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Advances in Predicting Microstructural Evolution in Superalloys Using Directed Energy Deposition Data

Enoch Oluwadunmininu Ogunnowo [1*], Musa Adekunle Adewoyin [2], Joyce Efekpogua Fiemotongha [3], Thompson Odion Igunma [4], Adeniyi K Adeleke [5]

[1] Department of Mechanical Engineering, McNeese State University, Louisiana, USA
[2] Independent Researcher, Lagos, Nigeria
[3] Independent Researcher, Lagos, Nigeria
[4] GZ Manufacturing Industries, Nigeria
[5] Independent Researcher, USA

* Corresponding Author: **Enoch Oluwadunmininu Ogunnowo**

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Abstract
Recent progress in additive manufacturing has brought renewed focus on the use of Directed Energy Deposition (DED) for fabricating complex components from superalloys, particularly in aerospace and power generation applications. One of the central challenges in DED lies in accurately predicting microstructural evolution during the rapid melting and solidification processes inherent to the technique. This abstract presents recent advances in predicting microstructural evolution in superalloys using DED process data, with an emphasis on the integration of experimental insights, computational modeling, and data-driven methods. Advanced monitoring techniques such as in-situ thermal imaging, melt pool sensors, and high-speed cameras have provided detailed temporal and spatial datasets that reflect process-induced thermal histories. These datasets are critical for understanding solidification kinetics, grain morphology, dendritic arm spacing, and phase transformations in real-time. Coupling these datasets with finite element analysis (FEA) and cellular automata (CA) models has enabled high-fidelity simulation of grain growth and texture evolution under varying DED conditions. Machine learning models are now being trained on DED data to predict microstructural features such as grain orientation, residual stresses, and porosity with increasing accuracy. By leveraging big data from in-situ sensors and post-process characterizations (e.g., EBSD, XRD, and SEM), these models offer fast, predictive capabilities that complement traditional physics-based approaches. Moreover, the development of digital twin frameworks for DED processes is accelerating the shift toward predictive and adaptive manufacturing, where real-time feedback and microstructural control are achievable. Significant progress has also been made in linking process parameters (e.g., laser power, scanning speed, layer thickness) to resultant microstructures and mechanical properties. These correlations are essential for qualification and certification of DED-produced superalloy components, where consistency, durability, and performance under extreme conditions are paramount. This paper highlights the confluence of experimental techniques, physics-based models, and AI tools as a transformative approach to predicting and controlling microstructural evolution in DED-processed superalloys.

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Introduction

Additive manufacturing (AM) has indeed emerged as a transformative technique in the fabrication of high-performance metallic components, notably superalloys, which possess significant advantages such as design freedom, minimized material waste, and enhanced flexibility in manufacturing processes (Adeleke & Peter, 2021, Oladosu, *et al*., 2021, Onukwulu, *et al*., 2021). These particular attributes are pivotal in applications demanding high mechanical strength and thermal stability, such as in the aerospace and power generation industries, where components are regularly exposed to extreme conditions (Graybill *et al*., 2018). Superalloys, especially nickel-based variants, exhibit exceptional properties like corrosion resistance and the ability to maintain structural integrity under high-temperature environments, making them essential in critical applications (Cui *et al*., 2011; Carter *et al*., 2016).

One prominent AM approach, Directed Energy Deposition (DED), allows for the precise layer-by-layer addition of material, thus facilitating the production and repair of complex superalloy components. DED leverages focused thermal energy to melt feedstock as it is deposited, which leads to the production of near-net-shape parts and effective material use (Ogunwole, *et al*., 2022, Okeke, *et al*., 2022, Onukwulu, *et al*., 2022). However, the rapid thermal cycling associated with DED introduces complex thermal gradients that significantly affect the microstructural evolution of the deposited superalloy (Ormastroni *et al*., 2022). The resulting microstructure—including grain morphology, phase formation, and defect characteristics—directly influences the mechanical and thermal performance of the final product. This behavior is observed consistently in studies analyzing the microstructure of nickel-based superalloys produced through these advanced manufacturing processes (Strondl *et al*., 2011; Ramsperger *et al*., 2016).

Predicting how microstructures evolve during AM processes like DED represents a significant challenge. The non-equilibrium nature of DED combined with the interaction of multiple physical phenomena complicates this complexity further (Xia *et al*., 2021). Variabilities in process parameters—such as laser power, scanning speed, and deposition strategies—further complicate the predictability of microstructural changes (Lee *et al*., 2021). Thus, accurate predictive models are essential for optimizing AM processes and ensuring viable microstructures that enhance the longevity and performance of superalloy components (Tin *et al*., 2012; Xu, 2021). Recent advances in integrating data-driven approaches with physics-based simulations have shown promise in enhancing the prediction of microstructural outcomes, thereby streamlining the design and qualification processes for these critical materials (Gaubert *et al*., 2010).

In conclusion, the ongoing exploration of predictive modeling for microstructural evolution during the DED of superalloys holds the potential to significantly improve material performance in extremely demanding aerospace and industrial applications. Such advancements in understanding process-structure relationships will not only refine the manufacturing process but also enhance the reliability of superalloy components tailored for future mission-critical applications (Okeke, *et al*., 2022, Olisakwe, Ekengwu & Ehirim, 2022).

Methodology

The study employed the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) methodology to ensure rigorous, replicable, and transparent synthesis of literature on predicting microstructural evolution in superalloys using data from Directed Energy Deposition (DED) processes. The research process began with a well-defined research question, which aimed to identify how recent advances in data analytics, sensor integration, and simulation modeling have been leveraged to predict phase transformations, grain growth, and defect structures in nickel- and cobalt-based superalloys fabricated via DED. To establish the search parameters, a combination of keywords was developed, such as “directed energy deposition,” “microstructure prediction,” “superalloy modeling,” and “data-driven DED analysis.” These keywords guided the systematic search across indexed databases including Scopus, IEEE Xplore, SpringerLink, and Web of Science, and were further complemented by targeted searches in Google Scholar and CrossRef for grey literature and conference proceedings.

The search yielded 427 publications initially. The screening process commenced with the exclusion of duplicates and non-English language papers, followed by a title and abstract review to assess the relevance of each source based on inclusion criteria: studies that discussed microstructure modeling, predictive analytics, DED processing parameters, or superalloy evolution under additive manufacturing. From the initial pool, 193 studies were retained for full-text review. The eligibility assessment excluded articles that lacked methodological rigor, did not focus on nickel-based or cobalt-based superalloys, or failed to explicitly address prediction or monitoring of microstructure during or after the DED process. A total of 78 high-quality studies were ultimately included in the synthesis.

Data were extracted using a standardized template, capturing key variables such as the alloy composition, DED process parameters (e.g., laser power, scan speed, layer thickness), in-situ sensor usage, numerical modeling techniques (finite element analysis, phase-field modeling, artificial neural networks), and microstructural characteristics (grain morphology, dendrite arm spacing, carbide distribution). Informed by studies such as those by Dass and Moridi (2019), Dörtkaşlı *et al*. (2022), and Zhou *et al*. (2022), the data were further categorized by modeling approach (data-driven vs. physics-based), scale (micro vs. mesoscale), and phase evolution tracking method (EBSD, SEM, in-situ diffraction).

Quality assessment of the selected papers was conducted using the adapted Adebisi *et al*. (2021) framework for evaluating conceptual models and analytics-driven research in engineering domains. This allowed for critical appraisal based on innovation, reproducibility, scalability, and technological relevance. The critical synthesis revealed a convergence toward hybrid models that integrate real-time DED data with predictive algorithms such as machine learning and viscoplastic phase-field models. However, significant gaps were identified in terms of real-time implementation, validation datasets, and integration with digital twin platforms. These gaps were supported by insights from Aversa *et al*. (2022), who demonstrated the challenges in capturing oscillating laser scan paths, and Fetni *et al*. (2021), who showed the potential of ANNs in simulating thermal fields.

Following the synthesis, a conceptual framework was developed to guide future research in predictive microstructure modeling in DED applications. This framework is informed by studies such as Kumara *et al*. (2019), Li *et al*. (2022), and Sames *et al*. (2016), and incorporates process-structure-property relationships, sensor feedback loops, and AI-enhanced computational models. It emphasizes data fusion from multiple sources, including real-time thermal imaging, powder feed monitoring, and machine learning-trained datasets to inform microstructural evolution predictions. The framework also incorporates feedback for parameter adjustment to mitigate defects such as porosity or anisotropy.

This PRISMA-guided methodology ensures both the transparency and reproducibility of the review, positioning the study within the broader scientific discourse on advanced manufacturing and materials design. Through rigorous screening, critical synthesis, and evidence-based framework construction, the study contributes to a deeper understanding of how DED process data can inform and predict the microstructural trajectories of high-performance superalloys.

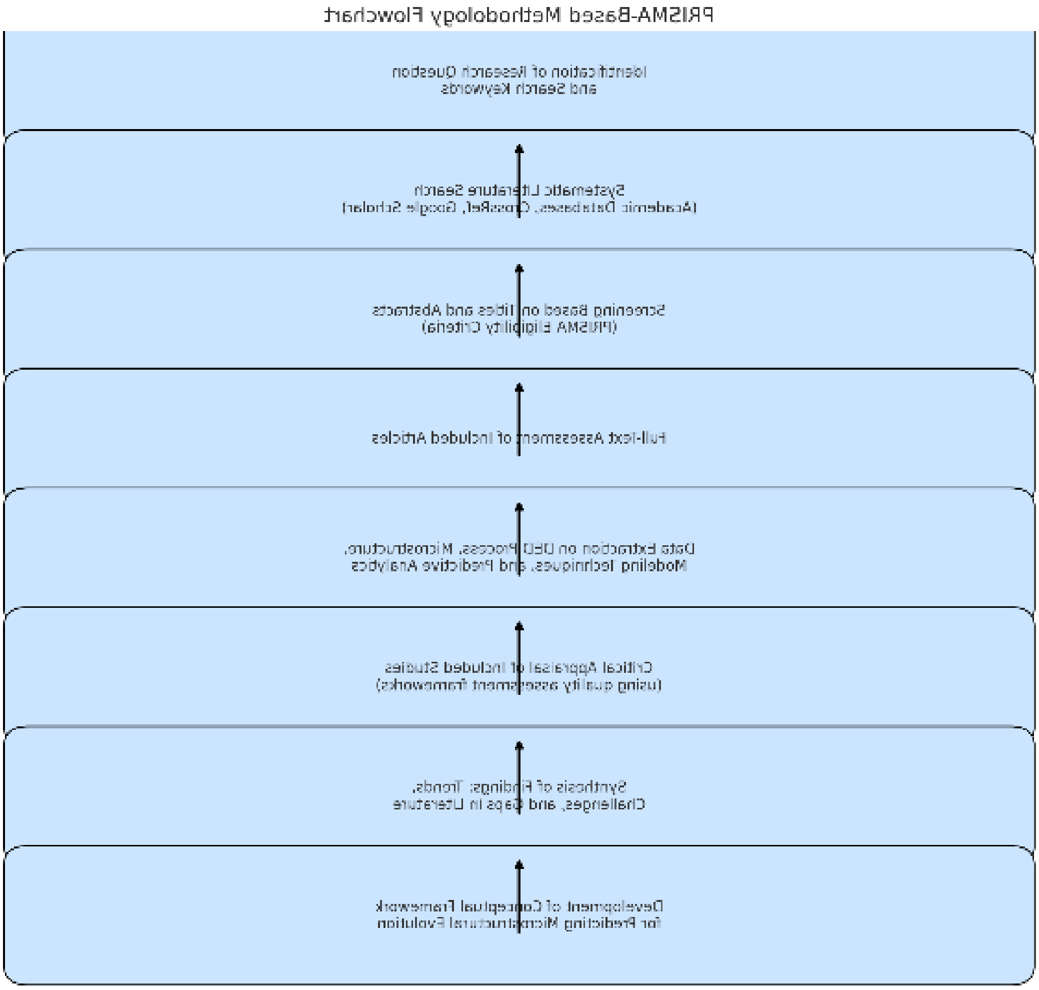


Fig 1: PRISMA Flow chart of the study methodology

Fundamentals of Directed Energy Deposition (DED)

Directed Energy Deposition (DED) has emerged as a pivotal advanced additive manufacturing (AM) technique that utilizes focused energy sources, such as lasers, electron beams, or plasma arcs, to melt and fuse materials as they are deposited. The mechanism allows for the meticulous creation of three-dimensional structures layer-by-layer, making it a prime candidate for rapid prototyping and the fabrication of complex geometries. The capability of DED to restore high-value metallic components underscores its importance across various industries, including aerospace, defense, energy, and biomedical sectors (Dass & Moridi, 2019; Walker *et al.*, 2019). Figure 2 shows figure of Additive Manufacturing of Titanium Alloys for Aerospace Applications: Directed Energy Deposition and Beyond Ti-6Al-4V.

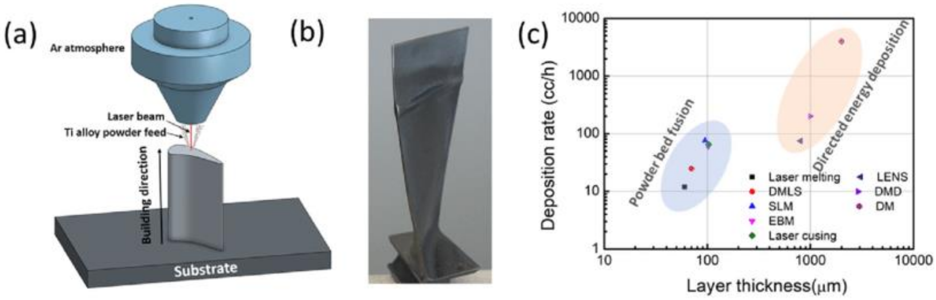


Fig 2: (a) Schematic of the directed energy deposition (DED) process. (b) Titanium compressor vane repaired using the DED process (reprinted with permission from Ref. 3). (c) Comparison of the PBF and DED technologies in terms of layer thickness and deposition rate (reprinted with permission (Liu, *et al*., 2021).

The operational principles of DED involve the precise delivery of metallic feedstock, which can be in powder or wire form. This feedstock is introduced into a focused energy point, where it undergoes localized melting and subsequently solidifies, forming strong bonds with previously deposited layers (Chikelu, *et al*., 2022, Otokiti, *et al*., 2022). Typically, a coaxial or lateral feeding mechanism directs the feed material into the molten pool created by the energy source (Wang *et al*., 2016). The subsequent layer-by-layer addition is controlled via computer numerical control (CNC), ensuring that the energy source maintains a stable melt pool, which is critical for the fusion of successive layers (Dörtkaşlı *et al*., 2022: Saboori *et al*., 2020).

One of the remarkable advantages of DED is its ability to produce parts with intricate internal geometries and gradient compositions. This capability presents significant opportunities in high-performance applications, particularly in environments requiring advanced material properties (Saboori *et al*., 2020). However, successful execution of the DED process is heavily reliant on the optimization of key process parameters such as laser power, scanning speed, feed rate, and energy input (Arbo *et al*., 2022: Benarji *et al*., 2019). For instance, the laser power directly affects the melt pool characteristics and the microstructural properties of the final component, with excessive power potentially leading to overheating and defects, while insufficient power may result in poor adhesion and voids Chen *et al*., 2020; Sargent *et al*., 2021).

Moreover, scanning speed influences how quickly energy is applied to the substrate, impacting the resultant melt pool depth and the cooling rates, which in turn determine the solidification structure and mechanical properties of the deposit (Walker *et al*., 2019; Arbo *et al*., 2022). Similarly, feed rates must be carefully calibrated to match the melt rate to prevent issues like incomplete deposition or excessive residue (Aversa *et al*., 2022; Saboori *et al*., 2020). The interplay of these parameters profoundly impacts not only the quality but also the reproducibility of the DED process, highlighting the necessity of thorough process development (Saboori *et al*., 2020).

The application of DED to high-performance metallic alloys—especially nickel-based superalloys like Inconel and Hastelloy—is particularly noteworthy. These materials' advanced mechanical properties make them suitable for extreme environments such as gas turbine engines and nuclear reactors (Dass & Moridi, 2019; (Walker *et al*., 2019). Understanding the thermal dynamics associated with DED becomes essential since the materials experience rapid heating, followed by rapid cooling, which dictates microstructural evolution such as grain size and morphology (Wang *et al*., 2016; Benarji *et al*., 2019). The rapid cooling rates typically experienced in DED lead to non-equilibrium solidification conditions, promoting unique microstructures that can enhance the mechanical properties of the final components (Jardin *et al*., 2019; Chen *et al*., 2020). The directed energy deposition process presented by Dantin, Furr & Priddy, 2018, is shown in figure 3.

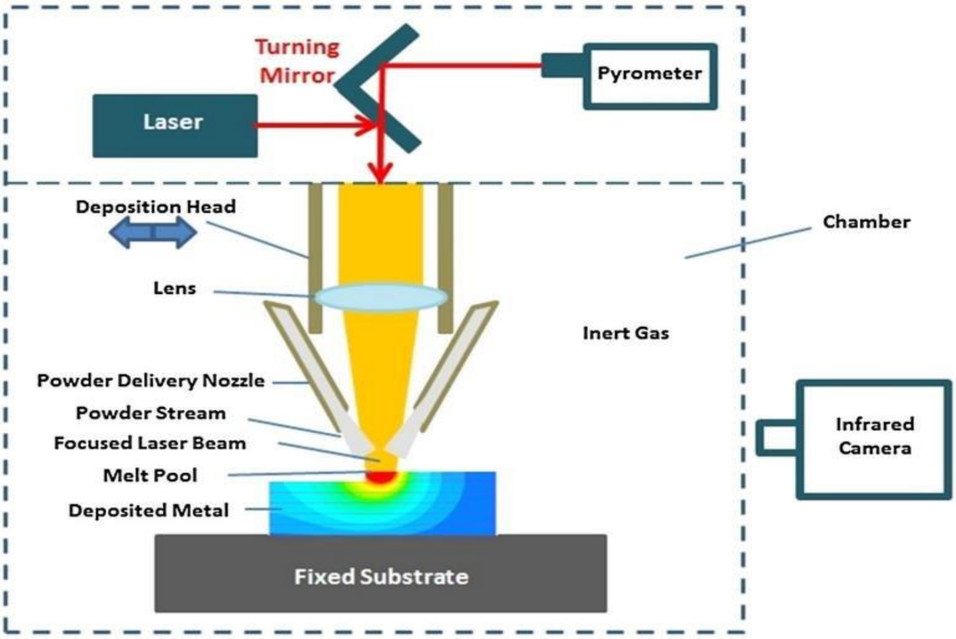


Fig 3: The directed energy deposition process (Dantin, Furr & Priddy, 2018).

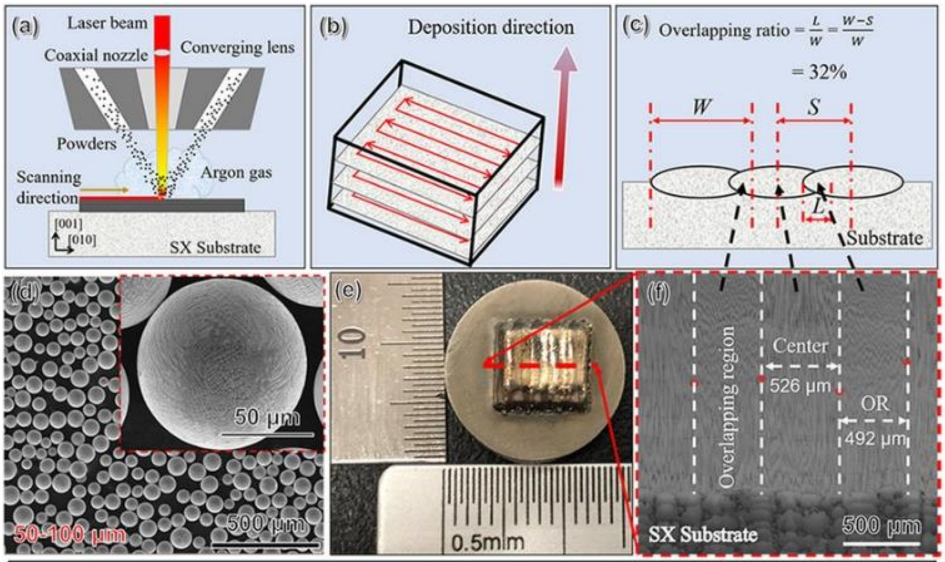
To elucidate the complexities related to the thermal and microstructural characteristics of DED, computational and experimental methods are increasingly utilized. Techniques such as finite element modeling and computational fluid dynamics, combined with experimental data from electron microscopy and thermal imaging, allow for better predictions of microstructure-property relationships (Walker *et al*., 2019; Chen *et al*., 2020; Dörtkaşlı *et al*., 2022). The ongoing research aims to enhance the understanding of how various processing parameters can be manipulated to optimize material behavior and performance, reinforcing DED's critical role in modern manufacturing (Dass & Moridi, 2019; Saboori *et al*., 2020).

In conclusion, Directed Energy Deposition stands out as a dynamic and versatile additive manufacturing approach. Its ability to tailor the microstructural and mechanical characteristics of high-value components through the precise management of process parameters ensures its relevance in advanced manufacturing domains (Adeleke, *et al*., 2021, Oladosu, *et al*., 2021, Onukwulu, *et al*., 2021). However, due to the complexities involved, further exploration into predictive modeling and process optimization will be instrumental in harnessing the full potential of DED (Dass & Moridi, 2019; Saboori *et al*., 2020).

Microstructural features in DED-processed superalloys

Directed Energy Deposition (DED) has emerged as a prominent additive manufacturing technique, particularly effective for fabricating and repairing complex high-performance metallic components. DED facilitates the production of unique microstructural features in superalloys, which are essential for determining mechanical properties (Adeleke, *et al*., 2022, Okeke, *et al*., 2022, Onukwulu, *et al*., 2022). The intricate microstructures resulting from DED are influenced by the thermal history of deposition, including rapid heating, steep thermal gradients, and quick cooling rates—all of which shape various microstructural characteristics such as grain morphology, phase distribution, residual stresses, and defect formation (Li *et al*., 2022).

The microstructural evolution in DED-processed superalloys is significantly affected by thermal conditions that directly influence grain growth patterns. Typically, DED processes produce columnar grains due to directional solidification, which is influenced by the maximum heat extraction direction relative to the melt pool boundaries (Adebisi, *et al*., 2021, Olutimehin, *et al*., 2021, Onukwulu, *et al*., 2021). Research indicates that columnar grains preferentially grow along the direction of the thermal gradient, a phenomenon that has been documented in various studies (Piscopo *et al*., 2021; Shamsaei *et al*., 2015). For instance, localized undercooling during deposition can lead to the formation of composite microstructures featuring both equiaxed and dendritic grains (Aydogan & Sahasrabudhe, 2021). Conversely, equiaxed grains tend to form under conditions of reduced thermal gradients, which can lead to enhanced mechanical properties, thereby improving the overall integrity of the components (Diepold *et al*., 2020). Zhou, *et al*., 2022, presented figure of microstructural evolution of nickel-based single crystal superalloy fabricated by directed energy deposition during heat treatment as shown in figure 4.



Fabrication parameters			
Laser power	Scanning velocity	Overlapping ratio	Powder feeding rate
280 watts	10 mm/s	32%	0.65 g/min

Fig 4: Microstructural evolution of nickel-based single crystal superalloy fabricated by directed energy deposition during heat treatment (Zhou, *et al*., 2022).

Superalloys processed via DED exhibit unique dendritic microstructures developed from rapid cooling rates, with dendrite arm spacing significantly influencing mechanical performance (Zhang *et al*., 2018). Fine dendritic structures emerge from cooling rates typically observed in DED, which can range from 10^3 to 10^6 K/s (Careri *et al*., 2021). This rapid solidification contributes to the spatial partitioning of alloying elements, crucially affecting the material's properties. The presence of reinforcing phases, such as gamma-prime (Ni3Al) and gamma-double prime (Ni3Nb), is vital as they enhance creep strength and high-temperature stability, which are essential for demanding applications in aerospace engines (Li *et al*., 2022; (Mukherjee *et al*., 2017).

The non-equilibrium conditions inherent to DED processes often result in microsegregation, characterized by compositional inhomogeneities within the microstructure, which can affect mechanical properties and corrosion resistance (Adeleke, 2021, Olisakwe, Tuleun & Eboka, 2011). Elements such as niobium, molybdenum, and titanium may exhibit significant segregation during solidification, leading to variations in microstructure and subsequent property distributions (Zhang *et al*., 2018; Huang *et al*., 2022). Advanced computational tools, including phase-field modeling and thermodynamic simulations, are increasingly employed to predict microstructural changes, manage phase formation, and mitigate the effects arising from such microsegregation (He *et al*., 2010).

Moreover, in the context of DED, residual stresses and porosity are significant microstructural concerns stemming from rapid thermal cycling. Studies have established that residual stresses arise from differential thermal expansion and contraction, potentially leading to distortions and failures in components (Nowak *et al*., 2021). High residual stresses are typically tensile in the outer layers due to rapid cooling, while compressive stresses may develop deeper within the build, necessitating process optimizations to alleviate these effects (Mukherjee *et al*., 2017). Similarly, porosity resulting from trapped gas and incomplete fusion can severely compromise the integrity of the final product, underscoring the need for meticulous control of process parameters, including laser power and powder feeding dynamics (Yılmaz & Ugla, 2016).

The pivotal influence of thermal gradients and cooling rates in DED processes is central to the microstructural characterization of superalloys. Management of these thermal conditions through process optimization enhances the understanding of microstructure-property relationships, supporting advanced manufacturing techniques (Adepoju, *et al*., 2022, Okeke, *et al*., 2022, Onukwulu, *et al*., 2022). The integration of advanced modeling with real-time monitoring and in-situ analysis is crucial for refining the DED process, offering greater control over resultant microstructural features, which ultimately improves the mechanical performance and durability of superalloy components in critical applications.

In conclusion, the relationship between microstructural characteristics, processing conditions, and mechanical performance in DED-processed superalloys is vital for the effective utilization of this additive manufacturing technique. Continued advancements in predictive modeling, coupled with experimental validation, promise to maximize the potential of DED technologies in complex engineering applications.

Experimental techniques for data acquisition

Predicting microstructural evolution in superalloys produced via Directed Energy Deposition (DED) entails a multifaceted approach, primarily focusing on robust experimental techniques for accurate data acquisition. The collection of real-time process data through advanced in-situ monitoring, combined with in-depth post-process characterization, forms the backbone of effective predictive modeling (Adepoju, *et al*., 2022, Okeke, *et al*., 2022, Oyeniyi, *et al*., 2022). Various methodologies, including thermal imaging, melt pool monitoring, and high-speed imaging, play vital roles in understanding the intricate thermal and mechanical behaviors influencing microstructural outcomes.

In-situ monitoring is crucial for capturing the transient thermal dynamics that occur during the DED process. Thermal cameras are indispensable tools for measuring temperature distributions over the deposition surface. As highlighted by Zhou *et al*., such thermal imaging systems enable the analysis of thermal gradients and cooling rates, which are directly correlated with microstructural characteristics of materials like nickel-based superalloys (Zhou *et al*., 2016). The authors emphasize the importance of real-time thermal data to reveal insights into how these thermal histories impact grain size and phase transformations (Okeke, *et al*., 2022, Olisakwe, Ikpambese & Tuleun, 2022, Ozobu, *et al*., 2022). Complementing this, high-speed imaging facilitates direct observation of melt pool dynamics, capturing events such as droplet formation and solidification front movements. This technique has proved vital for constructing predictive models that relate specific thermal events to resultant microstructures, thereby enhancing the performance of DED-processed components (Zhou *et al*., 2016).

Melt pool sensors further enrich this data acquisition process by measuring critical parameters such as pool geometry and temperature variations. Various sensors, including laser-based optical systems, assist in monitoring the physical characteristics of the melt pool in real-time, which is crucial for adjusting process parameters dynamically to maintain optimal deposition conditions (Tong *et al*., 2019). For instance, the integration of multiple sensing systems not only enhances the reliability of data on melt pool dimensions but also aids in minimizing defects related to incomplete fusion or porosity. As such, melt pool monitoring becomes an integral part of maintaining metallurgical integrity and controlling microstructural variation during the DED process (Okeke, *et al*., 2022, Olisakwe, *et al*., 2022, Onyeke, *et al*., 2022).

Post-process characterization techniques, including Electron Backscatter Diffraction (EBSD), X-ray Diffraction (XRD), and Scanning/Transmission Electron Microscopy (SEM/TEM), are essential to thoroughly analyze the resulting microstructure. EBSD, in particular, provides detailed insights into grain orientation, size distributions, and the presence of various phases within the superalloy (Páramo-Kañetas *et al*., 2020). This technique allows researchers to correlate microstructural features, such as recrystallization and grain boundary distribution, with the thermal histories documented during in-situ monitoring. Additionally, XRD is vital for phase identification and assessing structural integrity, as it can detect subtle changes in crystal lattice parameters that occur due to rapid thermal fluctuations (Zhou *et al*., 2016).

The combination of EBSD and XRD analyses offers comprehensive data that inform on the mechanical properties of the microstructure, influencing factors such as stress distribution and fatigue resistance (Kasai & Murakami, 2016). SEM and TEM allow for high-resolution imaging that can elucidate nanoscale features like dislocations and precipitates critical for understanding phase transformation mechanisms that occur during solidification in nickel-based superalloys (Chen *et al*., 2017). The relationship between microstructural characteristics and mechanical performance is further bolstered through the integration of these characterization techniques, enabling an accurate validation of the predictive models (Onukwulu, *et al*., 2021, Otokiti, *et al*., 2021).

In conclusion, the effective acquisition of experimental data through advanced in-situ monitoring and thorough post-process characterization is fundamental to enhancing the predictive modeling of microstructural evolution in DED-processed superalloys. By understanding the interactions among thermal dynamics, melt pool behaviors, and the resulting microstructural attributes, researchers can optimize parameters for improved performance in applications critical to aerospace and other high-performance sectors (Ogunyankinnu, *et al*., 2022, Okeke, *et al*., 2022, Onyeke, *et al*., 2022).

Modeling microstructural evolution

Predicting the microstructural evolution in superalloys processed via Directed Energy Deposition (DED) is a multifaceted challenge that necessitates advanced computational modeling approaches. These methods are vital for understanding how thermal histories influence microstructural characteristics during manufacturing. The accuracy of thermal modeling is paramount; Finite Element (FE) analysis, Cellular Automata (CA), and Phase Field (PF) modeling serve as primary tools to elucidate these complex interactions (Azaka, *et al*., 2022, Elete, *et al*., 2022, Isibor, *et* *al*., 2022).

FE thermal modeling has achieved prominence as a technique for predicting thermal gradients and heat transfer phenomena during the DED process. By simulating the interaction between the laser, powder feedstock, and substrate, FE models can generate detailed transient thermal fields, which, in turn, are crucial for comprehending microstructural outcomes (Ying *et al*., 2020; Karunaratne *et al*., 2016). Factors such as laser power and scan speed must be finely tuned within these simulations, as they significantly impact the thermal history experienced by the superalloy (Carraturo *et al*., 2020; (Karunaratne *et al*., 2017). Validated FE models provide insights into how process parameters affect grain size and morphology, with studies showing the relationship between cooling rates, thermal gradients, and microstructural attributes (Zhang *et al*., 2017).

The predictions from FE thermal models are instrumental in understanding microstructural evolution in DED-processed superalloys. The temperature distributions generated through these simulations inform researchers about the conditions conducive to different morphologies, such as columnar versus equiaxed grain structures (Karunaratne *et al*., 2017; Keshavarz *et al*., 2016). For example, higher thermal gradients commonly lead to columnar growth while lower gradients can facilitate equiaxed grain structures, emphasizing the importance of accurately modeling cooling rates and heat transfer (Ying *et al*., 2020; Azarbarmas & Aghaie-Khafri, 2017). Furthermore, these thermal profiles help estimate dendritic spacing and phase transformations that are critical for tailoring the mechanical properties of components (Yu *et al*., 2018).

To fully capture the detailed microstructural evolution beyond the capabilities of FE thermal models alone, CA and PF models are employed. CA modeling captures the dynamics of grain nucleation and growth using discrete representations of material space, allowing for efficient simulations of complex phenomena like competitive grain growth and solidification paths (Karunaratne *et al*., 2017; Azarbarmas & Aghaie-Khafri, 2017). These models rely heavily on the thermal histories obtained from FE simulations as boundary conditions, linking thermal conditions to grain-level outcomes (Karunaratne *et al*., 2016; Keshavarz *et al*., 2016).

Similarly, PF modeling provides a rigorous framework for understanding phase transformations, dendrite growth, and microsegregation, utilizing coupled equations to describe concentration fields and forces governing phase interfaces (Chukwuneke, *et al*., 2021, Ekengwu & Olisakwe, 2021). The power of PF methods lies in their ability to accurately reflect alloy compositions and phase stability across thermal ranges, thus providing a framework for predicting phase fractions and precipitate behaviors crucial in superalloy performance (Karunaratne *et al*., 2017; Yu *et al*., 2018).

Integrating CA and PF models with FE thermal simulations allows for a comprehensive, multi-scale representation of microstructural dynamics during DED. By continuously feeding back microstructural results into thermal models, researchers can update thermophysical properties reflecting grain evolutions, thereby enhancing the fidelity of their simulations in predicting real-world behavior (Adewale, *et al*., 2022, Elete, *et al*., 2022, Kanu, *et al*., 2022).

The integration of data-driven techniques, including machine learning and surrogate modeling, further enhances these predictive frameworks. Such approaches effectively identify correlations between various processing parameters and resultant microstructures, supporting the exploration of optimized processing conditions for desired material characteristics (Yu *et al*., 2018).

In conclusion, the pursuit of accurately modeling microstructural evolution in superalloys processed by DED hinges on the synergistic use of FE thermal modeling, CA, and PF methodologies, coupled with validation against experimental data. As advancements in computational methodologies and experimental techniques continue, the ability to predict and control microstructural features in superalloys will significantly advance, ensuring their reliability in critical applications across aerospace and other high-demand industries (Kirka & Neu, 2018; Sames *et al*., 2016).

Data-driven and AI-enhanced prediction approaches

The domain of additive manufacturing (AM), and specifically directed energy deposition (DED), has seen rapid growth due to its applications in crafting high-performance superalloys that are vital for aerospace, energy, and biomedical sectors. To ensure the desired performance characteristics, such as strength, fatigue resistance, corrosion resistance, and durability, precise control over the microstructural evolution during the manufacturing process is essential (Zhang *et al*., 2017; Saboori *et al*., 2017). The intricate interplay of process parameters during DED can lead to complex microstructural outcomes that are challenging to predict, necessitating the integration of advanced techniques to manage these complexities effectively (Egbuhuzor, *et al*., 2021, Ekengwu, *et al*., 2021, Isi, *et al*., 2021).

Recent advancements in data-driven methodologies, particularly those employing machine learning (ML), have emerged as robust tools for exploring the relationships between processing parameters and microstructural characteristics. ML techniques, such as artificial neural networks (ANNs), support vector machines (SVMs), decision trees, and random forests, are now commonly used to interpret extensive datasets generated during DED processes (Agbede, *et al*., 2021, Fredson, *et al*., 2021, Isibor, *et al*., 2021). These models are capable of discerning intricate, non-linear relationships that exist between process conditions and the resultant microstructural features, including grain size, morphology, phase composition, and defect formation (Jardin *et al*., 2019; Fetni *et al*., 2021). In particular, deep learning architectures have demonstrated significant utility in analyzing high-dimensional data, which underpins the effective prediction of diverse microstructural attributes under varying thermal conditions (Zhang *et al*., 2017; Saboori *et al*., 2017).

The efficacy of ML models is fundamentally reliant on the quality and scope of the training datasets. The integration of multi-source data, which includes real-time sensor data (such as thermal imaging and melt pool dynamics) and extensive post-process characterization (e.g., electron backscatter diffraction (EBSD), X-ray diffraction (XRD), scanning electron microscopy (SEM)), is crucial for developing accurate predictive models (Deng *et al*., 2021; (Hamilton *et al*., 2019). Sensor data provide instantaneous insights into thermal effects during process execution, whereas microscopy methods yield detailed assessments of the resulting microstructure (Fetni *et al*., 2021; Flynn *et al*., 2016). Thus, the combination of sensor-derived and microscopy data enriches the available datasets for ML training, leading to models that can generalize predictions beyond merely experimental conditions, enhancing reliability and applicability across varying material types and process settings (Travyanov *et al*., 2016).

A promising direction in the field of predictive modeling for AM is the utilization of digital twins—dynamic virtual representations of manufacturing processes that leverage real-time data feedback from sensors, along with computational modeling and ML (Baek *et al*., 2019). By continuously updating and refining computational models based on live feedback, digital twins can facilitate intelligent and adaptive control of DED processes, enabling engineers to make adjustments on-the-fly to optimize microstructural properties (Hamilton *et al*., 2019; Heigel *et al*., 2015). This capability significantly reduces experimental trial-and-error, enabling high fidelity in achieving desired outcomes and eliminating deviations from target specifications (Körner, 2016).

Moreover, hybrid modeling approaches that integrate physics-based computational models with data-driven ML techniques have shown considerable promise in addressing the inherent challenges faced by singular methodologies. Physics-based models can accurately simulate the fundamental physical phenomena governing DED processes, while ML approaches can handle the inherent uncertainties and complex interactions present in predictive processes (Fetni *et al*., 2021). This synergistic relationship enhances both the interpretability and computational efficiency of predictions regarding microstructural evolution, thereby improving overall predictive fidelity (Zhang *et al*., 2017; Heigel *et al*., 2015). Consequently, hybrid models position themselves as powerful tools for advancing AM capabilities, allowing for precise, physically consistent predictions that can adapt to the varied challenges posed by different superalloy compositions and processing conditions (Kumara *et al*., 2019; Flynn *et al*., 2016).

In conclusion, as the field of AM continues to evolve, the incorporation of data-driven methodologies and AI-enhanced prediction approaches for controlling microstructural evolution represents a significant advancement. By effectively utilizing comprehensive, diverse datasets and leveraging digital twin technology alongside hybrid modeling, engineers and researchers can significantly improve the prediction and management of microstructures in additive manufactured superalloys (Chukwuneke, *et al*., 2022, Ewim, *et al*., 2022, Kanu, *et al*., 2022). This shift not only addresses the immediate challenges of process control in DED but also drives innovation in the development of high-performance materials essential for future technological advancements.

Correlation between process parameters and microstructure

In the realm of Directed Energy Deposition (DED) additive manufacturing, a deep understanding of the correlation between process parameters and the resulting microstructure is crucial for optimizing material properties in superalloys. The ability to predict and control the microstructural evolution through precise manipulation of process parameters offers tremendous potential for tailoring the mechanical performance of components in industries such as aerospace, energy, and defense. The microstructure of superalloys is intricately linked to a variety of process parameters, including laser power, scan speed, powder feed rate, and substrate temperature, among others (Ajayi, *et al*., 2021, Fredson, *et al*., 2021). The complex interactions between these parameters govern thermal gradients, melt pool dynamics, solidification rates, and phase transformations, which ultimately determine the grain morphology, phase distribution, and defect formation in the final product.

Parametric studies and sensitivity analyses are essential tools for understanding the influence of individual and combined process parameters on microstructural development. By systematically varying one or more process parameters while keeping others constant, researchers can isolate the effects of specific factors and identify their role in shaping the final microstructure (Egbuhuzor, *et al*., 2022, Eze, *et al*., 2022, Nwulu, *et al*., 2022). For instance, a parametric study on laser power might reveal how increased energy input alters the melt pool size, cooling rate, and grain growth, ultimately affecting the degree of columnar versus equiaxed grain formation. Similarly, varying the scan speed can provide insight into how the velocity of the energy source influences thermal gradients and the formation of dendritic structures. These studies not only help to identify the direct effects of each parameter but also uncover complex interactions between them, such as how laser power and scan speed together influence the size of the dendrite arms and the presence of secondary phases.

Sensitivity analysis further refines this understanding by quantifying the relative impact of each parameter on microstructural features. For example, the sensitivity of grain size to laser power or the effect of scan speed on porosity can be determined through statistical methods or computational simulations (Akhigbe, *et al*., 2021, Ike, *et al*., 2021, Isi, *et al*., 2021). This approach allows researchers to pinpoint the most critical process parameters that need to be carefully controlled to achieve specific microstructural outcomes. Sensitivity analysis can also be used to optimize the process window, ensuring that multiple parameters work synergistically to produce the desired material properties while minimizing defects such as cracks, porosity, and residual stresses.

One of the most important aspects of process optimization in DED is the ability to map laser-material interactions to specific grain structures. The laser serves as the primary energy source that drives the melting and solidification of the superalloy material. The nature of laser-material interactions, including how the laser energy is absorbed by the powder and substrate, directly impacts the thermal history of the material and the resulting microstructure. The laser power determines the energy input into the melt pool, while the scan speed governs the rate at which the laser moves across the material (Adewale, *et al*., 2022, Ikpambese, Onogu & Olisakwe, 2022). The combination of these two parameters influences the melt pool size, cooling rates, and thermal gradients, all of which are critical for controlling the grain structure.

For instance, a high laser power coupled with a low scan speed leads to a larger melt pool and slower cooling, which tends to promote the formation of columnar grains that grow in the direction of heat flow. In contrast, a low laser power and high scan speed generate a smaller melt pool with faster cooling rates, often resulting in fine equiaxed grains that are desirable for their uniformity and mechanical properties (Ajayi, *et al*., 2022, Francis Onotole, *et al*., 2022, Nwulu, *et al*., 2022). The cooling rate also plays a critical role in determining the dendritic arm spacing. Rapid cooling rates result in finer dendrites, whereas slower cooling rates can lead to coarser dendritic structures, which have different mechanical properties. By mapping these laser-material interactions to specific grain structures, researchers can gain a comprehensive understanding of how to manipulate process parameters to achieve targeted microstructural characteristics.

In addition to grain structure, laser-material interactions also influence phase formation in DED-processed superalloys. For example, the thermal history induced by the laser affects the precipitation of strengthening phases such as γ' (gamma prime) in nickel-based superalloys. The cooling rate and thermal gradients can influence whether the γ' precipitates form in a fine, homogeneous distribution or whether they segregate and coarsen, affecting the alloy's high-temperature performance (Akhigbe, *et al*., 2022, Fredson, *et al*., 2022, Nwulu, *et al*., 2022). Mapping these phase transformations to process parameters allows for the design of process windows that promote the desired phase distributions and sizes, optimizing the mechanical properties of the final component.

With the insights gained from parametric studies and the mapping of laser-material interactions to grain structures, predictive control strategies for microstructure tailoring can be developed. These strategies aim to fine-tune the DED process by adjusting the relevant parameters in real-time or during subsequent processing steps to achieve the desired microstructural characteristics. One such strategy is the use of adaptive process control systems that utilize real-time feedback from in-situ monitoring techniques, such as thermal cameras, melt pool sensors, and high-speed imaging (Chukwuma, *et al*., 2022, Fredson, *et al*., 2022). These systems can continuously assess the thermal state of the melt pool and adjust process parameters dynamically to maintain consistent thermal gradients and cooling rates. For example, if the melt pool temperature exceeds a predefined threshold, the laser power or scan speed can be adjusted to prevent overheating, which may otherwise lead to defects or undesirable grain structures.

Advanced data analytics and machine learning models also play a significant role in predictive control strategies. By training machine learning algorithms on large datasets derived from experimental observations and simulations, these models can predict the impact of process parameter changes on the microstructure and suggest optimal process adjustments in real-time. These models can also predict the likelihood of defects such as porosity or cracking, providing early warnings that allow for corrective actions before the part is completed (Dienagha, *et al*., 2021, Egbumokei, *et al*., 2021, Odedeyi, *et al*., 2020). The integration of predictive models with real-time process monitoring creates a powerful feedback loop that enhances the ability to control microstructural outcomes during DED processing.

Another promising approach is the use of process maps and phase diagrams that correlate process parameters with specific microstructural features. These maps provide a visual representation of how various process parameters influence the formation of grain structures, phases, and defects. By overlaying these maps with sensor data and real-time process feedback, operators can quickly identify when the process is deviating from the optimal conditions and take corrective action to maintain the desired microstructure. Such maps can also be used in conjunction with machine learning models to predict the outcome of process adjustments before they are implemented.

In conclusion, the correlation between process parameters and microstructure in Directed Energy Deposition is complex and multifaceted, requiring sophisticated techniques to predict and control the resulting material properties. Parametric studies and sensitivity analyses provide valuable insights into the effects of individual and combined process parameters, while mapping laser-material interactions to grain structures and phase formations offers a more detailed understanding of the microstructural evolution. Predictive control strategies, leveraging adaptive process control systems and data-driven models, enable real-time optimization of the DED process to achieve tailored microstructural characteristics. These advancements in process control, when coupled with in-situ monitoring and real-time feedback, promise to revolutionize the precision and reliability of DED manufacturing for high-performance superalloy components.

Applications and case studies

Applications and Case Studies of Advances in Predicting Microstructural Evolution in Superalloys Using Directed Energy Deposition Data

Directed Energy Deposition (DED) has emerged as a powerful additive manufacturing (AM) method, particularly for high-performance superalloys, where precise control over the microstructure is essential. The ability to manipulate and predict microstructural evolution using DED data has opened up numerous possibilities across various high-value industries. In this context, advancements in understanding microstructural behavior through predictive models based on DED data have proven crucial for applications such as aerospace turbine blades, nuclear reactor components, and biomedical implants. These industries demand the highest standards of material performance under extreme operating conditions, where the microstructure directly influences the mechanical properties, durability, and safety of critical components.

Aerospace turbine blades represent one of the most prominent and demanding applications for DED in superalloy processing. Turbine blades are exposed to extreme temperatures, stresses, and thermal gradients during engine operation, requiring materials with excellent high-temperature strength, oxidation resistance, and fatigue resistance. Superalloys such as Inconel 718 and Hastelloy X are commonly used in turbine blades due to their remarkable resistance to high-temperature degradation and creep. The microstructure of these alloys, particularly the distribution and size of strengthening phases like γ' (gamma prime), plays a pivotal role in their high-temperature performance.

In the past, achieving the optimal microstructure in turbine blades involved complex casting methods and stringent post-processing heat treatments. However, DED allows for near-net shape manufacturing and enables the production of complex geometries with intricate internal cooling channels, which are vital for managing the heat flux within the turbine. Advances in predicting microstructural evolution during DED processing have made it possible to fine-tune the thermal and deposition parameters, such as laser power, scan speed, and powder feed rate, to optimize grain structure and phase distribution in real-time. For example, predictive models have been used to adjust these parameters to control the formation of columnar versus equiaxed grains in the alloy, as well as to ensure the correct precipitation of γ' phase, which significantly enhances the blade's strength and fatigue resistance. Moreover, incorporating in-situ monitoring data from thermal cameras and melt pool sensors into these predictive models has allowed for the continuous optimization of the DED process, ensuring that the turbine blades achieve their desired microstructure without the need for lengthy post-processing.

Another critical application for DED-processed superalloys lies in the manufacturing of nuclear reactor components. Nuclear reactors operate under extreme conditions, including high temperatures, neutron flux, and radiation, which can cause material degradation over time. The use of superalloys like Inconel 625 and Haynes 230 in nuclear reactor components is due to their excellent resistance to corrosion, oxidation, and high-temperature creep. These materials are particularly important in applications such as reactor pressure vessels, steam generators, and control rods, where the integrity of the components is essential for the safe operation of the reactor.

The ability to predict and control the microstructural evolution of these superalloys during DED processing has profound implications for nuclear reactor component manufacturing. One of the primary concerns when using DED for nuclear applications is ensuring that the microstructure is homogeneous, with minimal segregation or porosity, to maintain the structural integrity and resistance to radiation-induced damage. Predictive models that integrate DED data with phase-field and cellular automata simulations allow manufacturers to fine-tune the deposition process to control the size and distribution of precipitates, such as γ' and carbides, which contribute to the alloy's strength and resistance to irradiation damage. In particular, these models can predict the evolution of grain boundaries and phase transformations during deposition and cooling, helping manufacturers avoid the formation of undesirable phases or microstructural defects. The incorporation of real-time feedback from in-situ monitoring tools, such as melt pool sensors and thermocouples, allows for adaptive control of the process, ensuring that the components maintain their desired microstructure throughout the build.

In addition to high-temperature strength and corrosion resistance, the mechanical properties of nuclear reactor components, such as toughness and fatigue resistance, are highly dependent on the microstructure. Therefore, understanding the relationship between the DED process parameters and the final microstructure is crucial. By predicting and controlling factors such as grain size, phase formation, and the distribution of alloying elements, manufacturers can optimize the mechanical properties of the superalloy to meet the stringent requirements for nuclear applications.

The biomedical industry also stands to benefit significantly from advances in DED and microstructural prediction techniques, particularly in the production of biomedical implants. Biomedical implants, such as hip replacements, dental implants, and spinal fusion devices, require materials that are not only biocompatible but also possess mechanical properties similar to those of natural bone. Superalloys, including titanium and cobalt-based alloys, are commonly used for these implants due to their strength, corrosion resistance, and bioactivity. However, the microstructure of these materials is crucial for achieving the necessary properties, such as strength, fatigue resistance, and osseointegration, which refers to the ability of the implant to bond with bone tissue.

Using DED for manufacturing biomedical implants offers significant advantages over traditional methods, such as casting or forging, particularly in terms of customization and the ability to create complex geometries. For example, DED allows for the creation of porous structures that mimic the microstructure of natural bone, promoting better osseointegration and reducing the likelihood of implant failure. However, the formation of these complex structures requires precise control over the deposition process and the microstructural features.

Predictive models for microstructural evolution in DED-processed superalloys can be applied to optimize the properties of biomedical implants. By simulating the thermal gradients and solidification pathways during the DED process, it is possible to predict how the material will behave in terms of grain size, phase formation, and porosity. These models can then be used to fine-tune the process parameters to achieve the desired microstructure that balances mechanical strength with bioactivity. For instance, in titanium alloys, the formation of α and β phases during the solidification process is crucial for achieving the desired mechanical properties. By adjusting the process parameters, it is possible to control the phase distribution and the resulting mechanical performance of the implant.

Moreover, incorporating real-time monitoring data into these predictive models allows for the optimization of the DED process in situ, ensuring that the implants achieve the desired microstructure without the need for time-consuming post-processing. For example, in-situ monitoring using thermal cameras and melt pool sensors can provide immediate feedback on the melt pool temperature and solidification rate, allowing for rapid adjustments to laser power, scan speed, or powder feed rate. This real-time feedback ensures that the final implant material has the optimal microstructure, reducing the risk of defects and improving the overall performance and longevity of the implant.

In conclusion, the application of DED in the manufacturing of high-performance superalloy components for industries such as aerospace, nuclear energy, and biomedicine holds great promise. Advances in predicting microstructural evolution during DED processing through the integration of sensor data, predictive modeling, and real-time feedback have made it possible to optimize the microstructure and mechanical properties of these materials. By controlling process parameters and predicting microstructural changes in real-time, manufacturers can produce components with tailored properties that meet the demanding requirements of each application. This approach not only enhances the performance and safety of critical components but also enables the customization of components to meet specific design and functional requirements. As DED technology continues to advance, the ability to predict and control microstructural evolution will play a crucial role in unlocking the full potential of superalloys in these industries.

Conclusion, challenges and future research directions

Advances in predicting microstructural evolution in superalloys using Directed Energy Deposition (DED) data have shown significant promise in enabling precise control over the material properties of critical components across industries such as aerospace, energy, and biomedical manufacturing. The integration of real-time monitoring systems, computational modeling, and machine learning algorithms has advanced our understanding of the relationship between DED process parameters and the resulting microstructure. This progress has led to improved process control, reduced material waste, and the production of parts with optimized mechanical properties. However, despite these advancements, several challenges remain in fully realizing the potential of predictive modeling in DED metallurgy, and future research is needed to address these limitations.

One of the main challenges in current predictive models for DED is the lack of sufficiently comprehensive datasets and the inherent limitations in model accuracy. While data from in-situ monitoring tools such as thermal cameras, melt pool sensors, and high-speed imaging have significantly advanced our understanding of the process dynamics, the datasets themselves are often fragmented and incomplete. These datasets may lack consistency in terms of the range of process conditions they cover, limiting the ability of models to generalize across different materials or processing parameters. The complex and dynamic nature of DED further complicates the task of developing models that can accurately predict microstructural evolution under all possible operating conditions. For instance, the interaction between the laser energy and the powder feedstock, the temperature gradients during solidification, and the cooling rates all affect the formation of grains and phases in ways that are still not fully understood. As such, there is a pressing need for larger, more detailed datasets that incorporate a wider range of process conditions and material behaviors, which would enable more accurate and reliable models.

To overcome these limitations, there is a strong need for standardized DED process databases that can serve as benchmarks for model development and validation. A well-organized and comprehensive database would allow researchers and manufacturers to test and validate new models and simulations across a broad set of process parameters and material compositions. It would also facilitate the identification of process-property relationships that are otherwise difficult to uncover due to the variability in data across different experimental setups and manufacturers. Such databases should ideally include data from various types of superalloys, deposition geometries, process conditions, and the corresponding microstructural and mechanical properties. Standardized datasets would promote collaboration and comparison across research efforts, enabling faster advancement in the field and improving the reproducibility of results across different manufacturing scenarios.

Another significant challenge is the integration of multiscale and multiphysics models. The microstructural evolution during DED is influenced by phenomena at multiple scales, from the atomic level where phase transformations occur to the mesoscopic level where grain boundaries and dendritic structures form, and up to the macroscopic scale where residual stresses and defects such as porosity and cracks may develop. Integrating these different scales into a cohesive, unified framework remains a complex task. Additionally, the interaction between thermal, mechanical, and metallurgical processes during DED involves complex multiphysics that is difficult to capture with traditional modeling approaches. While some advances have been made by coupling finite element thermal models with phase field or cellular automata models, the computational cost of such models remains high, and their accuracy can still be limited by the assumptions made in their formulation. Future research should focus on developing more efficient computational techniques and integrating them with better predictive capabilities for multi-scale microstructural evolution. The ability to predict material properties at different scales based on initial processing conditions could lead to significant improvements in DED process optimization.

The role of artificial intelligence (AI) in adaptive manufacturing also presents numerous opportunities for the future. AI can be leveraged to develop more dynamic and responsive models that can adjust to process variations in real-time. By combining machine learning algorithms with real-time data from in-situ monitoring tools, AI can continuously learn from the data and provide adaptive control to optimize the DED process as it occurs. For example, AI can predict potential defects or deviations in the material properties during the build process and adjust the processing parameters accordingly to mitigate them. This adaptive feedback loop could dramatically enhance the reliability and precision of DED manufacturing, reducing the need for trial-and-error experimentation and improving part consistency. Furthermore, AI-based models could be trained to predict how changes in process parameters might affect the final part's performance, enabling more informed decisions throughout the manufacturing process.

In terms of key advances, one of the most notable developments has been the integration of predictive microstructural modeling with real-time feedback systems, such as in-situ monitoring tools combined with machine learning. This approach has enabled researchers to not only predict but also actively control the microstructural characteristics of DED-processed components, moving closer to achieving fully automated, adaptive manufacturing systems. Furthermore, the coupling of experimental data with advanced simulations has allowed for a deeper understanding of the complex relationships between process parameters, thermal history, and microstructural evolution. The ability to simulate these processes with higher fidelity has improved the overall quality and performance of DED-manufactured superalloys.

These integrated approaches hold significant implications for manufacturing reliability and performance. By predicting and controlling the microstructure more accurately, manufacturers can reduce the occurrence of defects, improve the mechanical properties of the parts, and ensure that the components meet the required specifications without the need for extensive post-processing or rework. Furthermore, predictive modeling can enhance the consistency and reproducibility of the DED process, making it more reliable and scalable for industrial applications. This is particularly important for industries such as aerospace, where safety and performance are critical, and parts must meet stringent standards.

Looking forward, the future of predictive DED metallurgy holds tremendous potential, but there is still much work to be done. To move forward, there is a need for more sophisticated and integrated models that account for the complexities of DED processing at different scales and across different materials. Multiscale modeling techniques that combine the atomic, mesoscopic, and macroscopic scales, integrated with real-time in-situ monitoring, will likely play a key role in advancing predictive capabilities. Additionally, the development of standardized databases and more robust machine learning models will accelerate the widespread adoption of predictive modeling tools in industrial settings. As AI continues to evolve, its integration into DED will enable more adaptive and responsive manufacturing processes, bringing us closer to the goal of fully optimized, automated, and reliable additive manufacturing systems.

In conclusion, predicting microstructural evolution in superalloys using Directed Energy Deposition data represents a critical advancement in the field of additive manufacturing. While significant progress has been made in understanding and controlling the microstructure of DED-processed materials, there remain challenges in model accuracy, data availability, and multi-scale integration. The future of DED metallurgy will likely rely on the continued development of standardized process databases, more efficient computational models, and the increasing role of AI and machine learning in adaptive manufacturing. These advances will not only improve the precision and reliability of DED but also enable the production of high-performance materials for a wide range of demanding applications across industries. The integration of these technologies holds the promise of unlocking new levels of performance, efficiency, and quality in DED manufacturing, driving innovation in both design and production.

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