-based MAM in the last 5 years.

Year	Article	Emphasize
2020	[150]	Integrating ML with the PSP-performance paradigm to optimize alloy selection, process parameters, and microstructural predictions Application of Integrated Computational Materials Engineering approaches and DD methods to improve the understanding and control of AM processes.
2021	[147]	Proposes a framework for implementing PIML in manufacturing, Presents a roadmap for future research, emphasizing the need for collaboration and standards for PIML methodologies.
2021	[151]	Developing multiscale-multiphysics models and their surrogates for digital twins in MAM.
2021	[152]	Explores the integration of ML with LPBF in MAM, Provides a roadmap for future research, emphasizing applications of ML to improve efficiency and quality control in LPBF.
2021	[153]	Explores integration of metallurgy, mechanistic models, and ML in MAM, Highlights the potential of combining mechanistic models with ML to predict microstructures, defects, and mechanical properties.
2021	[154]	Explores data-driven models for predicting relationships between process parameters, microstructures, and mechanical properties without explicit equations, Focuses on modeling the PSP relationships and the advantages and disadvantages of physics-driven and data-driven modeling in MAM.
2022	[155]	Focuses on ML algorithms for defect detection in laser-based additive manufacturing.
2022	[156]	Explores the use of artificial intelligence and digital twins in MAM to transition from open-loop to closed-loop systems. Reviews applications of artificial intelligence in areas with a focus on achieving consistent quality in MAM parts.
2022	[157]	Focuses on the applications of CNNs in AM, addressing image, video, and acoustic signal data. Explores 3D CNNs for volumetric analysis and semantic segmentation for pixel-level defect detection in AM processes.
2022	[158]	Proposes a digital twin hierarchy for MAM with four levels of increasing complexity: Implicit, Instantiated, Interfaced, and Intelligent Digital Twins. Emphasizes the potential of reinforcement learning and deep reinforcement learning for developing intelligent control policies to optimize laser parameters, improve build quality, and reduce defects in real-time.
2023	[159]	Focuses on artificial intelligence into WAAM, Proposes future research directions, including the adoption of digital twins, human–robot collaboration, and imitation learning to enhance automation and control in WAAM.
2024	[160]	Focuses on applying ML to WAAM for addressing key challenges like porosity, deformation, and residual stresses, Identifies gaps in material analytics and Design for WAAM as underexplored areas requiring further research.
2025	[161]	Focuses on PIML in MAM, Suggests future research directions, including exploring Fourier Physics-Informed Neural Operators as a next-generation modeling approach for AM.

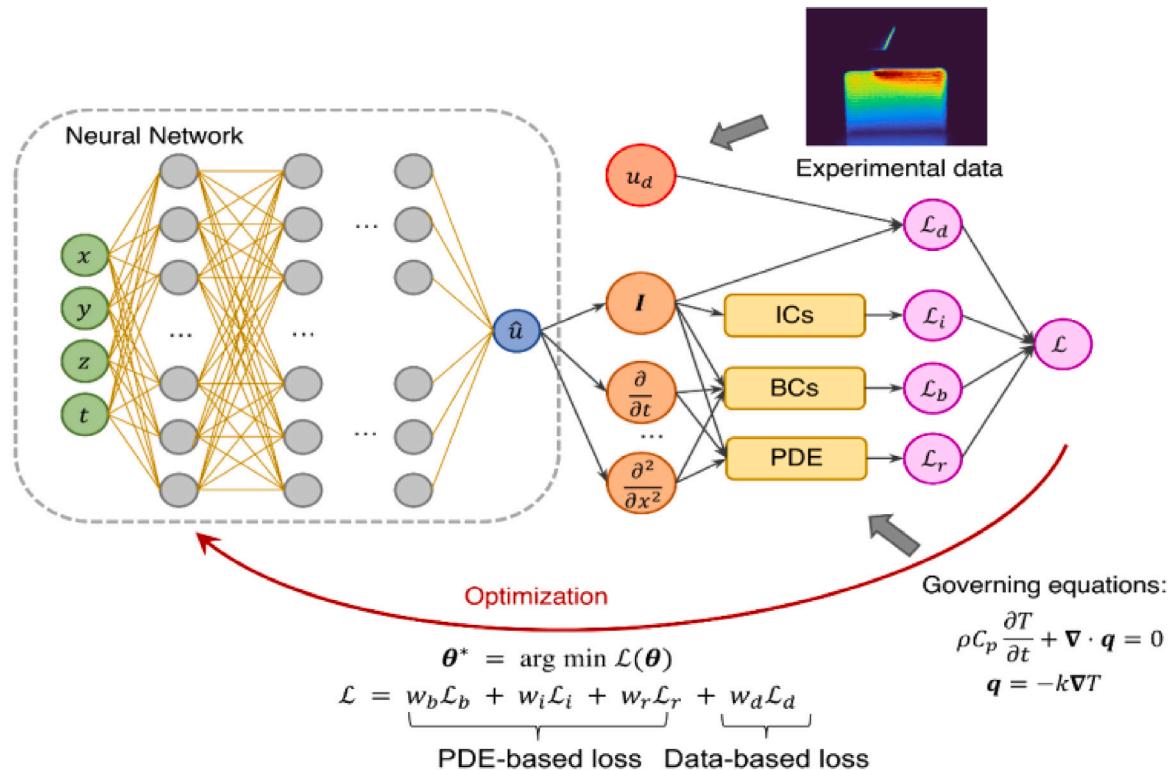


Fig. 14. Hybrid thermal modeling framework for AM based on PINNs [162].

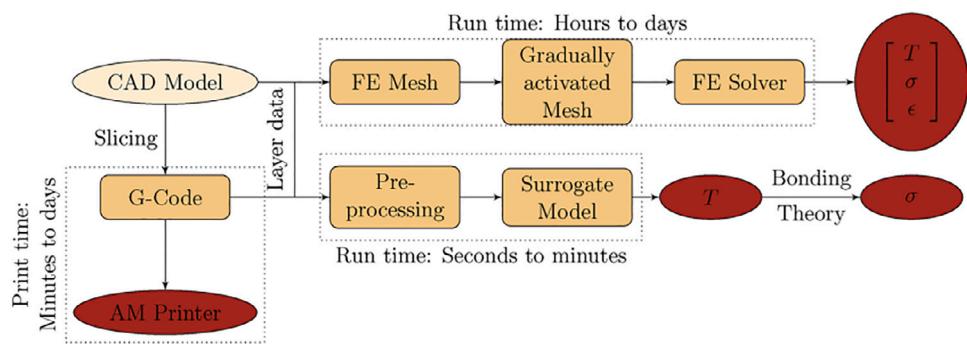


Fig. 15. Basic methodology for the surrogate model of any FEM study in AM [188].

emphasized predicting temperature distributions [179] and melt pool size [180]. Fatigue life has also been a significant focus, with studies examining AMed Hastelloy X under various conditions [181–183]. These investigations provide essential insights into the performance and durability of HT alloys in AM applications.

As mentioned, much research has been done in applying PIML into AM fabrication of HT alloys but not refractory materials, even though they share characteristics such as high melting point, thermal stability, and high strength. The reason is due to various challenges such as, data scarcity and quality [8], and complex PSP relationships [184]. Therefore, the success of PIML for HT alloys show the potential of PIML for understanding the PSP relationship in AM fabricated refractory metals and alloys.

#### 4.2. Thermal history and temperature profile

Refractory metals and alloys undergo complex thermal cycles during AM. These processes make them susceptible to the formation of defects [185]. Therefore, modeling thermal history is essential for optimizing the mechanical properties, dimensional accuracy, and overall performance of manufactured components [186,187].

To address the mentioned challenges, data-driven and PIML models have been developed to serve as surrogate models of physics-based models and speed up computations as illustrated in Fig. 15. Liao et al. [162] created a NN model that takes input as the spatio-temporal coordinates of a point and outputs the predicted temperature. For training, they applied sum of squares loss function to the error in initial conditions, boundary conditions, and PDE error. Such approach was used to solve the forward (thermal prediction) and backward (initial conditions) problems in thermal simulations of Ni-based alloys. Abedi et al. [189] developed NN models to predict transformation temperatures in NiTiHf alloys fabricated via LPBF. Their approach leveraged experimental data and optimized features such as laser power, speed, and heat treatments to improve accuracy, highlighting the potential of ML to refine thermal predictions and material design in AM. Zhu et al. [190] demonstrated the applicability of the penalized boundary condition approach for not only thermal but also pressure prediction in melt pool fluid dynamics in AM for multiple metallic materials. An alternative approach is the use of graph theory to approximate the expensive FEM for heat dissipation solutions [191] which has been demonstrated in laser-powder DED process of Ti-6Al-4V parts [192, 193].

#### 4.3. Microstructural evolution

Materials' microstructures consist of spatially distributed phases with different compositions or crystal structures, grains with varying orientations, domains characterized by distinct structural variants or polarizations, and various structural defects [194]. These features, typically ranging in size from nanometers to microns, are crucial in determining a material's physical properties [195]. Microstructural

evolution is influenced by external factors such as applied stress, temperature, electrical, and magnetic fields. Due to the coupled and non-linear nature of these phenomena, predicting microstructural evolution presents a significant challenge. Data-driven and PIML approaches are indispensable in studying the microstructural evolution of refractory metals and alloys, given their ability to analyze complex datasets and predict material behaviors under diverse conditions [196]. Kim et al. [197] demonstrated the use of Convolutional Neural Networks (CNNs)-based real-time monitoring in the Wire Arc Additive Manufacturing (WAAM) process for Mo, which aids in maintaining consistent deposition conditions by detecting process anomalies that influence microstructural uniformity.

Several data-driven and PIML methodologies have been proposed for efficient solutions of PFM in MAM, regardless of material. Xue et al. [193] integrated physics knowledge into a graph network to solve PFM efficiently in the LPBF process using 316L stainless steel. Grains were represented as graph nodes embedded with properties like temperature, grain orientation, and solidification fraction, while graph edges captured material attributes such as thermal conductivity. This approach effectively replaced traditional numerical methods by leveraging an NN equivalent for solving ordinary differential equations. Montes et al. [198] extract two-point statistics and their corresponding principal component analysis scores as low-dimensional representations of phase fields for a two-phase mixture undergoing spinodal decomposition in an unspecified material. The evolution of this representation is trained using a long short-term memory network whose input is the latest microstructure condition as well as the phase fraction and mobilities. Choi et al. [199] reduce the surrogate model complexity by working with only a limited region of interest, typically close to the power source during AM. They utilize the current grain structure map, temperature field, and future temperature field as inputs for a UNet to predict the future grain structure. This approach was demonstrated by printing stainless steel parts; however, it is limited by the requirement of full thermal history. In contrast, Riensche et al. [200] first predict the thermal history using a graph theory approach, then extract the thermal features to train a support vector machine classifier to predict melt pool depth in LPBF of Inconel 718.

#### 4.4. Process optimization

Process optimization in melt-based AM of refractory metals and alloys is crucial for enhancing material properties and minimizing defects. Achieving this requires a deep understanding of the complex interplay between process parameters, adjusting factors, material behavior, and resulting microstructures [201]. Wu et al. [202] employed a hybrid methodology combining DEM, CFD, and back propagation NNs (BPNN) as shown in Fig. 16 to optimize powder bed formation and molten track properties during LPBF of Mo. Their results demonstrated that careful adjustment of spreading velocity and gap height can significantly improve powder bed density and surface uniformity, directly influencing molten track performance.

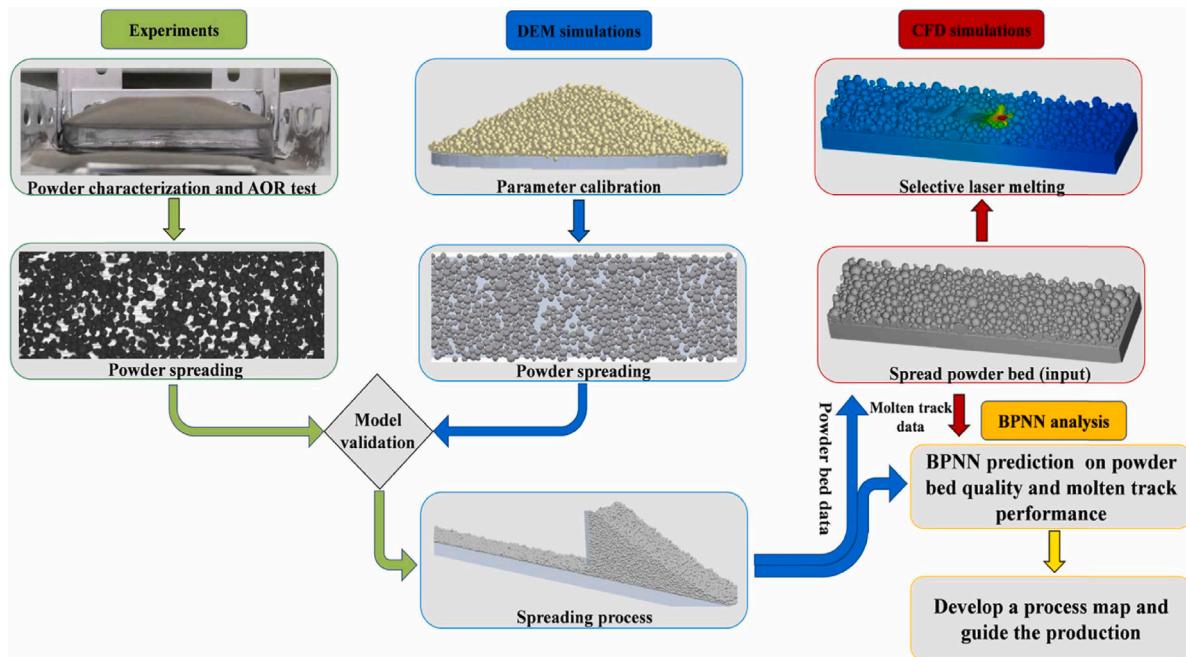


Fig. 16. Flowchart of process optimization by Wu et al. [202]. BPNN: back propagation neural network.

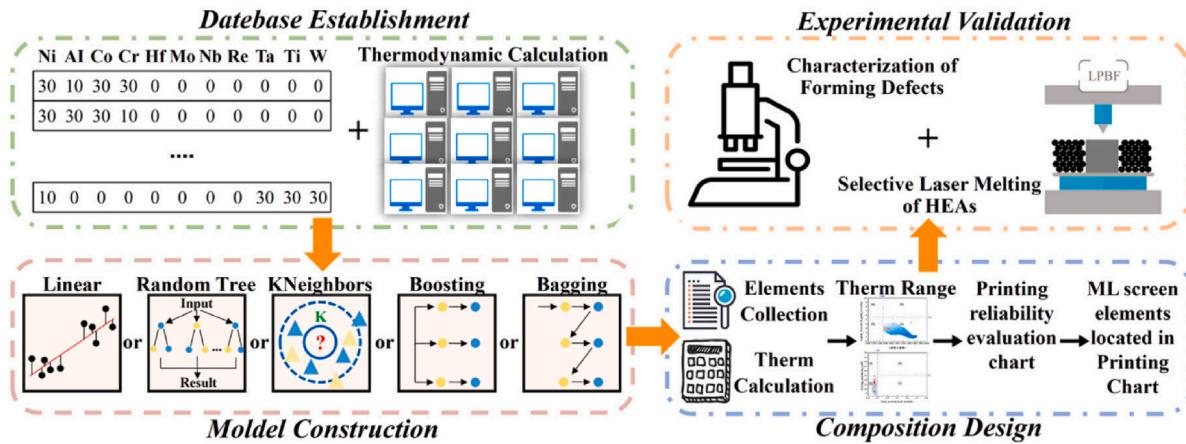


Fig. 17. ML framework for LPBF-MPEAs in [203], covering the creation of a thermodynamic database, selection of ML models, and choice of experimental components for validation.

Wang et al. [204] developed a process optimization model that considers uncertainties in the process such as fluctuations in powder properties and power absorption coefficients in EBPBF of Ti-6Al-4V. They model both the thermal history and microstructure evolution as a Gaussian process of low-dimensional representations of the field data. The uncertainties are evaluated through MC simulations during the parameter optimization process. To optimize the printability of MPEAs, Duan et al. [203] focuses on reducing defects that occur during solidification, as shown in Fig. 17. By predicting essential thermodynamic parameters such as liquid temperature range and liquid viscosity, their ensemble model identifies alloy compositions that minimize porosity and cracking. This allows for better filling during solidification and reduces thermal deformation, streamlining the design process for defect-resistant refractory alloys. Sun et al. [205] integrated ML with CALPHAD to design Nb-Ta-Ti-Zr RMPEA systems with targeted hardness. They created a comprehensive database of 100 quaternary alloys, trained the ML model, and verified predictions through experiments. Similarly, Buranich et al. [206] evaluate RMPEAs using ML to predict their thermal and mechanical properties, highlighting their

potential for AM and mechatronic applications. By identifying optimal compositions, such as HfNbTaTiW and CrHfNbTaW, the findings provide a valuable foundation for optimizing manufacturing processes to achieve superior performance in HT and mechanically demanding environments.

#### 4.5. ML-based interatomic potentials

Section 3.1 reviewed MD simulations for the metal AM process at the atomic-scale. The accuracy of MD simulations largely depends on the quality of the interatomic potentials (IAPs) used [207]. Unfortunately, most available IAPs are inadequate for accurately modeling refractory metals and alloys [208]. However, the recent advancements in ML-based IAPs [209–212], which offer near-density functional theory (DFT) accuracy at a fraction of the computational cost, present a promising opportunity for overcoming this limitation. To date, ML-based IAPs have been developed for many refractory metals and alloys,

including pure metals [213], binaries [214], and RMPEAs [215]. Defects in RMPEAs, which are prevalent in AM materials, have been extensively studied in recent years. Li et al. [216], Zheng et al. [217], Yin et al. [218], and Wang et al. [219] developed ML-based IAPs for several RMPEA systems including MoNbTaTi, MoNbTaW, and MoNbTaVW, and have conducted detailed research of effects of lattice distortion and chemical short-range order on dislocation glide. Byggmaster et al. [220] trained a Gaussian approximation potential and investigated multiple types of defects in MoNbTaVW RMPEA. More recently, several universal ML-based IAPs have been developed, covering dozens of chemical elements in the periodic table [221–223]. Also known as the foundation potentials, they can be fine-tuned for specific properties or material systems (e.g., refractory metals and alloys) [224]. Indeed, some of them have been applied to model defects such as vacancies, dislocations, and voids [225], which are potentially important for AM. To our best knowledge, no ML-based IAPs have been applied to AM of refractory metals and alloys. Nevertheless, there is no challenge in applying those potentials to AM in future work, as more powerful computers have enabled very large-scale MD simulations.

#### 4.6. Future research opportunities

In this section, the integration of ML with AM processes has been explored, particularly for refractory metals, alloys, and HT alloys [146, 147, 161]. Significant advancements in AM have enabled the fabrication and characterization of challenging refractory materials, as reviewed in Tables 1 and 2. These include Mo [51], Nb [56], Ta [61], W [21], and Re [23]. The studies highlight both challenges and opportunities in processing these materials, primarily due to their high melting points and unique properties. Significant advancements have been achieved, such as fabricating crack-free Mo with EB-PBF [51], processing Zr into near-net shape components using laser techniques [226], and producing high-purity Nb for superconducting applications [56].

ML techniques have further advanced research on refractory metals and alloys, offering powerful tools for optimizing their properties and accelerating material discovery as outlined in Table 4. For instance, Kedharnath et al. used ML to predict flow stress [227] and analyze dislocation velocity in Ta-W alloys [228]. Similarly as discussed in Section 4.3, ML has been effective in evaluating the microstructures of materials such as Mo [229] and Zr [230]. Interatomic potentials for Ti–Nb–Zr alloys now leads to run detailed simulations, showing how their elastic properties change with temperature, including predictions of near-constant modulus behavior (Elinvar effect) [231]. In HT NiTiHf shape memory alloys, ML-guided approaches have identified compositions with precise transformation temperatures and thermal properties [232]. Additionally, ML-driven methods have simplified the discovery of novel materials, such as Re-based systems, by providing accurate property predictions across vast chemical spaces while minimizing time and computational costs [233]. Finally, as mentioned in Section 4.1, although ML and PIML models offer powerful tools for modeling AM processes, further investigation is still needed, especially in the promising yet underexplored intersection of AM, ML, and refractory metals as highlighted in Fig. 18. However, there are still several challenges that need to be overcome to fully bridge this gap. To address these limitations, future research must tackle several critical challenges such as follows.

##### 4.6.1. Data scarcity and quality

Data scarcity and poor-quality datasets prevent the optimization of AM for refractory metals and alloys. Limited and inconsistent data on powder properties, thermal behavior, and mechanical performance reduce the accuracy of predictive models and process control [244]. This lack of standardized, high-quality datasets limits the integration of ML with AM for refractory materials, making it difficult to predict defects, optimize parameters, and ensure consistent material performance [8, 41, 245]. In future work, by establishing standardized

protocols for data collection, creating open-access datasets, and integrating in-situ monitoring systems such as knowledge-constrained clustering methods [246], researchers can enhance data fidelity and comparability. These improvements will enable the development of robust ML and PIML models, ultimately improving process optimization and reliability.

##### 4.6.2. Complex process-material interactions

Complex process-material interactions in AM of RMPEAs make it challenging to apply ML effectively. The nonlinear links between process parameters (like thermal gradients and melt pool behavior) and material changes (such as microstructural evolution and defect formation) complicate predictive modeling for refractory metals and alloys. Elemental segregation, residual stresses, and microstructural defects introduce additional variability, reducing the accuracy of ML-driven optimization [247–249]. In the future, by integrating multi-scale simulations with ML methods and employing active/reinforcement learning [8] to iteratively refine models, researchers can better capture and control these complex interactions. Targeted experiments, guided by physics-based feature engineering, can further enhance model fidelity and process consistency.

##### 4.6.3. Anisotropy and microstructural variability

Anisotropy, the directional dependence of material properties, and microstructural variability in AM of refractory metals and alloys, such as Nb [56] and Ta [250, 251], create challenges for consistent material performance. Layer-by-layer fabrication leads to uneven grain growth and directional properties, causing mechanical behavior to vary across different orientations. This variability makes it difficult for ML models to generalize predictions and accurately optimize process parameters for uniform quality [252]. Future researchers may better understand and quantify the microstructural variability in refractory metals by leveraging anisotropy-specific modeling techniques, such as ultrasonic testing combined with advanced anisotropy indices [253]. Implementing real-time scanning strategies, such as adaptive laser pathing and dynamic thermal control, helps mitigate directional grain growth and stabilize local microstructures during the additive process [253, 254]. Furthermore, integrating deep learning-based predictive frameworks optimized with genetic algorithms can significantly improve the accuracy of microstructure–property correlations [36, 255] and guide post-processing treatments [256], such as heat treatment or hot isostatic pressing, to homogenize anisotropic properties and enhance reliability.

## 5. Conclusions and perspectives

In recent years, AM has emerged as a transformative approach for fabricating refractory materials, enabling the creation of complex geometries with precision and offering real-time control over composition and microstructure. This paper provides a comprehensive review of melt-based AM methods, including PBF and DED, as applied to refractory metals and alloys. It explores experimental advancements, physics-based modeling efforts across scales (atomic to macroscale), and ML applications for optimizing process parameters, microstructure, and mechanical properties. The success of melt-based AM for refractory metals and alloys hinges on continued innovations in both experiments and modeling. By refining these elements, melt-based AM can more fully unlock the potential of refractory materials in high-performance, HT applications. The subsequent sections provide a detailed summary and perspective on experiments, physics-based models, and ML approaches, respectively.

**Table 4**

Summary of ML techniques in analyzing refractory metals and alloys.

ML(t)	ML Technique	Material/Alloy	Input data	Output data
Data-driven	XGBoost	TaW [228]	Experimental dataset with features: Vickers hardness, sintering temperature, W particle size	Predicted dislocation velocities, Importance ranking of influencing factors
Data-driven	Gradient boosting decision trees	W-Ni-Fe alloy [234]	Experimental parameters: Temperature, applied voltage, Electrolyte concentration, wire length	Predicted mechanical properties
Data-driven	Artificial neural network	W [235]	Experimental parameters	Predicted W tip curvature radius and aspect ratio
Data-driven	PINNs, XGBoost	TaW [227]	Experimental parameters: Temperature range, Strain rate, alloying content	Predicted flow stress
Data-driven	NN regression with bond-order potential	Ta [236]	DFT-generated dataset of supercells covering various atomic environments, Local structural descriptors	General-purpose interatomic potential, Predictions of physical properties
Data-driven	NN regression with bond-order potential	Re-based compounds [233]	DFT-generated dataset, Local structural descriptors	Predictions of physical properties
Data-driven	Random forest, Generative adversarial networks	U-10Mo alloy [229]	SEM images and features	Classification of microstructures
Data-driven	Multilayer perceptron Neural network	U-10Mo alloy [237]	Irradiation test parameters and post-irradiation experimental	Predicted thermal conductivity and identification of key factors affecting it
Data-driven	Moment tensor potential	Ti-Nb-Zr alloy [231]	DFT + special quasirandom structure for training and validation	Predicted elastic constants, Mechanical stability
Data-driven	XGBoost	Nb [238]	Process parameters, Microstructure characterization	Predicted mechanical properties
Data-driven	Support vector classifier, Elastic net regression	Al-Cr-Nb-Ti-V-Zr [239]	Experimental parameters, Physicochemical descriptors	Predicted ductility classification, Identification of optimal compositions
Data-driven	XGBoost	Ni-Nb alloy [240]	Analytical thermal model, Experimental morphology	Optimized printability map, Processing windows
PIML	Support vector machines, Random forest	Mo-Re alloy [241]	Experimental and simulated data	Predicted mechanical and electronic properties
PIML	Sequential deep learning NN, Random forest regressor	Mo-Re-W alloy [242]	First-principles DFT Data, Special quasirandom structure, Thermodynamic data	Predicted elastic constants, Thermal properties
PIML	Artificial neural network, Random forest	Nb-Ti-Zr alloy [243]	First-principles DFT calculations, Computed material descriptors	Predicted elastic constants, Classification of mechanically stable and unstable alloys, identification of optimal compositions
PIML	Spectral neighbor analysis potential	Mo-Re alloy [241]	DFT calculations for elastic properties, Special quasirandom structure, HT MD data	Predicted mechanical properties

### 5.1. Experiments

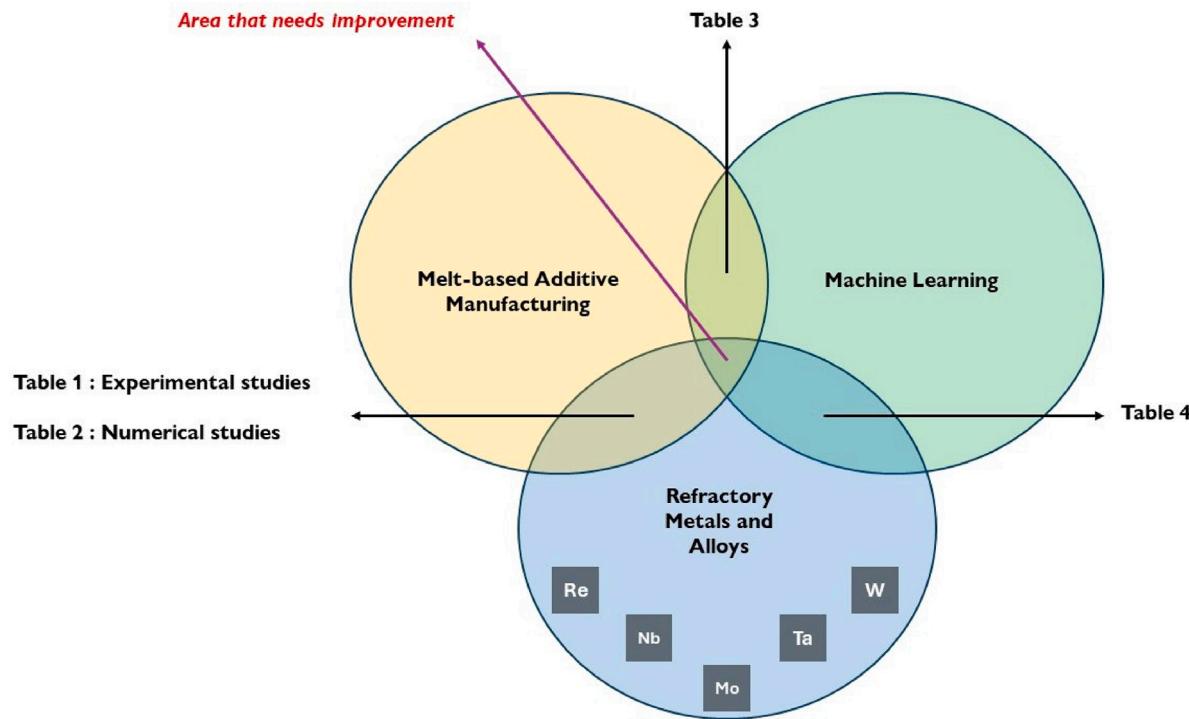
Significant advancements have been made in melt-based AM techniques for fabricating refractory metals and alloys. For example, much effort has been devoted to minimizing defects such as cracking and residual porosity, which are prevalent due to the high melting points and brittleness of refractory materials. Detailed studies on laser and electron beam processes reveal how parameters like scanning speed, beam power, and preheating influence microstructures, including grain size, texture, and phase distribution. For instance, tailoring these parameters has enabled the production of high-density RMPEAs with enhanced mechanical properties, including improved strength and ductility. Additionally, heat treatments and post-processing techniques have been found to mitigate thermal stresses and optimize microstructures.

Despite these successes, several issues persist that demand further research and process optimization. These include (i) cracking and distortion induced by steep thermal gradients, (ii) residual porosity linked to melt pool instabilities and the vaporization of certain alloying elements, (iii) sensitivity to impurities and high melting temperatures that restrict the permissible process window, and (iv) the ongoing challenge of achieving uniform microstructures, controlling phase formation, and ensuring reproducibility. Looking ahead, one critical step

is to strengthen real-time process monitoring and control. Future experimental work should emphasize the integration of advanced *in-situ* diagnostic techniques, such as high-resolution thermal imaging, high-speed synchrotron-based tomography, and real-time X-ray diffraction. Leveraging these tools will facilitate a deeper understanding of defect formation mechanisms, thermal dynamics, and microstructural evolution, ultimately guiding improved processing strategies and more effective validation of computational models.

### 5.2. Physics-based models

Physics-based models from atomic to macroscale have been developed to understand and optimize AM of refractory metals and alloys. At the atomic scale, MD simulations provide insights into atomic-level phenomena such as laser-powder interactions and defect formation, enabling predictions of material behavior under extreme conditions. At the microscale, MC, CA, and PFM simulate microstructural evolution, capturing grain growth, solidification, and phase transitions under varying processing conditions. These models have been applied to predict the effects of process parameters on thermal histories and microstructural features such as dendritic growth and defect distributions. At the macroscale, CFD and FEM simulate heat transfer, melt



**Fig. 18.** Summary of studies in three areas of melt-based AM, ML, and refractory metals and their subscriptions.

pool dynamics, and residual stresses, providing guidance for optimizing large-scale builds.

However, challenges such as computational costs, scale coupling, and incomplete understanding of material behavior highlight the need for further refinement and integration of these models. Parallel to the experimental innovations, researchers must refine multi-scale and multi-physics simulations to improve the understanding of how defects initiate and propagate, while also bridging insights from the atomic scale to bulk material behavior. Efforts to develop compositionally complex and RMPEAs should continue, as these systems can offer a broader range of HT capabilities and enhanced mechanical stability when processed via AM.

### 5.3. Machine learning approaches

PIML supplies a fast, physically consistent surrogate to traditional simulations: by embedding governing equations and boundary conditions into model features, architectures, or loss terms, it yields near-DFT accuracy for thermal histories, grain-scale evolution, defect prediction, and process-window optimization while avoiding the overfitting, poor transferability, and opacity that beset purely data-driven surrogates. ML-derived interatomic potentials further extend this capability to atomistic scales, underscoring the technique's value for rapid alloy screening and process design.

Yet several limitations still constrain regular use in melt-based AM of refractory metals and alloys. Scarce, heterogeneous, and sometimes noisy datasets hinder both model training and cross-laboratory validation; complex, nonlinear couplings between process parameters and evolving microstructures challenge generalization; directional grain growth and property anisotropy introduce additional predictive uncertainty; and physics-informed networks demand substantial computational resources and rigorously standardized metadata. Overcoming these hurdles will require coordinated data-generation protocols — shared test matrices, common metadata schemas, and routine release of raw and processed results — alongside open, version-controlled repositories. It also calls for tighter coupling of in-situ sensors (thermal cameras, X-ray, acoustics) with multi-fidelity simulations so models can

update on the fly, community benchmarks to track progress, and scalable cloud or HPC resources for training. Together, these measures will make future PIML frameworks both trustworthy and broadly applicable, paving the way for closed-loop, certifiable additive manufacturing of next-generation refractory alloys.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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