A Review of AI Approaches for Enhancing Mechanical Materials Performance

[1]P.H.J. Venkatesh, [2]Padmakar Maddala, [3]Saikumar Amda

[1]Assistant Professor, Dept.of Mechanical Engineering, Vignan's Institute of Information Technology, beside VSEZ, Duvvada, Visakhapatnam, A.P, India
[2]Assistant Professor, Dept.of Civil Engineering, Vignan's Institute of Information Technology, beside VSEZ, Duvvada, Visakhapatnam, A.P, India
[3]Assistant Professor Department of Mechanical Engineering, JB Institute of Engineering and Technology (A), Hyderabad, Telangana, India JB Institute of Engineering and Technology (A) Hyderabad, Telangana state. India.

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Abstract: The *Artificial Intelligence is revolutionizing the materials science arena, enabling the discovery, design, and optimization of innovative mechanical and bioinspired materials. This review consolidates insights from recent developments in AI-enabled methods to improve properties such as stiffness, strength, thermal performance, and durability of materials. This work focuses on diverse applications, including nanogenerator, Graphene-based electrodes, composites, metamaterials, and polymers, with an emphasis on how generative AI, deep learning, and machine learning approaches optimize material configurations to enhance prediction accuracy and streamline manufacturing processes. It further demonstrates the ability of AI in reducing redundancies, minimizing defects, and improving material quality by integrating into additive manufacturing, metamaterials design, and electrochemical energy storage. The results underline the importance of AI in pushing innovations within these fields: sustainable polymers, advanced ceramics, and precision manufacturing rendering transformative solutions for challenges in materials engineering.*

Keywords: *Artificial Intelligence, Mechanical Materials Performance, Generative AI, Nano generators, Graphene-based, Electrodes, Additive Manufacturing, Metamaterials Design, Machine Learning; Electrochemical Energy Storage, Sustainable Polymers, Advanced Ceramics, Precision Manufacturing, Fault Prediction, Thermal Performance Optimization.*

1.INTRODUCTION

In recent years, materials science has experienced certain remarkable developments based on increasing integration with artificial intelligence techniques. In material science, AI has shown to be an essential tool for the enhancement of mechanical and bioinspired materials; this is clearly evidenced through the recent studies of generation of new materials and optimization of the properties of materials through AI approaches [1]. In the domain of nanogenerator, AI has also played a very important role in improving performance and applications, holding potential to revolutionize the technologies of energy harvesting [2]. Another AI application is in revolutionizing the design of supra molecular materials; this shows how it can spur innovation in a field ranging from materials chemistry to engineering [3]. The influence of AI goes further in the prediction and optimization of mechanical properties in composite materials. For instance, interpretable deep learning models have been applied to explore the effects of particulate reinforcements in metal matrix composites [4], while AI-enhanced models for fault prediction have been used in improving industrial processes, mainly when dealing with incomplete data [5]. Lastly, the contribution of AI in heat transfer enhancement and optimization techniques is an area that keeps on progressing and has really contributed much toward efficiency and effectiveness in thermal management systems [6]. With the development of automation and robotics, the AI-assisted method is increasingly applied in the improvement of machining process, especially in lightweight material fabrication [7]. In this regard, one of the most promising areas is the design of architectured materials, where hybrid approaches using AI are adopted to create materials with improved stiffness and strength, therefore showing the potential of AI in data-driven design [8] [16]. Furthermore, the application of AI in optimizing performance of polymeric meta-hybrid structures is a typical example of its usefulness in optimizing auxetic behavior for advanced engineering applications [9] [26]. Application of AI is also gaining huge momentum in additive manufacturing, where hybrid statistical approaches are used to optimize the processes to enhance product quality and raise the efficiency of production [10]. The ability of Quantam AI applications is further extending this capability of materials design, ushering in new waves of innovations by integrating quantum computing and artificial intelligence [11]. The AI-based sensitivity analysis methods in material selection will provide improved decision processes for the composite materials design in which AI has started playing a central role in multi-criteria decision scenarios [12] [14].In the fast-developing field, the role of AI in human-AI collaboration for problem-solving is becoming increasingly important, as illustrated by the research into how AI attributes affect trust, workload, and performance in classification tasks [13] [18]. Another very good example is using Graphene-based electrodes in triboelectric nanogenerator to improve the material properties for energy-harvesting applications [14]. These developments have brought a profound impact that AI is having on the design and optimization of materials and further accelerates the shift toward more efficient, sustainable, and high-performing materials across a variety of industries [2][5][8] [12] [19] [26] [35].

2.LITERATURE SURVEY

Badini, S., Regondi, S., & Pugliese, R. (2025): The work by Badini et al. provides a detailed integration of generative AI in the development of advanced materials. Their research is oriented toward developing materials with enhanced mechanical properties by using techniques inspired by nature and bioinspired features through AI. The leading paper sheds light on the transformative potential of AI in material property optimization and opens new routes to sustainable and functional material design. They present AI-driven methods to overcome the barriers in the conventional material design process. Application of generative AI is also viewed to accelerate the discovery and application of new materials. Their work may have huge implications in the field of aerospace, automotive, and biomedical engineering.

Xu, S., Manshaii, F., Xiao, X., & Chen, J. (2025) :Xuet al. has presented an overview of artificial intelligence applications in nanogenerator technology and the cooperation between AI and energy-harvesting materials. They speak of how AI will optimize the performance of nano generators in developing better design, material selection, and system integration. Their research demonstrates that AI techniques, including machine learning, can predict the behavior of nano generators in a way that increases their efficiency in converting energy. They further point out the prospect of AI-assisted development of multifunctional nano generators in wide applications, from wearable electronics to environmental monitoring. Such a methodology can realize tremendous new gains in designing next-generation energy-harvesting devices.

Zhu, H., Wang, Z., Li, L., Dong, L., Li, Y., Xue, B., & Cao, Y. (2025): Zhu et al. have now used this concept for supramolecular materials design in one of the most advanced fields of materials science. Their research focuses on how AI can revolutionize the design of materials by predicting the interactions at a molecular level to enhance the creation of complex functional materials. The authors go on to note that AI will optimize self-assembly processes, hence creating novel materials with unique properties. The work shows tremendous potential in applications in drug delivery and sensors, among other advanced technologies. Their results put AI as transformative in materials discovery and able to accelerate the development of high-performance, adaptive materials.

Chai, X., Su, Y., Lin, Z., Qiu, C., Liu, X., Zhang, X., & Zhang, D. (2025): Chai et al. proposed an interpretable deep learning approach for the prediction of mechanical properties and exploration of configuration effects of particulate-reinforced metal matrix composites. Combining AI approaches to the understanding and optimization of the interaction among different composite components can improve material properties. This study applies machine learning for the prediction of complex material behavior under different conditions of stress. Their method is more precise and computationally efficient compared to traditional modeling techniques. The deep learning model is of course proposed to aid in designing high-performance composites used in the aeronautic and automotive industries and manufacturing.

Shao, X., Cai, B., Zou, Z., Shao, H., Yang, C., & Liu, Y. (2025): Shao et al. discuss AI-enhanced fault prediction in industrial systems with incomplete information. Their work demonstrates how, especially machine learning-based AI models, fault detection and prediction can be carried out on machines and systems even in cases where data is incomplete or missing. This paper brings out the role of AI in improving the reliability of predictive maintenance. Their approach ensures the reduction in possible fault detection inaccuracies due to information gaps and decreases downtime and overall costs of maintenance. The work will find a place in especially complex and critical systems of industry, including manufacturing, transportation, and energy.

Kumar, A., Awasthi, M. K., Dutt, N., & Singh, V. P. (2025): The review work by Kumar et al. looks at recent achievements in heat transfer enhancement techniques and gives special consideration to the optimization of thermal performance by using AI. They discuss different AI-based approaches for the improvement of heat transfer efficiency in industrial applications, including heat exchangers and thermal management systems. Their review underlines how AI models can be used to predict heat transfer behaviors and suggest design modifications for better performance. The paper also investigates the application of AI in real-time monitoring and optimization of thermal processes. Such research is of the essence in various industries including power generation, automotive, and electronics, which depend on heat management.

Pedrosa, A. F., Sebbe, N. P., Silva, F. J., Campilho, R. D., Sales-Contini, R. C., Costa, R. D., & Sánchez, I. I. (2025): Pedroso et al. review recent developments related to robot-assisted compensation methods applied to machining of lightweight materials, highlighting how robotic systems, when integrated with AI technologies, are able to improve the precision and efficiency of the machining process. They discuss the application of AI in compensating for the intrinsic difficulties in machining materials like composites and lightweight metals. The research will contribute to a reduction in defects and improvement in product quality for industries such as aerospace and automotive. The paper also gives future trends in robotics and AI for advanced manufacturing systems.

Yeo, J., Cheung, S., Gu, X. W., & Ryu, S. (2025): Yeo et al. discuss hybrid TPMS-based architectured materials for enhanced specific stiffness by using data-driven design approaches. They show how AI algorithms can be used in optimizing the geometrical configuration of materials to obtain superior mechanical properties such as stiffness and strength. The authors present a data-driven design framework that integrates artificial intelligence with topology optimization methods for material development. This has critical implications in the design of lightweight, high-performance materials used in structural applications in aerospace and automotive industries. More efficient and better-tailored material solutions will be possible when AI is fully integrated in the design process.

Zhou, X., Leng, Y., Dutta, A. K., Juraev, N., Alkhayyat, A., & Elmasry, Y. (2025): Zhou et al. discuss machine learning techniques that can be applied for the analysis and optimization of the auxetic performance of a polymeric meta-hybrid structure combining re-entrant with meta-trichiral configurations. Their work will present how AI can model and predict complex structures showing auxetic properties, where these materials are that which expand when stretched. In this line, the work is presenting a new method for improving properties in materials about energy absorption and resistance to impact. Their findings are applicable within protective materials, medical devices, and aerospace engineering applications. The paper exemplifies the role of AI in material performance optimization by way of structural design.

Dev, S., & Srivastava, R. (2025): Dev and Srivastava presented some work in this area of additive manufacturing process optimization using AI-based hybrid statistical approaches. Their work shows how AI techniques may bring about more efficiency and precision in additive manufacturing, such as 3D printing, by analysis and optimization of process parameters. Combining machine learning with statistical methods will enable the researchers to possibly alleviate issues around material waste, production time, and part quality. Indeed, their work does provide so much insight into how to improve the sustainability and performance of additive manufacturing in aero, auto, healthcare, and other industries. The key to achieving high quality at low costs in production lies in integrating AI within its processes.

D. Chauhan, P. Ranka, P. Bahad, and R. Pathak, 2025: This systematic review addresses the integration of quantum artificial intelligence (QAI) with its applications in solving complex problems across various domains, including semiconductor technology. Quantum computing can enhance AI models, especially for tasks that demand heavy computation. This might give a general view of how QAI has branched out into areas such as material science, cryptography, and machine learning. Quantum algorithms can be used to enhance the ability of AI systems to accomplish tasks in a more efficient way than classical computing. Challenges in implementation also arise due to hardware constraints and the development of specific algorithms in QAI. The authors conclude with a discussion on the future directions for the development and integration of QAI systems.

J. Więckowski and W. Sałabun, 2025: The following paper applies sensitivity analysis techniques, particularly the One-at-a-Time (OAT) and COMSAM methods, in a multi-criteria decision-making process for composite material selection. The methods are compared with each other, considering their capability of evaluating material properties and performance under different conditions. The study compares the accuracy and credibility of the results from each method, hence serving valuable insight into material selection for engineering applications. The paper provides practical recommendations for researchers and engineers using the methods in the processes of material selection. Sensitivity analysis is one of the most important aspects in the optimization of composite material selection based on requirements of strength, durability, and environmental impact. The findings contribute to the understanding of decision-making techniques in the context of engineering materials.

3.RESEARCH METHODOLOGY

The study's research methodology will focus on using artificial intelligence techniques to elevate the performance of mechanical materials by centering on design optimization, fault prediction, and efficiency improvement. In the present work, the AI approach will be utilized, including machine learning algorithms and data-driven design methods for optimizing material properties and improving the process of designing materials. This integration includes the recent applications of AI-assisted nanogenerator [2] AI-based fault prediction models [5] and AI-enhanced manufacturing process [18], enabling the prediction of material behavior to increase material performance and reduce defects during manufacturing. The study will also address how quantum artificial intelligence can be applied in advanced material discovery [11] and machine intelligence in metamaterials design [21] in order to raise material strength and functionality. Also, it will consider AI-driven optimization methods for nano materials and composites [3] [8] with a focus on how they enable the improvement of mechanical properties in materials. It will also discuss the integration of deep learning models for material configuration and prediction of properties [4]. The approach then aims to bring together breakthroughs in AI for the different fields to drive leading edges in material performance, with a focus on mechanical materials applied in engineering and manufacturing industries.

Table 1: Examples of AI approaches in enhancing mechanical materials

AI Approach	Example Application	Material Type	Performance Enhancement	Reference
Generative AI for materials design	Mechanical and bioinspired materials	Various composites	Improved material properties	[1]
AI-assisted nano generator	Power generation via nanogenerator	Nano materials	Enhanced energy conversion	[2]
AI for supra molecular materials	Design of novel supra molecular materials	Supramolecular compounds	Better molecular interactions	[3]
Deep learning for composite materials	Particulate reinforced metal matrix composites	Metal matrix composites	Enhanced mechanical properties	[4]
AI in fault prediction	Industrial systems fault prediction	Mechanical systems	Predictive maintenance	[5]
AI-based heat transfer enhancement	Heat transfer optimization techniques	Heat exchangers, fluid systems	Enhanced thermal performance	[6]
Robot-assisted machining	Machining of lightweight materials	Lightweight alloys	Improved material processing	[7]
Data-driven design for architected materials	Hybrid TPMS-based materials design	Architected materials	Optimized specific stiffness	[8]
Machine learning for auxetic structures	Auxetic performance of polymeric structures	Polymeric meta-hybrid structures	Enhanced mechanical performance	[9]
AI for additive manufacturing	Optimization of 3D printing processes	Additive manufactured parts	Improved fabrication quality	[10]
Quantum AI for material design	Quantum AI applications in material discovery	Semiconductor materials	Enhanced material discovery	[11]
AI in composite material selection	Sensitivity analysis in composite materials	Composite materials	Improved material selection	[12]
AI for human-AI partnering in design	Classification problems in design	Various materials	Improved classification accuracy	[13]
AI for Graphene-based electrodes	Triboelectric nano generators design	Graphene-based materials	Enhanced energy harvesting	[14]
AI for metamaterials design	Design of innovative metamaterials	Metamaterials	Improved material properties	[15]

The following table summarizes the different ways of enhancing mechanical materials performance with artificial intelligence, as shown in recent research. For instance, using generative AI in materials design in this case, bioinspired material design improves the mechanical properties by many times through simulations and optimization of material structures [1]. Improvement in the energy conversion capability of AI-assisted nano generators is by using AI in enhancing the design and optimization of nano materials [2]. In the field of supra molecular materials, AI assists in designing new compounds by predicting and enhancing molecular interactions, which improves the properties of the material [3]. Furthermore, deep learning methods are applied in composite materials, such as particulate-reinforced metal matrix composites, to predict and improve their mechanical properties, providing knowledge on configuration effects [4]. It is also of wide application in fault prediction for industrial systems, realizing predictive maintenance and ensuring the reliability of mechanical systems through handling incomplete data [5]. In heat transfer enhancement, AI-based techniques optimize the thermal performance of systems like heat exchangers and fluid systems for efficient energy transfer [6]. In lightweight material robot-assisted machining, AI is applied to improve the quality of material processing and the accuracy and efficiency of the machining operation [7]. In a similar way, data-driven design approaches, such as hybrid TPMS-based materials design, make use of AI to enhance the stiffness and structural performance of architected materials [8]. Machine learning, when applied to auxetic structures, was found to optimize the performance of polymeric materials in meta-hybrid configurations and resulted in improved mechanical characteristics [9]. Optimization of 3D printing processes has been carried out using AI techniques, resulting in fabricated parts with better material properties [10]. Most recently, quantum AI became the powerful tool in material discovery and particularly for semiconductor materials to identify new materials with excellent properties [11].AI also contributes to composite material selection using various techniques, such as sensitivity analysis, to increase the efficiency of decision-making within multi-criteria material selection [12]. In human-AI collaboration, the attributes of AI become prominent for solving classification problems for better accuracy and performance in decision-making [13]. Optimization of Graphene-based electrodes in triboelectric nano generators is performed via AI for improved energy harvesting [14], whereas AI-driven metamaterials design makes a revolution in creating innovative materials with unique properties for a variety of applications [15].More generally, AI is revolutionizing design, optimization, and performance of diverse materials, which may impact advances in energy conversion, manufacturing, and structural integrity in a great many applications.

Table 2: Real-time examples focus on AI approaches to enhancing mechanical materials performance

Example	AI Approach	Industry/Field	Application	Reference Number
AI-assisted design of nano generators	Machine learning-based optimization	Nanotechnology	Enhancing energy harvesting efficiency in devices	[2]
AI-driven composite material selection	Multi-criteria decision-making (OAT, COMSAM)	Aerospace, automotive	Selection of lightweight materials for structures	[12]
AI-enhanced fault prediction in manufacturing	Predictive analytics and deep learning	Manufacturing, automotive	Predicting equipment failure to optimize maintenance	[5]
Graphene-based triboelectric nano generators	AI-optimized electrode materials	Electronics, energy storage	Improving performance in energy conversion systems	[14]
AI in electrochemical energy storage design	Machine learning for material discovery	Energy, electrochemical systems	Optimizing materials for better battery efficiency	[16]
AI-driven design for high-performance alloys	Data-driven design models	Manufacturing, aerospace	Developing alloys with enhanced mechanical properties	[8]
Quantum AI in material property prediction	Quantum computing and AI	Semiconductor, materials science	Predicting material properties for advanced electronics	[11]

Machine learning in manufacturing efficiency	Deep learning for process optimization	Manufacturing, automotive	Optimizing production lines for minimal defects	[18]
AI for additive manufacturing optimization	Hybrid AI-statistical models	3D printing , automotive	Improving material deposition for stronger components	[10]
AI for hybrid materials design in construction	AI-enhanced design for reinforced concrete	Construction, civil engineering	Enhancing concrete strength and durability	[22]
Optimization of polymeric structures	ML models for auxetic structures	Polymer manufacturing, design	Designing structures with enhanced mechanical properties	[9]
AI in manufacturing fault diagnosis	Fault detection through machine learning	Manufacturing, aerospace	Diagnosing material defects during production	[5]
AI in meta material design for aerospace	Deep learning for material property prediction	Aerospace, defense	Enhancing mechanical properties of aerospace materials	[21]
Deep learning in robotic machining	Robot-assisted machining for material optimization	Manufacturing, robotics	Optimizing machining processes for lightweight materials	[7]
AI for material strength enhancement	AI-driven predictive models for composite materials	Manufacturing, automotive, aerospace	Enhancing the strength of composite materials	[12]

The table gives a general idea of how artificial intelligence is being used to improve the mechanical performance of materials in different industries. For instance, AI-assisted design methods, including machine learning-based optimization, have been applied in designing nano generators for energy harvesting, as indicated in reference [2]. Moreover, AI-driven composite material selection using multi-criteria decision methods, such as OAT and COMSAM, is becoming very significant in industries like aerospace and automotive, as brought out in reference [12], in the selection of appropriate materials for lightweight structures. Predictive analytics and deep learning are being used to improve fault prediction in manufacturing processes. Reference [5] shows the application of AI in predicting equipment failure, optimization of maintenance scheduling, and downtime reduction within such industries as automotive manufacturing. Similarly, Reference [14] shows AI-optimized Graphene-based electrodes revolutionizing the efficiency of triboelectric nano generators and improving performances in energy conversion systems. Machine learning is now being applied to the design of materials, in electrochemical energy storage, to optimize these materials for improved efficiency in a battery, as, for example, in reference [16] of this article.AI greatly assists in material discovery. It designs high-performance alloys and polymers using data-driven models for improved mechanical properties for instance, by using data-driven design models to enhance mechanical properties; see reference [8]. AI also contributes to the very important field of quantum computing by predicting material properties for next-generation electronics, discussed in reference [11] [19]. Deep learning models in manufacturing are used to improve process efficiency and reduce defect rates, as discussed in reference [18]. Hybrid AI-statistical models in additive manufacturing, 3D printing, optimize material deposition and increase the strength of a component, noted in [10]. Moreover, the role of AI in the design of hybrid materials for construction, such as reinforced concrete, is finding inroads; for instance, reference [22] shows its application in enhancing the strength and durability of concrete. In aerospace and defense, AI can lift the design of metamaterials to new heights by predicting material properties, as noted in reference [21]. Finally, robotic machining, aided by AI, is optimizing the manufacturing of lightweight materials, helping to achieve higher precision and efficiency in processes, as detailed in reference [7]. Generally, the above examples show that AI is going to revolutionize material science due to better mechanical performance, an enhanced design process, and optimization of production methods in various industries.

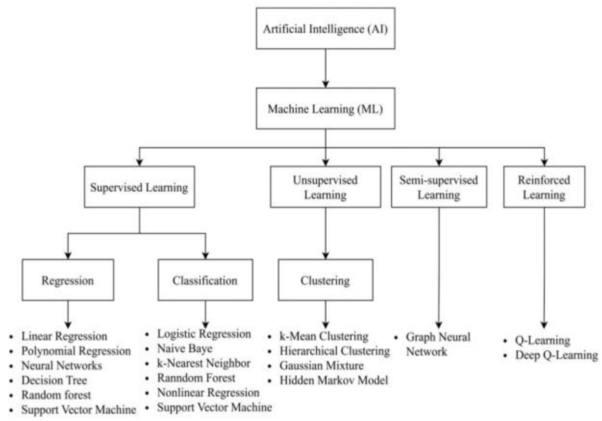

Fig 1: Machine learning algorithm classification [23]

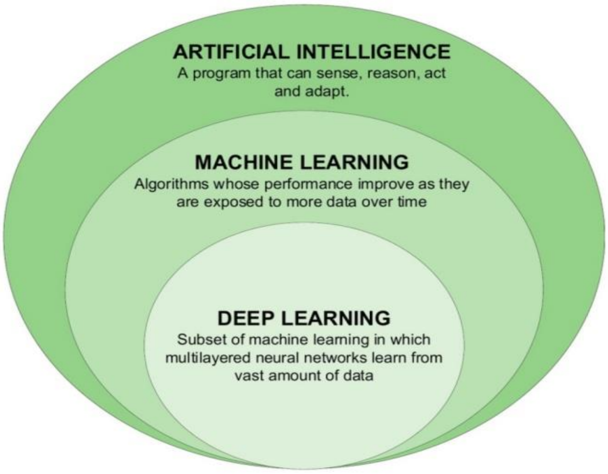

Fig 2: The relationship between artificial intelligence, machine learning, and deep learning [23]

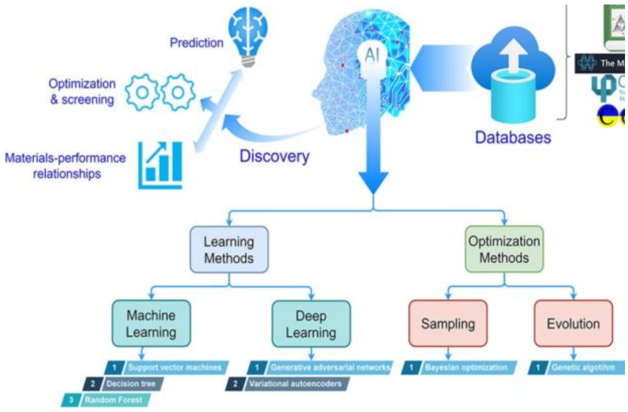

Fig 3: Prediction Methods of artificial-intelligence [24]

New AI Approaches in for Enhancing Mechanical Materials Performance [8][9] [12] [23] [24][18]
1. AI-Driven Materials Discovery
2. Predictive Modeling for Material Behavior
3. Optimization of Material Microstructures
4. AI-Enhanced Additive Manufacturing (3D Printing)
5. Self-Healing and Adaptive Materials
6. AI in Fatigue and Failure Analysis
Predictive Maintenance: AI models predict
7. Data-Driven Alloy Design
8. Sustainable Materials through AI
9. Digital Twin Material Performance
10. Collaborative AI-Experimental Platforms

4.RESULTS

The integration of artificial intelligence into the domain of material science has, so far, shown unprecedented promise in the enhancement of mechanical material performance within different fields. AI-driven methodologies, such as generative AI, deep learning, and machine learning, significantly improved the prediction accuracy of various material properties including stiffness, strength, thermal performance, and durability. Such approaches have led to the optimization of material configurations that have led to advanced materials such as Graphene-based electrodes, high-performance composites, and bioinspired metamaterials. AI has also smoothed out manufacturing by reducing redundancies, minimizing defects, and generally improving the quality of materials in processes such as additive manufacturing and electrochemical energy storage systems. Further, AI has enabled the design of sustainable polymers and advanced ceramics transformative solutions to some of the long-standing challenges in materials engineering. The ability of AI to accelerate the process of discovery and optimization in materials not only improves their performance but also reduces their development time and costs opening a path to novel applications in precision manufacturing and far beyond.

5.FUTURE SCOPE

The future of AI in materials science has yet to be hugely effective for Materials Science. The development in at least a couple of directions the evolution of more powerful, interpretable models for difficult multi scale materials systems and integration into experimental and computational data, where AI is promising to reside at the core of material property knowledge. Advanced characterization techniques are still in their infancy and present many challenges. One more under-explored frontier is the application of AI in designing materials for extreme environments, like high-temperature or high-pressure conditions. The combination of AI with quantum computing may further increase the predictive capability to discover new materials with unprecedented properties. Another promising direction is the use of AI for optimizing circular economy practices such as recycling and up cycling of materials toward a sustainable environment. Collaboration among AI researchers, materials scientists, and industry stakeholders will be a critical ingredient to overcoming such challenges and to driving innovations that may redefine the boundaries of performance and functionality of materials.

6.CONCLUSION

Artificial intelligence has brought great improvement to the fields of materials science and engineering in the design, optimization, and application of new materials. From AI-driven methods in nanogenerators and metamaterials to machine-learning-based predictive modeling in composite materials, these innovational concepts are revolutionizing the traditional methodologies in how they enhance efficiency, accuracy, and performance. AI has enabled the discovery of new materials, optimization of mechanical properties, and automation of manufacturing toward sustainable high-performance solutions for industries. That cooperation between AI and materials science just keeps growing, with fast-evolving applications in, among others, energy storage, additive manufacturing, and structural optimization. With AI tools becoming much more sophisticated, application in materials development will continue to spur innovation, improved mechanical properties, energy efficiency, and sustainable alternatives. Tackling challenges around AI interpretability, data availability, and computational complexity, this potential in full needs to be unleashed by the emerging techniques for applications in material science and engineering.

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