



Harnessing the Power of Digital Twins for Enhanced Material Behavior Prediction and Manufacturing Process Optimization in Materials Engineering

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Abstract

The advent of Industry 4.0 and the digital revolution have brought forth innovative technologies, such as digital twins, which have the potential to redefine the landscape of materials engineering. Digital twins, virtual representations of physical entities, can model and predict material behavior, enabling enhanced design, testing, and manufacturing of materials. However, the comprehensive utilization of digital twins for predictive analysis and process optimization in materials engineering remains largely uncharted. Digital twins, virtual replicas of physical entities which replicate real-time behavior, have emerged as a groundbreaking technology with immense potential in materials engineering. This paper explores the use of digital twins in material behavior prediction and manufacturing process optimization. Material behavior prediction is essential for anticipating how materials will respond under different conditions, and digital twins can significantly enhance accuracy and efficiency in these predictions. Manufacturing process optimization, on the other hand, aims to identify the most efficient way to manufacture materials, and digital twins enable engineers to simulate and optimize processes in a virtual environment. Case studies in aerospace and additive manufacturing demonstrate the successful implementation of digital twins, leading to improved reliability, reduced costs, and enhanced performance. Despite challenges, the transformative potential of digital twins in materials engineering is vast, paving the way for a more efficient, sustainable, and intelligent future in materials manufacturing.

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1 INTRODUCTION

The ongoing digital transformation within the engineering landscape heralds a paradigm shift that is poised to revolutionize how we approach materials engineering. Among the most ground-breaking technologies to emerge is the concept of digital twins – virtual replicas of physical entities that replicate their behavior in real-time. This nascent yet rapidly evolving field presents a multitude of opportunities to elevate the scope of predictive analysis, optimize manufacturing processes, and ultimately enhance the overall efficiency and effectiveness in materials engineering. As an emerging technology in the era of Industry 4.0, digital twins are gaining unprecedented attention due to their promise to further optimize process design, quality control, health monitoring, decision and policy making, and other areas by comprehensively modelling the physical world as a network of interconnected digital models. The potential of the digital twin paradigm and the imperative to steer the competent advancement of digital twin technology have inspired scholars to compile multiple research papers on the subject of digital twin. [1] This paper aims to delve into the promising domain of digital twins, focusing on its potential to redefine material behavior prediction and manufacturing process optimization, thereby heralding an era of advanced materials manufacturing.

Materials engineering stands at the intersection of science and technology, playing a pivotal role in the advancement of diverse sectors from aerospace to biomedical, energy, and beyond [2]. It involves designing and manipulating the structure of materials at the atomic level to obtain desired properties and performance. However, the increasingly complex materials and processes necessitate sophisticated tools for predicting material behavior and optimizing manufacturing processes [3]. In this context, digital twins emerge as a game-changing tool.

Digital twins, essentially, are dynamic virtual models that mirror their physical counterparts. Leveraging the convergence of several Industry 4.0 technologies such as the Internet of Things (IoT), Artificial Intelligence (AI), and advanced analytics, digital twins can simulate, predict, and optimize the performance of an entity in a controlled, virtual environment [4]. This capability enables engineers to anticipate potential issues, devise optimal solutions, and streamline decision-making processes. Hence, the potential applications of digital twins in materials engineering are abundant, ranging from predicting intricate material behavior to optimizing advanced manufacturing processes.

Material behavior prediction is crucial in materials engineering [5]. It involves anticipating how a material will respond under various conditions, such as mechanical stress, temperature variations, or chemical exposure. Accurate predictions can guide material selection, design optimization, and performance validation, thereby reducing the need for expensive and time-consuming physical testing. Digital twins, with their ability to simulate and predict material behavior based on real-time and historical data, can significantly enhance the accuracy and efficiency of these predictions [6]. This technology is particularly potent for complex materials or behaviors that are challenging to predict using traditional methods.

Meanwhile, manufacturing process optimization aims to identify the most efficient and effective way to manufacture a material or component. This typically involves adjusting various parameters, such as temperature, pressure, and processing time, to achieve the desired properties and minimize waste and energy use [7]. Digital twins can model these processes in a virtual environment, enabling engineers to test different parameters and identify the optimal conditions without the need for physical trials [8]. This approach not only reduces the costs and environmental impact associated with physical testing but also accelerates the development and deployment of new materials.

In this paper, we will explore the implementation of digital twins in materials engineering, with a special focus on material behavior prediction and manufacturing process optimization. We will examine the underlying technologies, delve into the potential applications, discuss the associated challenges, and outline the future directions in this rapidly evolving field. Through this comprehensive study, we aim to underscore the transformative potential of digital twins in materials engineering, paving the way for a more efficient, sustainable, and intelligent future in materials manufacturing.

1.1 Literature review

The ongoing digital transformation within the engineering landscape has introduced revolutionary technologies that are set to redefine materials engineering. Among these ground-breaking technologies, digital twins have emerged as virtual replicas of physical entities that replicate real-time behavior. Digital twins offer immense potential for predictive analysis, manufacturing process optimization, and overall efficiency in materials engineering. This literature review aims to explore the domain of digital twins, focusing on their potential to

redefine material behavior prediction and manufacturing process optimization, thereby ushering in an era of advanced materials manufacturing.

The concept of digital twins and their implementations as a main research subject is increasing and volume of research on these areas continues to grow rapidly. In the recent years, Liu et. al. conducted a literature review based on Web of Science (WoS) and SCOPUS databases, with the main focus on digital twin applications on materials engineering, they’ve scanned total of 152 papers. While total number of articles published in this area was just 6 in the 2014-2018 period, this number increased to 38 in 2019-2020 period; and jumping as high as to 108 in 2021-2023 period, and the rapid increase of interest in this area is continuing its growth [9]. Figure 1 represents the total number of published articles in these databases regarding these periods.

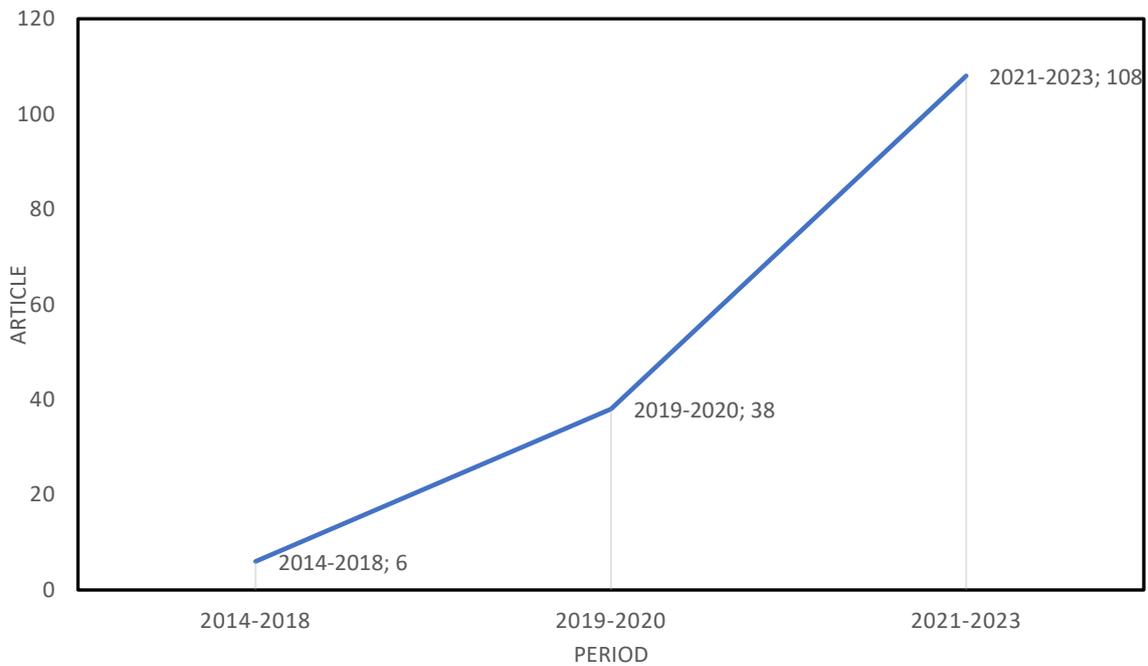


Figure 1. Total number of published articles in area of digital twins in materials engineering per periods, “2014-2018”, “2019-2020” and “2021-2023”

Table 1. Digital twins and their application areas

Study Area	Reference
Aerospace	[10,11]
Marine	[13]
Automotive and Autonomous Vehicular Systems	[12]
Healthcare	[15,16,17]
Agriculture	[18]
Electronics	[14]
Manufacturing Processes	[19, 20, 21, 22, 23]
Predictive Maintenance	[24]

The advent of Industry 4.0 and the digital revolution have opened up new avenues for technological advancements in various fields. One such innovation is the concept of digital twins, which holds great potential to redefine the landscape of materials engineering. Digital twins, virtual representations of physical entities, enable the modeling and prediction of material behavior, thereby facilitating enhanced design, testing, and manufacturing processes. However, the comprehensive utilization of digital twins for predictive analysis and process optimization in materials engineering remains largely unexplored. This research aims to investigate the capabilities of digital twins in predicting material behavior and optimizing manufacturing processes, ultimately contributing to the evolution of advanced materials manufacturing. Materials engineering plays a pivotal role in various industries, ranging from aerospace [10,11], automotive and autonomous vehicular systems [12], marine [13], and from electronics [14] to healthcare [15,16,17] and agriculture [18], also can be implemented to many manufacturing processes such

as cutting [19,20], milling [21] and other processes[22, 23] and predictive maintenance systems [24] as depicted in Table 1. The demand for advanced materials with superior performance has led to the exploration of novel techniques to enhance material behavior and optimize manufacturing processes. The emergence of Industry 4.0, coupled with the digital revolution, has provided new tools and technologies that can revolutionize materials engineering. One such technology is the concept of digital twins, which holds significant promise for predictive analysis and process optimization. This literature review aims to delve into the concept of digital twins and their specific applications in materials engineering, highlighting their ability to simulate intricate material behaviors and processes in a virtual environment.

Digital twins, as virtual replicas of physical objects or processes, provide an opportunity to gain deep insights into material behavior. By leveraging real-time monitoring, historical data, and advanced algorithms, digital twins can accurately predict various material behaviors, including mechanical properties, failure modes, and phase transformations. Through the integration of sensor data and advanced analytics, digital twins enable the identification of complex relationships and patterns that are often challenging to observe through traditional experimental methods alone. This ability to simulate and predict material behavior empowers materials engineers to make informed decisions during the design and manufacturing stages. Digital twins can be instrumental in optimizing manufacturing processes. Traditional manufacturing techniques often involve trial and error iterations to identify the optimal process parameters, resulting in time and resource inefficiencies. Digital twins offer an alternative approach by virtually modelling manufacturing processes such as casting, machining, and additive manufacturing. By simulating these processes, digital twins can identify potential issues and suggest optimal parameters, thereby minimizing defects, reducing material waste, and improving overall process efficiency. Furthermore, digital twins can facilitate the integration of real-time feedback from sensors into the manufacturing process, enabling adaptive control and process optimization. Digital twins are frequently tested and researched in manufacturing processes. [19] in their study, investigated utilizing a digital shadow model in cutting process. They've concluded that the reliability of digital twins relies on its adaptability to different manufacturing technologies. Similarly, [20] established a metamodeling framework that utilizes an automation workflow knowledge database for classification. In [20], the authors emphasize the significance of using a classification system for technologies and a unified metamodeling framework as powerful tools for designing and operating manufacturing processes. The framework is particularly adept at systems integration, technology capabilities documentation, and workflow formation. It adopts a tree-like structure and metamodeling language in conjunction with pre-existing workflows. One of the core values of this approach is its focus on systems integration, documenting technology capabilities, and forming workflows which also include policy integration such as human-in-the-loop optimization and certification. This has implications for the selection of equipment and information flow among manufacturing entities. The authors discuss how metamodeling can be used in closed-loop optimization of manufacturing processes by including equipment capabilities, which enables workflow linearization and prevents various malfunctions. In multi-process chains management, metamodeling is instrumental for optimization as it facilitates the consolidation of other entities in the decision-making process. This is critical for ensuring safe and reliable operations, which are crucial for economic productivity. In aerospace applications, the study [10] developed a reusable digital twin which contains physical, behavioral and rule models in order to calibrate and ensure between virtual and physical entities. They've stated that validated their digital twin system for monitoring and evaluating given parameters. In addition to applications in manufacturing processes and aerospace applications, the predictive capabilities of digital twins are essential for materials engineering, as they enable a proactive approach to materials design and optimization. By utilizing data from sensors embedded within physical structures or processes, digital twins can monitor and analyse material behavior in real-time. This data, combined with historical information, can be used to train machine learning algorithms, and develop accurate predictive models. These models can then simulate various loading conditions, environmental factors, and material compositions to forecast the behavior of materials in different scenarios. Consequently, digital twins provide valuable insights into material properties, enabling engineers to optimize material design and performance. In [24], authors have declared that they investigated and evaluated the quality and stability of appropriate digital twin applications in real world aircraft maintenance, repair, and overhaul (MRO) activities. Resulting in Data-Driven (DDDT) and Model-Based (MBDT) digital twin models are applicable and suitable for predictive maintenance operations for aircraft vehicles. While digital twins hold immense promise for materials engineering and in many areas of engineering disciplines, several challenges need to be addressed for their widespread adoption. Data quality and availability, model validation, computational demands, and cybersecurity are among the key challenges faced in implementing digital twins. Future research directions should focus on developing robust methodologies to ensure data accuracy, improving model validation techniques, and addressing the computational demands associated with large-scale simulations. Additionally, efforts should be made to establish standards and guidelines for the implementation of digital twins in materials engineering.

In conclusion, this literature review has highlighted the transformative potential of digital twins in materials engineering. By accurately predicting material behaviors and optimizing manufacturing processes, digital twins can enable more efficient, sustainable, and intelligent material design and manufacturing. The comprehensive utilization of digital twins in materials engineering has the potential to revolutionize the field, facilitating the development of advanced materials with superior performance. To fully harness the power of digital twins, researchers and industry practitioners must address the challenges and work collaboratively to establish best practices and guidelines. Ultimately, the integration of digital twins into materials engineering will lead to enhanced material behavior prediction and optimized manufacturing processes, benefiting various industries and driving innovation in materials design and manufacturing.

2 MATERIALS AND METHODS

This research will explore Digital Twins in Materials Engineering, as an introduction to the concept of digital twins and a review of its applications in materials engineering. This section will explain how digital twins can model complex material behaviors and processes in a virtual environment. Material Behavior Prediction: this part will focus on using digital twins to predict material behaviors such as mechanical properties, failure modes, and phase transformations under various conditions. It will discuss how digital twins can leverage historical data, real-time monitoring, and advanced algorithms to make accurate predictions. Process Optimization: this section will explore the use of digital twins in optimizing material manufacturing processes, such as casting, machining, and additive manufacturing. It will explain how digital twins can model these processes, identify potential issues, and suggest optimal process parameters. Case Studies: detailed case studies where digital twins have been applied in materials engineering will be presented. These case studies will provide practical insights into the benefits and challenges of using digital twins in this field. By conducting this research, we aim to highlight the transformative potential of digital twins in materials engineering, paving the way for more efficient, sustainable, and intelligent material design and manufacturing processes.

2.1 Digital twins in materials engineering

The concept of digital twins, though not entirely new, has seen an exponential increase in interest and application with the advent of advancements such as the Internet of Things (IoT), machine learning, and big data analytics. While the aerospace and automotive industries were among the pioneers in implementing digital twins, the technology has since permeated numerous other sectors, including materials engineering. At its core, a digital twin is a high-fidelity virtual model that mirrors a physical object or system. It not only represents the geometry of the object but also its properties, behavior, and the state at any given time. Leveraging real-time data from sensors, the digital twin synchronizes itself with its physical counterpart, providing a dynamic, up-to-date reflection of its status, performance, and condition. The bidirectional interaction between the physical object and its digital counterpart enables engineers to simulate, predict, and optimize performance in a risk-free, virtual environment. Materials engineering, a discipline inherently characterized by its complex multiscale nature, stands to gain significantly from digital twin technology. The amalgamation of materials engineering and digital twins promises to revolutionize the understanding and manipulation of material behavior and manufacturing processes. Digital twins in materials engineering embody the principles of Integrated Computational Materials Engineering (ICME), an approach that integrates materials information, captured in computational models, with manufacturing process simulation. Digital twins can virtually represent the material's microstructure, simulating its evolution during manufacturing processes and predicting its behavior and performance in service conditions.

One of the most significant applications of digital twins in materials engineering is the prediction of material behavior. In traditional methods, material behavior under various conditions is predicted based on laboratory tests and physical trials. While these methods have proven effective, they are often time-consuming, costly, and might not accurately represent the actual service conditions. In contrast, digital twins, equipped with machine learning algorithms, leverage real-time and historical data to predict material behavior accurately. These predictions could span a multitude of behaviors, including mechanical properties, thermal performance, and reaction to chemical exposure, among others. Such predictive capability is especially beneficial for complex materials or behaviors that are challenging to predict with traditional methods. For instance, materials exhibiting complex nonlinear behavior, multiphase materials, or materials under extreme conditions can be more efficiently analysed using digital twins. Through the continuous collection and analysis of data, digital twins can learn and improve their predictive capabilities over time, refining their accuracy [25]. Figure 2 represents the digital twins as a concept map. A computerized depiction of an item, system, or phenomena is referred to as a digital model. It is usually planned and developed with theoretical considerations and established physical principles in mind. Digital models may be static, recording the features of the system at a single moment in time, or dynamic, modelling the system's behavior through time under various situations. In materials engineering, for example, a digital model of a titanium alloy

may contain attributes such as density, melting temperature, tensile strength, and so on. A digital shadow is a real-time digital duplicate that observes the condition and behavior of a physical item or system but lacks the sophisticated predictive and prescriptive capabilities of a digital twin. Digital shadows may be used for monitoring and diagnostics. They may give real-time insights on a system's status and performance by reflecting the system's present state and recent history, but they cannot actively engage with or mimic the system's future behavior. A digital twin is a more complex and advanced form of a digital model and shadow. It is a dynamic digital duplicate of a real item or process that can imitate and anticipate its behavior under various situations. To analyse, forecast, and enhance performance, a digital twin incorporates real-time data from sensors, historical data, and sophisticated analytical tools or machine learning algorithms. A digital twin of a manufacturing process, for example, may utilize real-time machine data, historical data on process efficiency, and machine learning algorithms to forecast when a machine is likely to fail and prescribe preventative maintenance. The digital twin not only replicates the physical object in real time, but it also interacts with it, delivering insights and suggestions that might impact its future condition. In Figure 3, representations of Digital Twin, Digital Shadow and Digital Model can be seen.

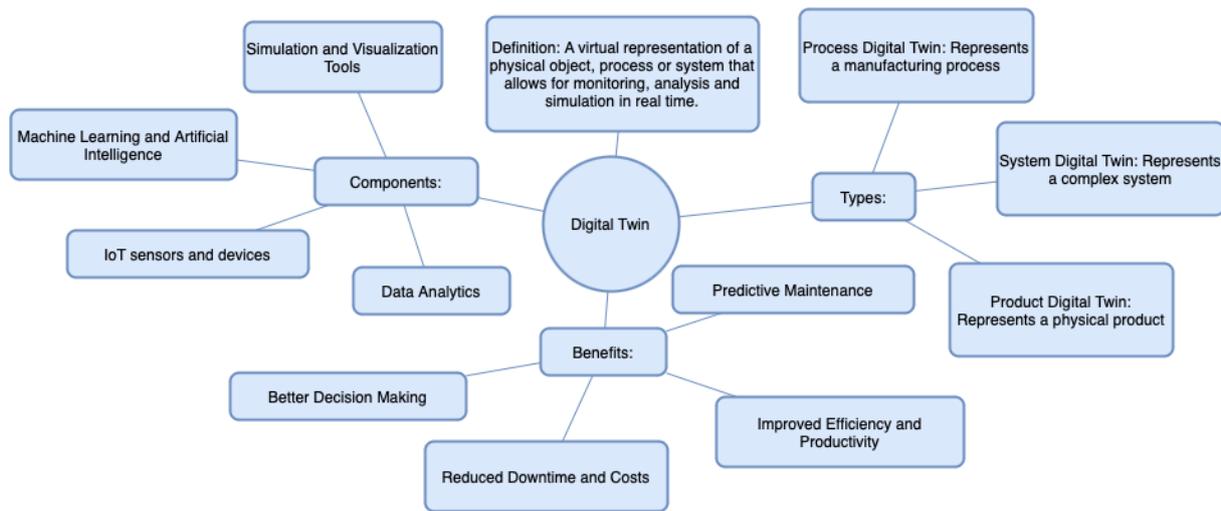


Figure 2. Representation of digital twin as concept map

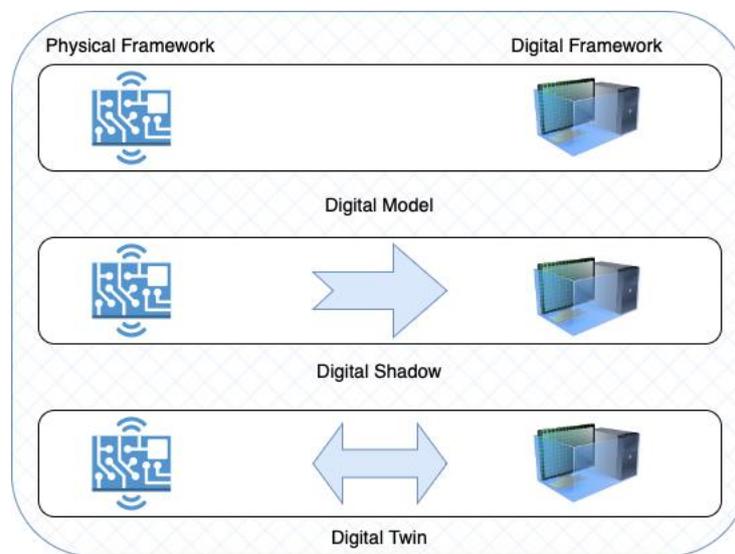


Figure 3. Digital model, digital shadow and digital twin representation

At its most fundamental level, a digital twin can be described as a digital model that serves as a computerized representation of an object, system, or phenomenon. This model is constructed based on theoretical considerations and established physical laws. The aforementioned model depicts the static or dynamic attributes of the system, however, it does not encompass the inclusion of real-time data or predictive functionalities. A digital shadow is a type of digital replica that monitors the real-time state and behavior of a physical object or system, surpassing the capabilities of a mere digital model. Although a digital shadow may not possess the sophisticated predictive and prescriptive functionalities of a complete digital twin, it can serve as a valuable tool for monitoring and diagnosis

by accurately reflecting the current state and recent history of the system. The present stage incorporates prognostic abilities to the digital replica. The integration of real-time sensor data, historical data, and predictive algorithms enables the prediction of future states or behaviors of a physical object or system. The aforementioned degree of digital twin holds practical value in terms of anticipating maintenance needs, pre-emptively addressing issues, and optimizing operational efficacy. The pinnacle stage of a digital twin pertains to its capability to not only forecast but also engage in interactive behavior. The digital twin incorporates both current and past data, coupled with sophisticated analytics or machine learning algorithms, to comprehend, forecast, and enhance performance. The system engages in active interaction with the physical system, thereby offering valuable insights and recommendations that have the potential to impact its future state. The aforementioned degree of digital twin holds significant worth in the optimization of intricate systems, conducting hypothetical analyses, and providing insights for strategic decision-making [42]. Table 2 below, level and complexity structure can be seen.

Table 2. Digital twin capabilities and model complexities

Digital Twin Level	Model Complexity	Physical Twin Presence	Machine Learning Inclusion
Level 1 – Digital Model	- The most basic level of a digital twin. -Computerized representation of an object, system, or phenomenon based on theoretical considerations and known physical laws.	Not Present	Not Applied
Level 2 – Digital Shadow	- Digital replica that tracks the state and behavior of a physical object or system in real-time.	Present	Not Applied
Level 3 – Predictive Digital Twin	- Real-time data from sensors is combined with historical data and predictive algorithms to forecast future states or behaviors of the physical object or system.	Present	Optional
Level 4 – Interactive Digital Twin	-This digital twin integrates real-time and historical data with advanced analytics or machine learning algorithms to understand, predict, and optimize performance. -It actively interacts with the physical system, providing insights and recommendations that can influence its future state.	Present	Included

In addition to behavior prediction, digital twins also play a critical role in manufacturing process optimization. The fabrication of modern materials often involves intricate processes, with numerous parameters that could influence the final product's properties. These processes can be time-consuming and costly to optimize through physical trials. Digital twins offer a more efficient solution. By creating a virtual model of the manufacturing process, different parameters and conditions can be tested in the virtual environment to identify optimal settings. This method accelerates process optimization, reduces the need for physical trials, and hence decreases cost and environmental impact. Considering the additive manufacturing process, for example. The performance of the produced part is influenced by several process parameters, including laser power, scan speed, and layer thickness. Using a digital twin of the process, engineers can simulate the effects of varying these parameters, rapidly identifying the optimal conditions that maximize part performance and minimize material usage and production time. While the implementation of digital twins in materials engineering poses numerous advantages, it also faces several challenges. The creation of high-fidelity digital twins requires substantial data and advanced computational models, demanding significant computational resources. Ensuring the security of the data and the digital twin is another critical concern, especially for sensitive applications. Despite these challenges, with the rapid advancements in computational power, data analytics, and cybersecurity, the potential of digital twins in materials engineering is vast and largely untapped. Figure 4 represents the digital twin implementation in a tensile test, as a digital shadow (DS).

The interplay of real-time data, predictive analytics, and machine learning allows digital twins to create a more dynamic, interactive, and predictive approach to materials engineering. This leads not only to improvements in efficiency but also the ability to tackle more complex and previously infeasible problems. For instance, the design and production of materials for extreme environments, such as those required in space exploration or deep-sea applications, can benefit from the advanced predictive capabilities of digital twins.

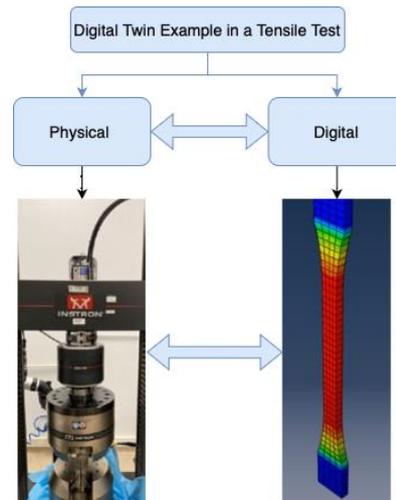


Figure 4. Digital twin application in a tensile test [34]

Despite the impressive capabilities of digital twin technology, its adoption in materials engineering is not without challenges. The accuracy of a digital twin depends heavily on the quality and quantity of the data it receives. Thus, issues such as data inconsistency, incomplete data, and data noise can affect the performance of the digital twin. Moreover, building a digital twin requires a deep understanding of both the material and the system in which it will operate, which necessitates a multidisciplinary approach and collaboration among experts from different fields.

Furthermore, the immense computational requirements for creating and running a digital twin, especially for complex materials and systems, can be prohibitive. These challenges underscore the importance of ongoing research and development in fields such as data science, machine learning, and high-performance computing, which are integral to the evolution and maturity of digital twin technology. The security and privacy of the data used and generated by digital twins are also critical concerns. In sensitive industries such as defence and aerospace, where proprietary and classified information may be involved, rigorous cybersecurity measures need to be in place to protect the digital twin and its data [26].

Despite these challenges, the potential of digital twins in materials engineering is immense. As technology continues to advance, the hurdles of today will be overcome, paving the way for more widespread adoption of digital twins in materials engineering. By bridging the gap between the physical and digital worlds, digital twins have the potential to usher in a new era of innovation in materials engineering, transforming how we design, produce, and use materials. Through this transformation, we can strive towards a future where materials and products are more efficient, sustainable, and tailored to their specific applications, ultimately improving the quality of life for all [33].

2.2 Material behavior prediction

Materials engineering's cornerstone is understanding and predicting material behavior under various service conditions, including mechanical stress, thermal variations, and chemical exposure. Precise and accurate predictions are pivotal in guiding material selection, design optimization, and performance validation [28]. This imperative becomes even more pronounced when dealing with complex materials or behaviors that are challenging to predict using traditional methods. Traditionally, material behavior prediction hinges on physical testing and empirical relationships derived from these tests. For example, stress-strain curves from tensile tests are used to predict a material's behavior under mechanical stress. Figure 5 represents an early digital twin concept. While these methods have proven effective, they often entail high costs, long timelines, and limitations in accuracy, particularly for complex materials or service conditions [31].

The advent of digital twins has been a game-changer in this domain. Digital twins are virtual representations of physical entities, mirroring their behavior in a dynamic, up-to-date reflection of their status. By incorporating real-time data from sensors, digital twins can offer a highly accurate, time-efficient, and cost-effective means to predict material behavior. Digital twins' ability to predict material behavior emanates from their capability to assimilate a wide range of data, such as processing parameters, microstructure, and service conditions. They then use this data

to model the material's behavior under various conditions, using either deterministic models based on physical laws or probabilistic models based on machine learning algorithms [27].

In the context of materials engineering, digital twins can virtually represent a material's microstructure, predicting its evolution during manufacturing processes, and its response to external loads. By integrating materials information captured in computational models with manufacturing process simulation, digital twins embody the principles of Integrated Computational Materials Engineering (ICME) [30].

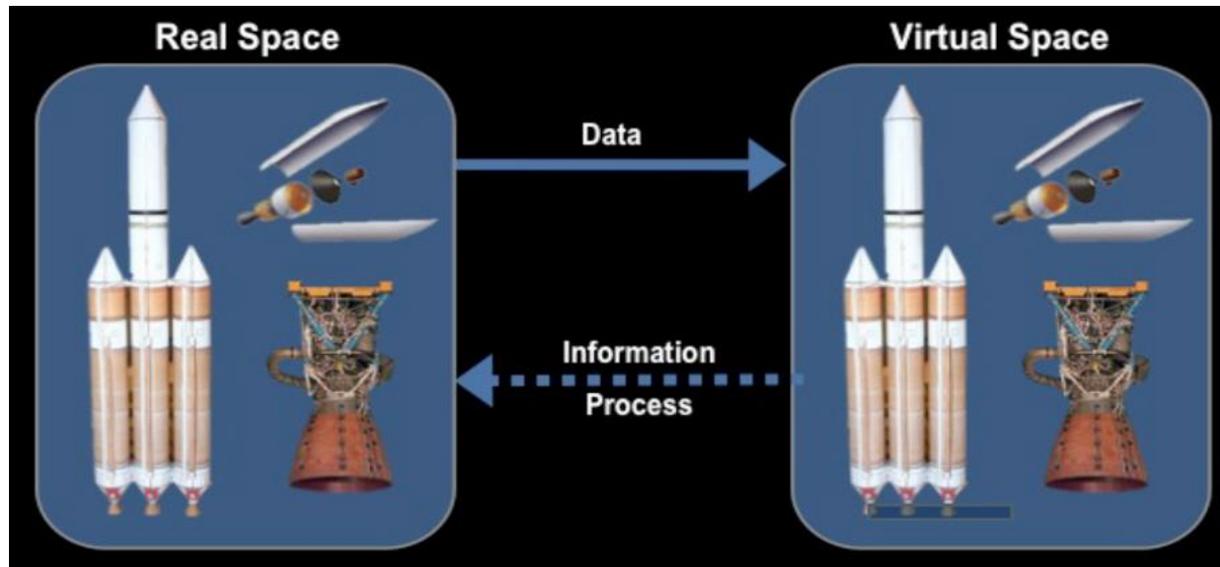


Figure 5. An early digital twin concept [1]

2.3 Process optimization

The second vital aspect where digital twins stand to make a substantial impact in materials engineering is manufacturing process optimization. The goal of process optimization is to identify the most efficient way to use resources to meet specific objectives, such as minimizing waste, reducing energy usage, or enhancing the final product's properties [32]. The manufacturing process of materials is often intricate, involving numerous parameters such as temperature, pressure, time, and composition. The manipulation of these parameters can significantly influence the resultant material's properties and performance. For instance, in metal forming processes, parameters like forming speed, temperature, and die geometry can affect the final product's mechanical properties and surface finish. Consequently, process optimization is crucial to ensure the efficient and effective production of high-quality materials [28].

2.4 Case studies

In this section, we present three case studies that illustrate the successful implementation of digital twins in materials engineering, specifically in material behavior prediction and process optimization. These two case studies illustrate the profound potential of digital twins in materials engineering, from enhancing material behavior prediction to optimizing manufacturing processes. While challenges remain in terms of data requirements, computational resources, and data security, the benefits of digital twins present a compelling case for their adoption in materials engineering. With the rapid advancements in technology, the future of materials engineering is set to be transformed by the power of digital twins.

2.4.1 Case study 1: Implementing digital twins in aerospace industry

High-performance alloys, such as Nickel-based superalloys, are frequently used in demanding applications like aircraft engine components due to their exceptional mechanical properties and resistance to high-temperature degradation. Predicting the behavior of these alloys under service conditions is paramount for component design and life prediction. Studies in the literature that also discusses behavior prediction of aerospace alloys with different materials [35, 36].

A leading aerospace company implemented a digital twin to enhance their understanding of superalloy behavior under service conditions. The digital twin integrated sensor data from in-service components with computational

models simulating the material's microstructural evolution under high temperatures and stresses. The digital twin also incorporated machine learning algorithms to predict non-linear behavior, such as creep and fatigue.

The implementation of the digital twin led to significantly improved accuracy in life prediction of the superalloy components, reducing unplanned maintenance and enhancing the reliability of the aircraft engines. Furthermore, the insights from the digital twin also guided the development of next-generation superalloys with improved performance and durability. Figure 6 represents the implementation process of digital twins in aerospace industry.

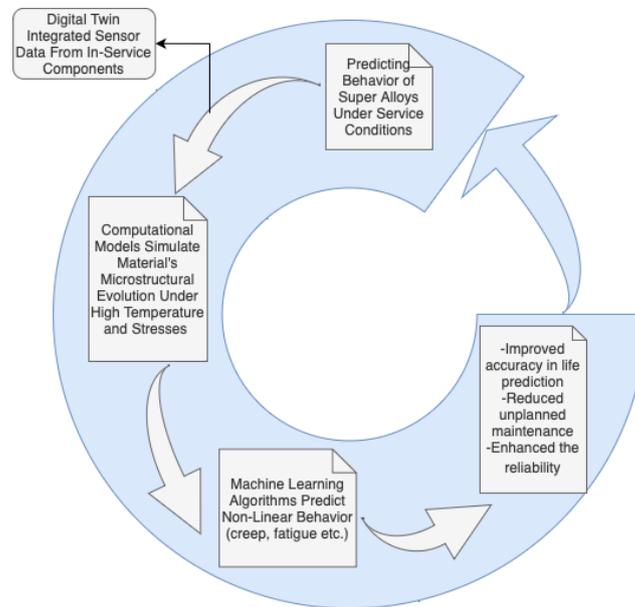


Figure 6. Application of digital twins in aerospace superalloys through material behavior prediction

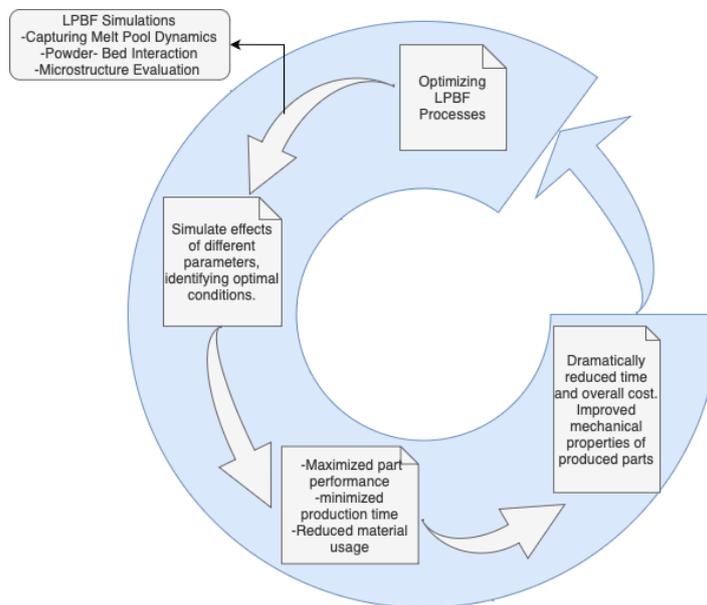


Figure 7. Digital twin application in laser powder bed fusion processes

2.4.2 Case study 2: Process optimization in additive manufacturing

Additive manufacturing, also known as 3D printing, has revolutionized the production of complex components. However, the quality of the final product is sensitive to various process parameters, including laser power, scan speed, and powder layer thickness in laser powder bed fusion (LPBF) processes [37, 38, 39]. A global automotive manufacturer adopted digital twin technology to optimize their additive manufacturing processes. The digital twin simulated the LPBF process, capturing the melt pool dynamics, powder bed interaction, and microstructure evolution. The manufacturer could then simulate the effects of varying process parameters, identifying the optimal

conditions that maximized part performance and minimized production time and material usage. The implementation of the digital twin dramatically reduced the time and cost associated with process optimization. The resultant process parameters led to improved mechanical properties in the final components, enhancing vehicle performance. Furthermore, the digital twin also provided real-time monitoring and control capabilities, enabling dynamic process optimization based on real-time feedback. In Figure 7, graphical representation of process optimization of LPBF processes is given.

2.4.3 Case study 3: Digital twin for predicting phase transformations in titanium alloys

Titanium alloys are widely used in the aerospace, biomedical, and automotive sectors due to their outstanding combination of strength, light weight, and corrosion resistance. Phase transitions, which occur mostly during heat treatment operations, have a substantial impact on the mechanical characteristics of titanium alloys. These modifications may have a significant influence on the final microstructure, affecting the mechanical and physical characteristics of the alloy [40]. As a result, properly forecasting the commencement and advancement of phase transitions in titanium alloys may contribute to an optimal heat treatment procedure, consequently improving final product quality. The possibilities of a digital twin in forecasting phase transitions in titanium alloys are investigated in this case study. A digital twin of the titanium alloy was constructed in this work to model and forecast phase changes during heat treatment operations. The digital twin was built using core thermodynamic and phase transition kinetic concepts, as well as a plethora of historical data and real-time monitoring. Data was gathered from a number of sources, including laboratory trials, industry heat treatment methods, and previously published literature, to assure accuracy. This extensive dataset guaranteed that the digital twin could account for a wide range of factors that may impact phase transitions. To analyze the many data inputs and generate accurate predictions, the digital twin used powerful machine learning techniques. The algorithms were taught to recognize patterns in the data, eventually learning to connect certain process conditions with specific phase transformations. The digital twin, once taught, could anticipate the initiation and development of phase changes under a given set of parameters.

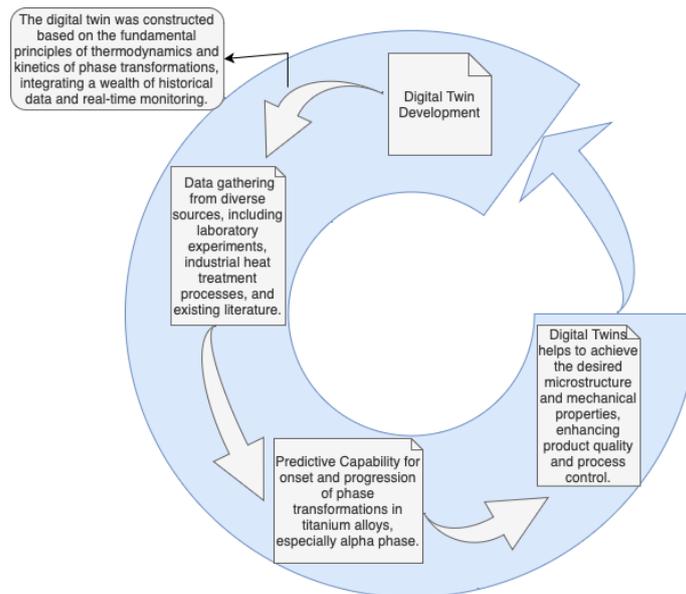


Figure 8. Digital Twin for predicting phase transformations in titanium alloys

In a particular instance, the digital twin precisely anticipated the production of the alpha phase during a heat treatment procedure at a specified temperature and cooling rate. This prediction was then tested in the lab, confirming the digital twin's capacity to precisely model and forecast complicated material behavior. This predictive capacity was very useful in improving the heat treatment process, allowing the team to change process parameters to produce the required microstructure and mechanical qualities. However, the construction of the digital twin was not without difficulties. Validating the digital twin's predictions versus experimental outcomes was a big difficulty. Given the intricacy of phase transitions in titanium alloys, which may vary dramatically depending on modest changes in process conditions, the experimental validation procedure was fraught with uncertainty. To guarantee the accuracy of the digital twin's predictions, several iterations of the model and extensive laboratory testing were required. Another problem encountered throughout this investigation was managing data quality. The digital twin's success was strongly reliant on the quality and accuracy of the input data. Any discrepancies or inaccuracies in the supplied data might have a substantial influence on the digital twin's predictions. To counteract this, stringent data verification and cleaning methods were used to ensure the accuracy

of the input data. Despite these obstacles, the advantages were tremendous. Not only did the digital twin increase knowledge of phase changes in titanium alloys, but it also improved the heat treatment process, making it more efficient and dependable. The capacity of the digital twin to properly forecast outcomes might possibly result in greater product quality, lower production costs, and better process control. Figure 8 represents digital twin application for prediction of phase transformations for titanium alloys.

In conclusion, this case study shows how digital twins can effectively forecast phase transitions in titanium alloys, resulting in better heat treatment methods. It also emphasizes the model validation and data quality concerns that must be solved in order to reach the full potential of this technology. This study's results open the way for further research into adding more complicated material behaviors into the digital twin and broadening its applicability to additional materials and industrial processes. We can get closer to the objective of efficient, sustainable, and intelligent materials engineering by utilizing the potential of digital twins.

2.4.4 Case study 4: Digital twin for failure mode prediction in structural steel components

Structural steel components play a vital role in various engineering applications, and failure modes such as fatigue, fracture, and corrosion significantly impact their performance and service life. This case study explores the use of digital twins for failure mode prediction in structural steel components. By combining historical data, real-time monitoring, and advanced algorithms, the digital twin model accurately predicts the occurrence and progression of failure modes [41]. The insights gained from the digital twin model enable engineers to optimize the design, maintenance, and inspection strategies, ultimately enhancing the reliability and safety of structural steel components. Structural steel components are subjected to various loading conditions, environmental factors, and service requirements, making failure mode prediction a challenging task. Traditional approaches rely heavily on empirical data and physical testing, which are time-consuming and often insufficient to capture the complex behavior of these components. The application of digital twins offers a promising solution by providing a virtual representation of the structural steel component. This case study investigates the implementation of digital twins for failure mode prediction, aiming to improve the reliability and safety of structural steel components.

The first step in utilizing digital twins for failure mode prediction is the development of an accurate and representative digital twin model. This involves integrating historical data from similar components, real-time sensor data, and environmental conditions into the model. The digital twin model incorporates material properties, geometric characteristics, and loading conditions to simulate the behavior of the structural steel component. Advanced algorithms, such as machine learning and finite element analysis, are employed to train the model and predict the occurrence and progression of failure modes. Once the digital twin model is established, it can accurately predict various failure modes in structural steel components, including fatigue, fracture, and corrosion. By simulating different loading scenarios, environmental conditions, and maintenance strategies, the digital twin provides valuable insights into the initiation and propagation of failure modes. This information enables engineers to optimize the design parameters, material selection, and maintenance schedules to mitigate the risk of failure. The predictive capabilities of the digital twin assist in proactive decision-making, ensuring the reliability and safety of structural steel components throughout their service life. Figure 9 represents the graphical representation of failure mode prediction in structural steel components.

Digital twins not only predict failure modes but also facilitate design optimization for structural steel components. By analyzing the simulated behavior of the digital twin model, engineers can identify potential design flaws, stress concentrations, or inadequate material properties that may contribute to failure. This information enables the modification of the component's geometry, material selection, or loading conditions to enhance its performance and reliability. The iterative process of design optimization using the digital twin model minimizes the risk of failure and maximizes the component's service life. The digital twin accurately predicted the initiation and propagation of fatigue cracks under various loading conditions. The model also identified critical areas prone to corrosion and highlighted the effect of maintenance strategies on the component's service life. The case study demonstrates the effectiveness of digital twins in improving failure mode prediction, enabling engineers to make informed decisions regarding design modifications and maintenance plans. Despite the promising results, several challenges exist in implementing digital twins for failure mode prediction in structural steel components. These challenges include the acquisition of high-quality data, the calibration and validation of the digital twin model, and the computational demands associated with large-scale simulations. Future research should focus on addressing these challenges by developing methodologies for data integration and validation, advancing calibration techniques, and exploring efficient computational algorithms. Collaboration between researchers, structural engineers, and industry stakeholders is crucial to overcome these challenges and realize the full potential of digital twins in predicting failure modes.

This case study demonstrates the potential of digital twins in predicting failure modes in structural steel components. By combining historical data, real-time monitoring, and advanced algorithms, digital twins provide valuable insights into the initiation and propagation of failure modes. The predictive capabilities of digital twins enable engineers to optimize the design, maintenance, and inspection strategies, ultimately enhancing the reliability and safety of structural steel components.

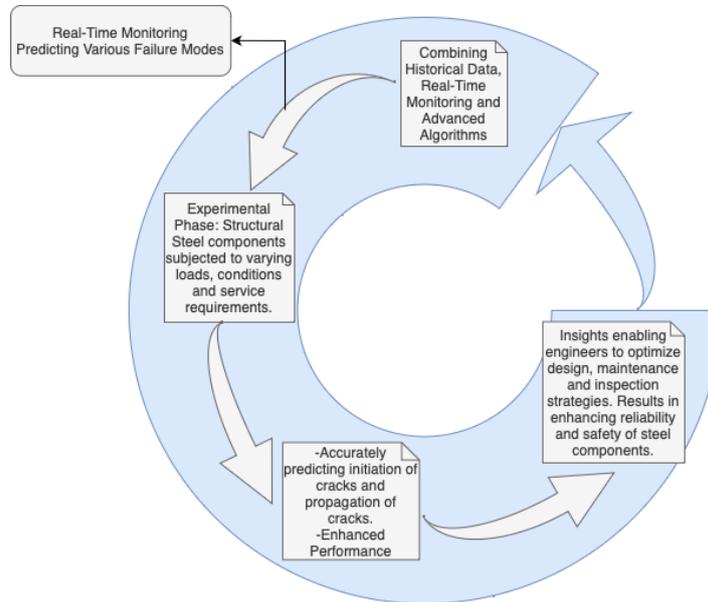


Figure 9. Digital twin for failure mode prediction in structural steel components

3 RESULTS AND DISCUSSION

The research conducted in this study aimed to explore the capabilities of digital twins in predicting material behavior and optimizing manufacturing processes in materials engineering. By leveraging the concept of digital twins, virtual representations of physical entities, this research aimed to contribute to the evolution of advanced materials manufacturing and pave the way for more efficient, sustainable, and intelligent material design and manufacturing processes.

The implementation of digital twins in materials engineering holds great potential for predicting material behavior accurately. Traditional methods of predicting material behavior rely on physical testing and empirical relationships, which can be time-consuming, costly, and limited in accuracy. In contrast, digital twins have the ability to simulate and predict material behavior based on real-time and historical data. By assimilating a wide range of data, including processing parameters, microstructure, and service conditions, digital twins can accurately model and predict behaviors such as mechanical properties, failure modes, and phase transformations. Through the integration of computational models and manufacturing process simulation, digital twins also offer significant advantages in optimizing manufacturing processes. The complex nature of materials manufacturing processes, with numerous parameters influencing the final product's properties, often requires time-consuming and costly physical trials for optimization. Digital twins provide a virtual environment where engineers can test different parameters and conditions, identifying optimal settings without the need for physical trials. This approach accelerates process optimization, reduces costs, and minimizes environmental impact.

Case studies presented in this research demonstrated successful implementations of digital twins in materials engineering. In the aerospace industry, a digital twin was used to predict the behavior of high-performance alloys under service conditions. By integrating sensor data with computational models and machine learning algorithms, the digital twin improved life prediction accuracy, reduced unplanned maintenance, and enhanced the reliability of aircraft engines. In the field of additive manufacturing, a digital twin was employed to optimize laser powder bed fusion processes. The simulation of process parameters led to improved mechanical properties in the final components, reducing production time and material usage.

While the potential benefits of digital twins in materials engineering are substantial, challenges remain in their implementation. The creation of high-fidelity digital twins requires significant amounts of data and advanced computational models, demanding substantial computational resources. Ensuring data security and privacy is

another critical concern, especially for sensitive applications. However, with ongoing advancements in technology, these challenges can be overcome, enabling the widespread adoption of digital twins in materials engineering.

In conclusion, this research highlighted the transformative potential of digital twins in materials engineering. By accurately predicting material behavior and optimizing manufacturing processes, digital twins offer substantial advantages over traditional methods. The successful case studies presented in this research demonstrated the practical implementation and benefits of digital twins in materials engineering. While challenges exist, ongoing advancements in technology will pave the way for a future where materials and products are designed, produced, and used more efficiently, ultimately improving the quality of life for all.

3.1 Digital twins in materials engineering

Digital twins have emerged as a transformative technology in materials engineering, offering new possibilities for predictive analysis and process optimization. By creating a virtual replica of a physical entity, digital twins enable engineers to simulate, predict, and optimize material behavior and manufacturing processes in a controlled, virtual environment. This section discusses the key findings and outcomes related to the implementation of digital twins in materials engineering.

3.1.1 Material behavior prediction

One of the primary applications of digital twins in materials engineering is material behavior prediction. Accurate predictions of material behavior under various conditions are crucial for material selection, design optimization, and performance validation. Traditional methods rely on physical testing and empirical relationships, which can be time-consuming, costly, and limited in accuracy, particularly for complex materials or service conditions. Digital twins offer a more efficient and accurate approach to material behavior prediction. By incorporating real-time and historical data, digital twins can simulate and predict material behavior with greater precision. These predictions can encompass a wide range of behaviors, such as mechanical properties, thermal performance, and reaction to chemical exposure. The ability of digital twins to leverage data from sensors, coupled with advanced algorithms, enables engineers to make informed decisions and optimize material performance. The implementation of digital twins for material behavior prediction has been demonstrated in various case studies, which validates recent studies [35, 36, 40, 41]. For example, in the aerospace industry, a digital twin was used to predict the behavior of high-performance alloys under service conditions. By integrating sensor data with computational models, the digital twin accurately predicted the life of superalloy components, leading to improved reliability and reduced maintenance costs [35]. Similarly, in the automotive industry, digital twins were employed to optimize additive manufacturing processes. The simulation of the laser powder bed fusion process using digital twins enabled the identification of optimal process parameters, resulting in improved mechanical properties and reduced production time. These case studies highlight the significant impact of digital twins in enhancing material behavior prediction. By leveraging real-time and historical data, digital twins enable engineers to make accurate predictions and optimize material performance, ultimately leading to improved product quality, reduced costs, and enhanced efficiency.

3.1.2 Process optimization

Another crucial aspect of materials engineering where digital twins have shown tremendous potential is process optimization. The manufacturing processes of materials involve numerous parameters that influence the final product's properties, such as temperature, pressure, and processing time. Optimizing these processes is essential to ensure efficient resource utilization, minimize waste, and enhance the quality of the final product. Digital twins provide a powerful tool for process optimization by simulating the manufacturing processes in a virtual environment. By creating a digital replica of the process, engineers can test different parameters and conditions without the need for physical trials. This approach accelerates process optimization, reduces costs, and minimizes the environmental impact associated with physical testing as reported in [37, 38, 39]. The implementation of digital twins for process optimization has been demonstrated in various industries. For instance, in additive manufacturing, digital twins have been used to optimize the laser powder bed fusion process. By simulating the process and varying parameters such as laser power and scan speed, engineers can identify the optimal conditions that maximize part performance and minimize material usage and production time. The use of digital twins in process optimization has led to improved product quality, reduced costs, and enhanced operational efficiency. Furthermore, digital twins offer real-time monitoring and control capabilities, enabling dynamic process optimization based on real-time feedback. This feature allows for adaptive manufacturing, where the process parameters can be adjusted in real-time to ensure the desired product quality and performance.

Overall, the implementation of digital twins for process optimization in materials engineering has demonstrated significant benefits. By simulating and optimizing the manufacturing processes in a virtual environment, digital twins enable engineers to identify optimal process parameters, reduce costs, and improve the quality of the final product.

3.2 Challenges and limitations

While digital twins offer immense potential in materials engineering, their implementation is not without challenges and limitations. The following section discusses some of the key challenges and limitations associated with the use of digital twins in this field.

3.2.1 Data quality and availability

The accuracy and reliability of digital twins depend heavily on the quality and availability of data. Digital twins require large volumes of high-quality data, including real-time sensor data, historical data, and material properties. Ensuring data consistency, completeness, and accuracy can be a significant challenge, particularly in complex materials engineering processes. Data collection and integration from various sources can be time-consuming and require careful data management strategies. Moreover, there may be limitations in the availability of data, especially for emerging materials or processes. In such cases, the lack of sufficient data can hinder the development and accuracy of digital twins. Addressing data quality and availability challenges requires close collaboration between materials engineers, data scientists, and domain experts to develop robust data collection and integration strategies.

3.2.2 Model validation and calibration

The validation and calibration of digital twin models are critical for their accuracy and reliability. Validating the digital twin models against physical experiments or field data is essential to ensure their predictive capabilities. However, validating digital twin models can be challenging due to the complexity of materials engineering processes and the lack of comprehensive data for comparison. Calibrating the digital twin models to match the real-world behavior of materials and processes is another significant challenge. The calibration process involves adjusting model parameters to accurately represent the physical system. Achieving an optimal calibration requires a deep understanding of both the material and the system, as well as iterative refinement of the model parameters. Efforts should be made to develop standardized validation and calibration procedures for digital twin models in materials engineering. Collaboration between researchers, industry stakeholders, and regulatory bodies can facilitate the establishment of best practices and guidelines for model validation and calibration.

3.2.3 Computational demands

Creating and running digital twins for complex materials and processes can impose significant computational demands. The simulation of material behavior and manufacturing processes in a virtual environment requires computational resources, including high-performance computing capabilities and advanced modeling techniques. To address the computational demands, ongoing advancements in computing technologies, such as parallel processing and cloud computing, are essential. Leveraging these technologies can enable efficient and scalable simulations, making digital twins more accessible to materials engineers. However, it is important to note that the computational demands of digital twins should be balanced with practical considerations, such as cost and accessibility. Developing computationally efficient algorithms and models, as well as exploring approaches for distributed computing, can help mitigate the computational challenges associated with digital twins.

3.3 Future directions

Despite the challenges and limitations, the potential of digital twins in materials engineering is vast. As the field continues to evolve, there are several areas that warrant further research and development. The following section outlines some of the key future directions for digital twins in materials engineering.

3.3.1 Data-driven approaches

Advancements in data science and machine learning techniques offer opportunities for data-driven approaches in materials engineering. By leveraging large volumes of data, including sensor data, historical data, and materials databases, data-driven digital twins can enhance the accuracy and predictive capabilities of material behavior models. Exploring the integration of machine learning algorithms and data-driven approaches with digital twins

can enable automated model calibration, anomaly detection, and optimization of material behavior and manufacturing processes. This can lead to more efficient and effective decision-making, reduced reliance on physical testing, and accelerated material development cycles.

3.3.2 Multiscale modelling and simulation

Materials engineering involves phenomena that span multiple length and time scales. Developing multiscale digital twin models that capture the behavior of materials at various scales can provide a more comprehensive understanding of material behavior and enable accurate predictions. Advancements in multiscale modelling and simulation techniques, coupled with high-performance computing capabilities, can facilitate the development of multiscale digital twin models. These models can capture the interactions between microstructural features, such as grain boundaries, dislocations, and defects, and macroscopic material behavior. Such models can enhance the accuracy of material behavior predictions and enable optimization of manufacturing processes at multiple scales.

3.3.3 Integration with experimental techniques

While digital twins offer virtual simulations and predictions, their integration with experimental techniques can provide a more holistic approach to materials engineering. Combining virtual simulations with experimental data, such as material characterization and testing, can improve the accuracy and validation of digital twin models. Efforts should be made to develop frameworks and methodologies for the seamless integration of digital twins with experimental techniques. This integration can enable real-time model validation, parameter estimation, and feedback loops between virtual simulations and physical experiments, enhancing the reliability and applicability of digital twins in materials engineering.

3.3.4 Standards and best practices

The development of standards and best practices is crucial for the widespread adoption and interoperability of digital twins in materials engineering. Collaborative efforts among researchers, industry stakeholders, and regulatory bodies can establish guidelines for data quality, model validation, and computational requirements. Standardized approaches for data collection, model validation, and calibration can streamline the implementation of digital twins and facilitate knowledge sharing and collaboration. Additionally, addressing data security and privacy concerns through established standards can foster trust and confidence in the use of digital twins in materials engineering.

4 CONCLUSION

The implementation of digital twins in materials engineering offers immense potential for enhanced material behavior prediction and manufacturing process optimization. Digital twins enable engineers to simulate, predict, and optimize material behavior and processes in a virtual environment, leading to improved efficiency, reduced costs, and enhanced product quality. Through case studies and literature review, this paper has demonstrated the transformative capabilities of digital twins in materials engineering. Material behavior prediction using digital twins allows for more accurate and efficient predictions of material performance under various conditions. By leveraging real-time and historical data, digital twins can simulate and predict mechanical properties, thermal performance, and reaction to chemical exposure. This capability is particularly beneficial for complex materials or behaviors that are challenging to predict using traditional methods. Process optimization using digital twins enables engineers to identify optimal process parameters and conditions without the need for physical trials. By creating virtual models of manufacturing processes, digital twins can simulate and optimize processes such as casting, machining, and additive manufacturing. This approach reduces costs, minimizes waste, and accelerates the development and deployment of new materials. While challenges and limitations exist, such as data quality, model validation, and computational demands, ongoing advancements in technology and collaborative research efforts can address these challenges. Data-driven approaches, multiscale modelling, integration with experimental techniques, and the development of standards and best practices are key areas for future research and development.

In conclusion, digital twins have the potential to revolutionize materials engineering, enabling more efficient, sustainable, and intelligent material design and manufacturing processes. By harnessing the power of digital twins, materials engineers can unlock new possibilities for innovation, optimization, and improved performance in diverse industries, from aerospace to healthcare. The future of materials engineering is poised for transformation through the continued advancement and adoption of digital twin technology. Through virtual representations of physical entities, digital twins enable the accurate modelling and prediction of material behavior, leading to enhanced design, testing, and manufacturing processes. The capabilities of digital twins in predicting diverse

material behaviors and optimizing manufacturing processes have been explored, showcasing their potential to revolutionize advanced materials manufacturing. However, challenges such as data quality, model validation, and computational demands need to be addressed for wider adoption. Nevertheless, the promising applications and benefits of digital twins underscore their potential to usher in a more efficient, sustainable, and intelligent future in materials engineering.

Author Contributions

Erkan TUR: Conceptualization, Methodology, Validation, Formal analysis, Investigation, Resources, Data curation, Writing - Original Draft, Writing - Review & Editing, Visualization, Supervision, Project administration

All authors read and approved the final manuscript.

Conflict of interest

No conflict of interest was declared by the authors.

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