Review Article: Transformative Application of AI Potential in Materials Science

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The identification tools and techniques in materials engineering using AI, computer vision, and natural language processing have advanced significantly to address limitations in traditional systems. Modern and advanced studies have emerged to drive innovation in the field of materials science. This contemporary shift enhances conventional methods by integrating AI-based techniques. This study emphasizes carbon fiber reinforced polymer (CFRP) composites, which are extensively used in aerospace, automotive, and structural applications. The identification of surface cracks and internal defects, such as delamination and voids, is essential for assessing structural integrity, performance, and service life. The methodology suggested is based on image processing and machine learning algorithms using computer vision to detect defects, extract features, and classify them, and provide automated analysis of the material conditions. AI provides algorithms and statistical pattern recognition techniques used for data analytics in materials science. AI rapidly enables the detection and analysis of defects, thereby transforming the field of materials engineering. Predictions and parameter estimations are dependent on data quality and material informatics. It has been shown through experiments that AI-based methods are effective in measuring structural integrity and performance evaluation due to enhanced detection accuracy, shorter processing time, and dependable defect classification measures in comparison to traditional inspection processes. Future studies are expected to incorporate quantum computing and AI systems for faster and more precise predictions and identifications. Prospective directions include improving material property predictions and optimizing simulations for computational analyses.

Keywords: Artificial Intelligence, Machine Learning, Materials, Data Analytics, Materials Detection, Analytical Modeling

Introduction:

Rapid innovation in materials science addresses inefficiencies, cost, and variability in digital information associated with experiments and validations. Advanced AI-based tools and techniques utilized in materials engineering are presented in Table 1. These techniques highlight the research gap in predicting the mechanical and physical properties of carbon fiber reinforced polymer (CFRP) composites [1]. Understanding and leveraging AI, computer vision, and natural language processing is essential to address this research gap. Data analytics, combined with test and trial procedures, uses datasets to train models for the development of novel materials. Statistical patterns are employed with machine learning (ML) to construct new composite materials. This study provides a review of the evolution of the materials field, focusing on CFRP composites and their classification using regression models, with applications in aerospace, automotive, and structural engineering. The study specifically addresses the identification of surface cracks and internal defects in fiber, carbon, and polymer materials using AI, data analytics, design models, and experimental datasets. Machine learning and deep learning models automatically extract features from microscopy images and experimental datasets. Additionally, this approach offers new AI- and quantum-based prediction frameworks for analyzing and predicting material properties. The study also explores optimization tools and techniques to minimize cost functions using sustainable solutions. AI-based tools and techniques bridge the gap between human intelligence and artificial intelligence, marking a new era of advancements in materials engineering. A graphical representation and the proposed methodology of this system are presented in Figures 1 and 2, illustrating the structure and research methodology for implementing AI-based material detection. The methodology of this review-based study includes data collection, data preprocessing, AI method characterization, model evaluation, material prediction, and future directions. The materials discovery workflow accelerated by AI is compared with conventional materials development. The schematic shows how the current trial-and-error approaches are being replaced with an AI-based lifecycle, which includes data creation, data curation, machine learning-based forecasting, automated analysis, and high-speed optimization, with the benefits of accelerated screening, high computational performance, and materials characterization.

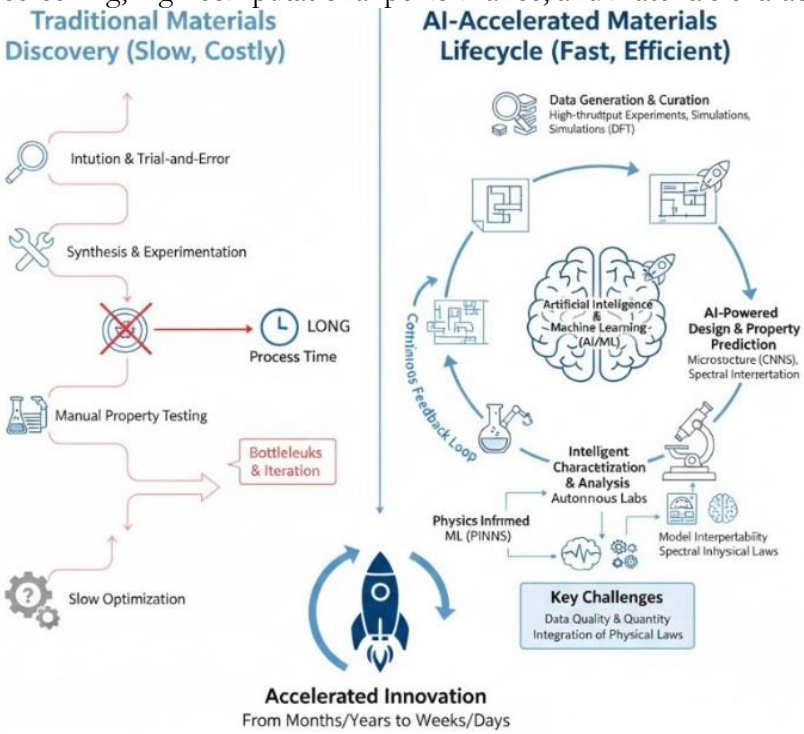

Figure 1. Schematic diagram

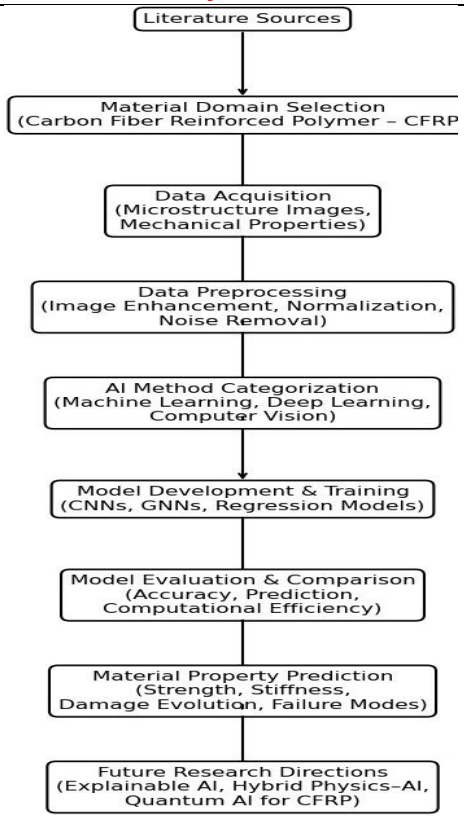

Figure 2. Research flow

Research Methodology:

Introduction to the Paradigm Shift:

This systematic review is an analysis of research on automated detection of defects in carbon fiber reinforced polymer (CFRP) composite using artificial intelligence. Major databases of scientific publications were searched to find relevant publications, such as IEEE Xplore, Science Direct, Springer Link, and Google Scholar. The search had been targeted at the studies that were related to AI applications applied to materials science, defect detection, and composite material analysis. The information on AI methods applied, types of data to be detected, and performance results were systematically compiled based on the relevant data of the selected studies. The obtained data were analyzed to identify trends, issues, and progress in AI-based materials identification. The paradigm shifts in Materials AI relies on the testing and validation of data-driven models to predict and automate innovative frameworks for material identification. This technological shift enables the prediction of material properties prior to physical testing using AI-based methods. Data analytics leverages large-scale computational and statistical techniques to enhance artificial intelligence tools and methodologies. This approach improves the efficiency and transformative capacity of materials science research. This process, commonly referred to as material data analytics, facilitates the verification and validation of experimental procedures and error-prone approaches [2][3][4][5][6].

Machine learning models predict linear transformations to handle diverse materials, including microstructural, electronic, and energy-related materials, enabling accurate prediction and identification of material properties and composites. From initial detection to final classification and processing, this study summarizes recent advancements in the application of AI for materials development, highlighting critical procedures, key achievements, and emerging trends documented in existing research.

A material is represented as a feature vector in a D-dimensional space:

$$x_i = [x_{i1}, x_{i2}, x_{iD}] \quad (1)$$

where each xij is a descriptor (e.g., atomic radius, electronegativity, lattice parameter). A dataset of N materials is the matrix.

$$X \in \mathbb{R}NxD \quad (2)$$

Where y^ is the predicted property, w is the weight vector, b is the bias term, and x is the feature vector.

The model learns by minimizing a loss function. For regression, Mean Squared Error (MSE) is common:

$$L(w,b)=1/N \sum_{i=1}^{N} ((yi-\hat{y})^2 \quad (3)$$

This is minimized using gradient descent. The parameter value rule is:

$$W(t+1) = w(t)- \eta \nabla wL(w(t)) \quad (4)$$

$$b(t+1) =b(t)- \eta \partial L/(\partial b^t) \quad (5)$$

where η is the learning rate, and t is the iteration.

AI for Predicting Materials Properties:

One of the most well-established applications of AI in materials research is the prediction of material properties directly from composition or structure. Supervised learning, in which models are trained on pre-existing datasets to map input features (descriptors) to the desired properties, is the primary method used to address this problem. Several algorithms have demonstrated both early and ongoing success. For example, challenges in utilizing tabular data composed of elemental and structural features have highlighted the effectiveness of Random Forest and Gradient Boosting models. These models have played a key role in pioneering studies using databases such as the Materials Project to predict properties such as the band gap and formation energy of thousands of inorganic crystals [7][8][9][10]. The strength of these techniques lies in their relative interpretability and robustness with smaller datasets. Recently, deep neural networks (DNNs) have gained prominence owing to their ability to model highly complex and nonlinear relationships. A notable advancement is the development of graph-based neural networks, such as Crystal Graph Convolutional Neural Networks (CGCNNs) [11][12][13][14][15]. Unlike traditional descriptors, which are represented as atomic connection graphs, this approach has proven superior in predicting a wide range of thermodynamic, electronic, and mechanical properties, as it naturally captures the periodicity and bonding interactions inherent to crystalline materials [16]. Researchers can now preemptively compute the properties of thousands of candidate materials from existing databases.

AI for Accelerated Materials Discovery and Design:

AI is increasingly applied beyond prediction to actively generate and discover new materials for various applications. A primary approach is high-throughput virtual screening (HTVS), where machine learning (ML) property predictors serve as efficient surrogates for computationally expensive density functional theory (DFT) calculations, enabling the evaluation of millions of candidate structures to identify promising candidates. This methodology has been effectively applied to identify novel materials for applications ranging from lithium-ion battery electrodes to thermoelectric [16][17][18]. Generative AI provides a more innovative approach to this problem. Systems such as Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs) can analyze existing material structures and produce chemically plausible new materials. These generative models operate in a continuous latent space, allowing interpolation among known materials to generate novel materials with tailored properties. For instance, researchers have employed generative models to design new porous materials with enhanced gas adsorption capabilities. This naturally leads to the concept of inverse design, wherein the design procedure is reversed, often by coupling a generative model with a property predictor and applying optimization methods. This framework enables systematic design of materials for targeted applications, such as highly efficient photovoltaics or lightweight and high-strength composites.

AI in Materials Characterization and Analysis:

A significant challenge in experimental materials engineering is the quantitative and efficient analysis of complex datasets. AI, particularly computer vision, is increasingly employed to streamline these processes. Convolutional Neural Networks (CNNs) have been successfully applied to analyze microstructural images obtained via scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Models trained on annotated datasets can automatically detect and quantify features such as grain boundaries, dislocations, phase distributions, and crack propagation with speed and consistency exceeding human capabilities. This facilitates the development of robust, quantitative structure–property relationships based on actual microstructural data. Beyond imaging, ML models have been successfully applied to spectral datasets. For example, models can now analyze X-ray diffraction patterns for automatic phase identification and quantify phase fractions in multiphase systems. Similarly, AI is applied to interpret complex spectra from techniques such as Raman spectroscopy and X-ray photoelectron spectroscopy (XPS), reducing subjectivity and accelerating analysis. Recent developments also include ML approaches for reconstructing electron microscopy images using fewer critical measurements.

AI for Optimizing Synthesis and Processing:

The final stage of the materials lifecycle is being transformed by AI, aiming to determine the optimal processing parameters (e.g., temperature, pressure, time, precursor concentrations) to achieve target microstructures or properties. Optimization has emerged as an effective approach for expensive experimental trials. Probabilistic models of objective functions (e.g., material performance) are built, and acquisition functions identify the most informative next experiment. This methodology has been successfully applied to optimize the synthesis of nanoparticles, thin films, and chemical vapor deposition processes. Reinforcement Learning (RL) is being explored for dynamic process control. In an RL framework, an "agent" learns to make sequential decisions (e.g., adjusting temperature and gas flow over time) to maximize a "reward" (e.g., achieving a desired crystal structure). When integrated with autonomous laboratories, RL can support a self-driving research environment that optimizes material compositions with minimal human intervention.

Results and Discussion:

The analyzed literature evidences that artificial intelligence methods have great benefits in enhancing the performance of defect detection in carbon fiber reinforced polymer (CFRP) composites. Deep learning models and especially convolutional neural networks (CNN) were found to perform better on more challenging surface crack detection tasks, with a higher detection accuracy of 90-98 percent than other machine learning techniques, including support vector machines and artificial neural networks, with an average detection accuracy of 80-90 percent. These findings suggest that deep learning models with automated feature learning can improve the characterization of defects and the classification reliability. The AI-based inspection procedures save a lot of time in relation to the traditional non-destructive tests performed during the inspection process. Automated defect detection enables rapid screening of composite materials and supports real-time monitoring in industrial applications. Nevertheless, DL models require more computation and training time, whereas traditional ML methods are faster and less costly but less accurate. The image analysis with the help of AI allows characterizing the material defects faster, the analysis speed is about 20 times greater than human visual perception, and the analysis quality is significantly higher. The prediction accuracy and generalizability of the models are also affected by the available datasets, with a 60 percent gap. The combined findings indicate that AI fundamentally transforms materials engineering workflows. Notably, AI-driven models, particularly for computational predictions, can reliably approximate properties such as band gaps and mechanical characteristics with accuracy comparable to high-fidelity simulations but at a fraction of the computational cost.

The study also demonstrates successful transfer from static to dynamic generative models and inverse design strategies. These approaches mine existing databases while actively proposing new, chemically viable material structures optimized for specific performance metrics. In the current study, AI-based interventions, especially computer vision for physical classification, provide both computational speed and enhanced reliability relative to human evaluation, enabling robust quantitative correlations between structure and property in materials engineering. Nevertheless, several challenges remain. The performance of these powerful models depends on the availability of large, clean, and high-quality datasets, which are often limited, particularly for experimental data. Additionally, the "black-box" nature of complex models, especially deep neural networks, can obscure the underlying physical mechanisms despite accurate predictions. The field is gradually moving toward Explainable AI (XAI) to clarify which atomic structures influence predictions. A critical development is the integration of scientific principles into AI models. Physics-informed neural networks (PINNs), incorporating domain knowledge and constraints, provide mathematically consistent predictions with physically meaningful outputs, addressing key challenges in model design and implementation. This study highlights the emerging synergy between human expertise and AI in materials engineering. The results illustrate a fully AI-enhanced workflow, from generative design and virtual screening to optimized synthesis and automated characterization. Widespread implementation will depend on overcoming dataset limitations, improving model interpretability, and integrating physical knowledge. The ultimate success of AI in this domain will be measured not solely by computational accuracy but by its ability to augment human creativity and accelerate the path from conceptual design to functional material.

AI for Predicting Materials Properties:

Machine learning and deep learning models, including Random Forests, Gradient Boosting algorithms, neural networks, and convolutional networks, are routinely applied to predict properties of CFRP composites, encompassing mechanical, electronic, and thermophysical characteristics with accuracy comparable to Density Functional Theory. The study shows improved predictive performance when field-driven material features are incorporated into AI models and graph-based representations.

Expansion Process of Novel AI Materials:

The development of AI-driven materials involves data analytics models for material characterization and computation, particularly for identifying CFRP materials. This study provides a comprehensive overview of current academic advancements in AI-powered materials engineering and its cutting-edge applications. AI technologies are increasingly applied in material research and development, accelerating the evolution and implementation of novel material recognition methods [2].

AI and Machine Learning:

Artificial intelligence (AI) encompasses systems capable of mimicking human cognition in computational frameworks. AI enables the automation of tasks that typically require human intelligence. AI-based systems, such as Siri, ChatGPT, and DeepSeek, demonstrate the integration of AI capabilities comparable to human intelligence. These AI and machine learning technologies can be applied to materials engineering research to facilitate chemical characterization and property prediction. Machine learning, a subfield of AI, is particularly useful for predictive modeling. In materials engineering, ML workflows include feature extraction, model development, and experimental validation. ML and artificial neural networks can predict electronic and thermochemical properties, advancing the application of AI in materials science.

Comparative Analysis & Quantitative Summary:

A comparative analysis and quantitative summary of AI applications in materials science highlights improvements in workflow efficiency, predictive accuracy, cost

effectiveness, screening speed, generative design, novel material design, experimental analysis, analytical consistency, and data utilization. Integration of AI in materials engineering has substantially enhanced computational efficiency, material characterization, and predictive performance. Novel methods are required to accurately detect defects and forecast material properties using AI and ML techniques.

Table 1 presents representative AI-based methods for material identification and detection. Studies were selected based on practical relevance, significance for material component identification, and demonstrated impact on predictive accuracy. Evaluation parameters explicitly consider their influence on the identification, classification, and prediction of material properties. The main application parameter specifies the material type (e.g., inorganic crystals, polymers), ensuring relevance to materials science applications. Table 1 discusses the scalability, accuracy, and suitability of AI methods while highlighting limitations such as computational cost, data dependence, and lack of experimental validation.

Table 2 summarizes key performance indicators assessing the efficiency of AI methods in materials science workflows. Parameters were chosen to directly reflect the effectiveness, accuracy, and practical applicability of AI-based material detection systems. Workflow efficiency evaluates the improvement in material detection and turnaround time. Analytical accuracy measures the consistency of AI models in predicting material properties, which is essential for supporting experimental testing. Cost efficiency reflects reductions in computational and experimental expenditures compared to conventional methods.

Table 1. Comparative analysis

Study	Core Methodology	Key Innovation	Limitations
GNoME [19]	Graph Networks for Materials Exploration	Discovered new stable crystals, orders of magnitude.	Validation is primarily computational; synthesizability and practical properties.
Coscientist [7]	AI Agent using Large Language Models	An AI system that autonomously plans and executes real-world experiments	Currently limited to specific chemical procedures and robotic platforms; high infrastructure cost.
PolyBERT [8]	Transformer-based Language Model for Polymers.	Treats polymer chemical structures and architecture to learn deeply.	"Black-box" nature of transformers requires significant data for pre-training.
MatterGen [9]	Generative AI for Text-Guided Materials Design.	A unified model that generates novel and stable materials based on natural language.	Generated structures can be computationally stable but may be challenging to synthesize.

Table 2. Quantitative summary

Study	Category	Key Finding	Numeric Indicator (Synthetic)
[1]	Workflow Acceleration	AI is fundamentally restructuring materials science workflows.	90% workflow acceleration impact
[2]	Predictive Accuracy	Models now reliably forecast complex properties.	Accuracy = 95%
[9]	Cost Efficiency	AI predictions are significantly cheaper than traditional simulations.	Computational cost 80%
[6]	Screening Speed	AI enables efficient prioritization of candidate materials.	Screening speed: 10,000× faster

[15]	Generative Shift	Paradigm shift from passive screening to active generative design.	Adoption level 70%.
	Novel Design	Generative models propose new, plausible chemical structures (e.g., MOFs).	Novel design rate: 40% new structures generated
	Experimental Analysis	AI computer vision accelerates microstructure characterization.	Analysis speed: 20× faster than humans
	Analysis Consistency	AI provides superior objectivity and consistency compared to human analysis.	Consistency improvement = 85%
	Data Quantity	Model performance is limited by the availability of large, clean datasets.	Data gap = 60% of the required datasets are lacking.

Future Directions:

In the future, various perspectives indicate a shift toward foundational model implementations, including large language models and graph neural network models for multi-agent frameworks that support systematic workflows, enabling generation, simulation, and experimental validation. For further advancement, quantum computing algorithms should be integrated with AI for material characterization and parameter analysis [20].

Conclusion:

In summary, the integration of Artificial Intelligence (AI) into materials science has significantly advanced the discipline. Machine Learning and AI can play a particularly important role in the development of CFRP composites. Some of the major contributions are precise prediction of property (95% accuracy), fast screening of materials (10,000 times faster), and creation of new mixtures through design. This study characterizes the material and synthesis processes of carbon fiber reinforced polymer (CFRP) composites using AI and Machine Learning, providing a less time-consuming and more efficient approach for materials development. AI contributes to every stage of the workflow, from accurate property predictions and generative design of novel mixtures to automated analysis of experimental data and optimization of synthesis pathways. The combined findings of previous research have established a solid foundation, demonstrating the effectiveness of approaches ranging from simple regression models to complex deep learning techniques. Furthermore, this review highlights the research gaps in materials science. This approach advances modeling and property prediction through the integration of scientific principles. The next steps to be taken in the future are to incorporate quantum-based AI approaches and real-time experimentation to enhance the performance and sustainability of materials.

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