SYNTHESIS, CHARACTERIZATION AND PROCESSING OF NEW MATERIALS FOR INNOVATIVE APPLICATIONS
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REVIEW

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Transformers in material science: Roles, challenges, and future scope

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ABSTRACT

This study explores the diverse applications, challenges, and future prospects of employing vision transformers in various material science domains, including biomaterials, ceramic materials, composite materials, energy materials, magnetic materials, electronics and photonic materials, materials synthesis, polymers, and nanomaterials. In the realm of biomaterials, the application of vision transformers has significantly improved our understanding of biological interactions, leading to the development of innovative medical implants and drug delivery systems. In ceramic materials, these transformers have revolutionized design and production processes, ensuring higher durability and efficiency. Likewise, in composite materials, they have enabled the creation of lightweight yet robust structures, transforming industries from aerospace to automotive. Energy materials research has greatly benefited from vision transformers, facilitating the discovery of novel materials for energy storage and conversion. Additionally, the study of magnetic materials has been transformed by their ability to analyze intricate magnetic patterns, aiding in the development of advanced data storage technologies. In electronics and photonic materials, vision transformers have accelerated the evolution of compact and high-performance devices. Integrating vision transformers poses challenges in managing vast and intricate datasets, ensuring model interpretability, and addressing ethical concerns related to data privacy and bias. As vision transformers continue to advance, their application in materials synthesis, polymers, and nanomaterials is anticipated to yield groundbreaking discoveries. This study highlights the way forward, underscoring the importance of collaborative efforts between computer scientists and materials researchers to unlock the full potential of vision transformers in reshaping the landscape of material science.

KEYWORDS

Transformer; Deep learning; Convolutional neural network; Features extraction; Materials

ARTICLE HISTORY

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Introduction

In the dynamic realm of material science, the fusion of cutting-edge technologies has paved the way for innovative research methodologies, with Vision Transformers (ViTs) emerging as a transformative force [1-4]. These ViTs, integrating deep learning and computer vision techniques, promise to revolutionize the exploration, analysis, and comprehension of diverse materials [3,5]. This research delves into the profound impact of ViTs within material science, focusing on specialized areas such as biomaterials, ceramic materials, composite materials, energy materials, magnetic materials, electronics, and photonic materials, materials synthesis, polymers, and nanomaterials. Traditionally, material studies have been propelled by experimental techniques and theoretical models, leading to significant discoveries and technological advancements. However, the digital era has ushered in a new paradigm, where the convergence of artificial intelligence and material science has unlocked unparalleled opportunities [6-10]. Vision Transformers, originally designed for image recognition tasks, have showcased exceptional capabilities across various domains, prompting researchers to explore their potential in material science [1,4].

The intricate and varied nature of materials demands advanced tools for characterization, analysis, and prediction. ViTs, with their ability to decipher intricate patterns and relationships within visual data, offer a fresh approach to tackle the challenges encountered in material science [1,3]. By harnessing the potential of ViTs, researchers can delve deeper into the microstructures, compositions, and behaviors of materials across different domains. This deeper understanding can expedite the development of innovative materials, enhance existing technologies, and pave the way for novel applications (Figure 1). This research aims to present a comprehensive overview of the applications, challenges, and future prospects of employing Vision Transformers in various subfields of material science. Specifically, the research explores how ViTs are being utilized in biomaterials, ceramic materials, composite materials, energy materials, magnetic materials, electronics and photonic materials, materials synthesis, polymers, and nanomaterials. By assessing the current state of research, analyzing challenges, and envisioning future trajectories, this paper contributes to the growing body of knowledge at the intersection of artificial intelligence and material science. As this research delves into the multifaceted applications of ViTs in material science, it aims to unravel the complexities of materials at a microscopic level, opening new avenues for exploration and innovation in this dynamic and vital scientific discipline.

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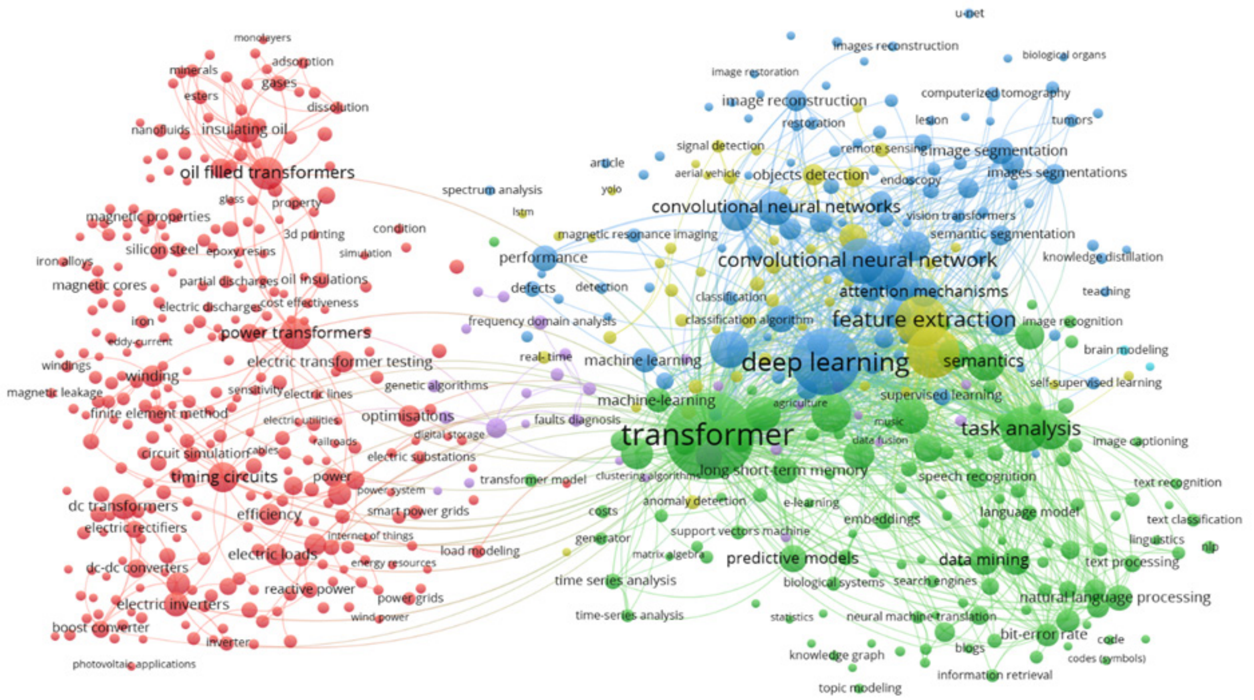

Figure 1. Co-occurrence analysis of the keywords in literature.

Vision Transformers in Biomaterials

Biomaterials represent engineered substances designed for interaction with biological systems in various medical applications, including tissue engineering, drug delivery, and medical devices [11-13]. Recent advancements in the field of biomaterials have been greatly influenced by the incorporation of artificial intelligence (AI) techniques [14,15]. An innovative approach in this regard involves the utilization of Vision Transformers (ViTs), a transformational technology rooted in the transformer architecture widely known for its remarkable performance in computer vision tasks. When applied to biomaterials, ViTs offer a distinct perspective, enabling efficient analysis, characterization, and design of a wide array of biomaterial types [16-20]. In contrast to conventional convolutional neural networks (CNNs), which process images in rigid grids, ViTs adopt a perspective of viewing images as sequences of patches. This sequence-centric approach empowers ViTs to grasp long-range dependencies within images, rendering them highly effective for tackling tasks involving intricate patterns and vast datasets [18,20]. Table 1 shows the applications and challenges of vision transformers in biomaterials.

Utilizing vision transformers for biomaterial characterization

Accurate characterization of biomaterials is pivotal for comprehending their properties and conduct in biological settings. ViTs present a robust tool for this purpose. By inputting microscopic images of biomaterial samples, ViTs can adeptly learn to identify and categorize various structures, such as nanofibers, pores, and surface textures. This capability holds particular significance in biomaterials research, where subtle structural differences can exert a substantial influence on the material's performance [19].

Polymeric biomaterials:

Polymeric biomaterials, encompassing polymers and copolymers, find widespread use in drug delivery and tissue engineering. ViTs can scrutinize scanning electron microscopy (SEM) images of polymeric biomaterials, facilitating the identification of features like polymer chains, cross-linking patterns, and porosity. This information is instrumental in refining the polymerization process and enhancing the mechanical and biological attributes of the biomaterial [16,18].

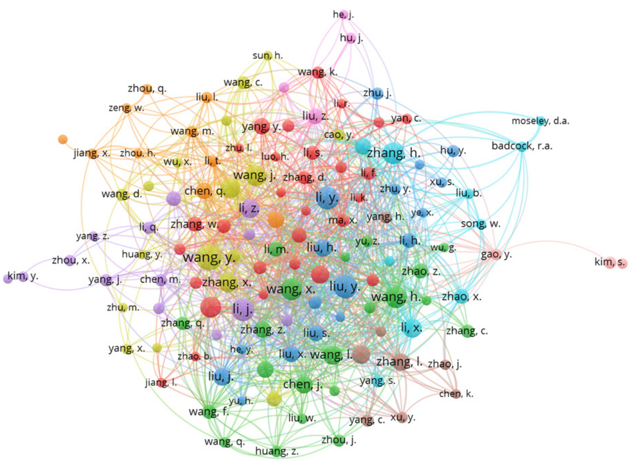

Figure 2. Co-authorship analysis in transformer for medical image analysis.

Ceramic biomaterials:

Ceramic biomaterials, exemplified by hydroxyapatite and bioglass, serve applications in bone tissue engineering and dental implants. ViTs excel in analyzing high-resolution images of ceramic structures, competently detecting crystal

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orientations, grain boundaries, and defects. This analysis is pivotal in understanding the mechanical strength and biocompatibility of the material, thereby leading to the development of more durable and efficacious implants [17].

Metallic biomaterials:

Metallic biomaterials, including titanium alloys used in orthopaedic implants and medical devices, benefit from ViTs' capabilities. These technologies can process images of metal surfaces obtained through techniques like atomic force microscopy (AFM) to identify surface roughness, corrosion patterns, and wear characteristics. This information is vital in the design of implants with enhanced wear resistance and biocompatibility [18,19].

Enhancing biomaterial formulations with vision transformers

ViTs also play a pivotal role in optimizing biomaterial formulations through the analysis of intricate datasets related to material composition, processing parameters, and performance metrics.

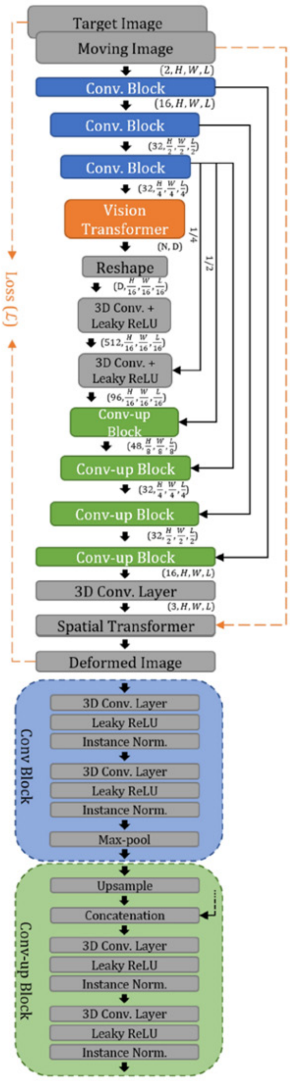

Figure 3. Network architecture of ViT-V-Net proposed by Chen et al. 2021 [1]

Composite biomaterials:

Composite biomaterials merge two or more distinct materials to attain specific properties. ViTs are adept at processing images of composite microstructures, effectively distinguishing between individual phases and interfaces. This ability streamlines the optimization of composite ratios, ensuring a harmonious balance of strength, flexibility, and bioactivity. Potential applications encompass the development of reinforced scaffolds for tissue engineering and composite coatings for medical devices (Figure 3) [20].

Nanomaterials:

Nanomaterials, exemplified by nanoparticles and nanocomposites, showcase unique properties due to their diminutive size. ViTs can analyze transmission electron microscopy (TEM) images of nanomaterials, enabling the quantification of particle size, shape, and distribution. This analysis is indispensable for designing nanoparticles for targeted drug delivery, where particle size directly influences cellular uptake and drug release kinetics [16,17].

Vision transformers in biomaterials simulation and prediction

In addition to experimental data, ViTs can leverage computational simulations and predictive modeling to expedite biomaterials research [21-23].

Molecular dynamics simulations:

Molecular dynamics (MD) simulations offer insights into biomolecular interactions at the atomic level. ViTs can scrutinize simulation trajectories and visualize molecular structures, assisting researchers in understanding how biomaterials interact with biological molecules. This knowledge is invaluable for designing drug delivery carriers and studying protein adsorption on biomaterial surfaces [24].

Property prediction:

ViTs possess the ability to predict various biomaterial properties, encompassing mechanical strength, biodegradation rate, and thermal conductivity, based on microstructural features. Through training on a diverse dataset of biomaterial images and corresponding properties, ViTs can generalize their learning to predict the properties of unseen biomaterials. This predictive capability expedites the material screening processes, enabling researchers to concentrate on the most promising candidates for specific applications [21,22].

Vision transformers for personalized biomaterial design

The concept of personalized medicine aims to tailor medical treatments to the unique characteristics of individual patients. In the context of biomaterials, ViTs contribute to the realization of personalized therapies and implants.

Patient-specific implants:

ViTs can process medical imaging data, such as computed tomography (CT) scans, to construct detailed 3D models of anatomical structures. By integrating these models with biomaterial design, ViTs facilitate the production of patient-specific implants customized to the anatomy of individual patients. This personalized approach enhances implant fit, reduces recovery time, and minimizes the risk of complications [25].

Drug response prediction:

ViTs can analyze cellular images to predict the responses of individual cells or patient-derived cell cultures to specific biomaterials or drug formulations. By correlating cellular morphology and behavior with treatment outcomes, ViTs enable the identification of biomaterials that are most effective for particular patient populations. This information proves invaluable in the design of personalized drug delivery systems and tissue engineering constructs [22,24].

Vision Transformers in Ceramic Materials

Ceramic materials have been an integral part of human civilization for millennia, finding applications in diverse fields, including construction, electronics, healthcare, and aerospace [24-26]. In recent years, the fusion of ceramics with artificial intelligence has led to groundbreaking advancements in material science and engineering [27,28]. Among the most

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revolutionary technologies in artificial intelligence is Vision Transformers (ViTs). ViTs, a category of deep learning models, have demonstrated exceptional performance in computer vision tasks, particularly in image recognition and analysis. Table 2. Shows the role and challenges of vision transformers in ceramic materials [29].

Applications of vision transformers in ceramic materials

Defect detection and quality control:

ViTs can automate the inspection process of ceramic materials. By training ViTs on extensive datasets of images showcasing various defects and imperfections in ceramics, the model can accurately identify and classify defects, such as cracks, chips, and impurities. This application ensures that only high-quality ceramic products reach the market, thereby enhancing the overall reliability and safety of ceramic materials in various applications (Table 1) [30].

Table 1. Applications and challenges of vision transformers in biomaterials.

S/N.	Biomaterial Type	Vision Transformer Applications	Challenges in Vision Transformer Implementation
1	Bioceramics	Example: Analyzing bioceramic coatings for orthopedic implants. - Studying material composition and predicting behavior. - Identifying structural properties for enhanced performance.	Example: Limited labeled data for specific bioceramic compositions. - Standardizing imaging techniques for accurate analysis. - Integrating vision transformers into complex manufacturing processes.
2	Biopolymers	Example: Studying biopolymer-based drug delivery systems. - Analyzing polymer morphology for controlled drug release. - Predicting biodegradation patterns for sustainable applications.	Example: Complex interactions between polymers and drugs. - Variability in natural polymer structures. - Real-time analysis for dynamic drug delivery systems.
3	Composite Biomaterials	Example: Investigating composite materials for dental applications. - Identifying material interfaces and bonding properties. - Predicting mechanical properties for optimal performance.	Example: Integrating data from diverse imaging modalities. - Limited understanding of long-term composite behavior. - Developing algorithms for real-time composite analysis.
4	Biosensors	Example: Developing biosensors for glucose monitoring. - Analyzing sensor surface for effective biomolecule binding. - Predicting sensor sensitivity and selectivity for accurate detection.	Example: Ensuring reliability of sensor readings under varying conditions. - Noise reduction in sensor data for precise measurements. - Integrating vision transformers with biosensor technologies seamlessly.
5	Biodegradable Metals	Example: Studying biodegradable metal stents. - Analyzing corrosion behavior in physiological environments. - Predicting mechanical integrity during degradation.	Example: Limited availability of in vivo degradation data. - Understanding complex interactions with biological systems. - Developing accurate simulation models for degradation behavior.
6	Hydrogels	Example: Developing hydrogel-based tissue engineering scaffolds. - Studying hydrogel structure for cellular attachment and growth.	Example: Controlling hydrogel swelling and degradation rates. - Real-time monitoring of hydrogel properties in dynamic physiological environments.

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Material composition analysis:

Ceramic materials often involve complex compositions comprising various elements and phases. ViTs can analyze the microstructure of ceramics at a granular level, identifying the composition of different phases and elements. This capability is invaluable in research and development, enabling scientists and engineers to optimize ceramic formulations for specific properties, such as strength, conductivity, or thermal resistance [29,30].

Predictive modelling and simulation:

ViTs can create predictive models for the behaviour of ceramic materials under different conditions. By training ViTs on data from experiments and simulations, researchers can develop accurate models predicting properties like mechanical strength, thermal expansion, and electrical conductivity. These models are invaluable for designing advanced ceramic materials for cutting-edge applications in industries such as aerospace and electronics [31].

Process optimization:

Ceramic manufacturing processes are complex and often involve multiple stages such as mixing, moulding, sintering, and glazing. ViTs can analyze data from various stages of the manufacturing process to optimize parameters like temperature, pressure, and composition. This optimization leads to increased efficiency, reduced energy consumption, and minimized waste, making ceramic production more sustainable and environmentally friendly [32].

Vision transformers and different ceramic material types

Traditional ceramics:

Traditional ceramics, such as clay-based products, have a long history in pottery and construction. ViTs can improve the quality control processes in traditional ceramics manufacturing by accurately detecting imperfections in the final products. Additionally, ViTs can analyze the composition of raw materials, ensuring consistency and quality in the production of traditional ceramic items (Table 2) [33].

Refractory ceramics:

Refractory ceramics are engineered to withstand extreme temperatures and harsh conditions, making them ideal for applications in kilns, furnaces, and the aerospace industry. ViTs can assist in the development of refractory ceramics with enhanced thermal and mechanical properties. By analyzing the microstructure of refractory ceramics, ViTs can optimize the material composition, resulting in improved heat resistance and longer lifespans in high-temperature environments [34].

Advanced ceramics:

Advanced ceramics, including oxides, nitrides, and carbides, are tailored for specialized applications in electronics, cutting tools, and biomedical devices. ViTs play a pivotal role in the development of advanced ceramics with customized properties. Their ability to analyze the crystal structure and grain boundaries of these materials enables researchers to design ceramics with superior electrical conductivity, hardness, and biocompatibility. ViTs also facilitate the detection of nanoscale defects in advanced ceramic components, ensuring the reliability of these critical components in various high-tech applications [30,32].

Bioceramics:

Bioceramics, such as hydroxyapatite and bioactive glasses, are used in medical implants and dental applications due to their biocompatibility and ability to integrate with natural tissues. ViTs can aid in the precise analysis of bioceramic surfaces and interfaces, ensuring the biocompatibility of implants and prosthetics. By detecting subtle surface irregularities or defects, ViTs contribute to the development of safer and more effective bioceramic materials for medical use [33].

Table 2. Role and challenges of vision transformers in ceramic materials.

S/N.	Ceramic Material Type	Applications of ViTs	Challenges
1	Porcelain Ceramics	1. Quality Control in Production 2. Surface Defect Detection 3. Ceramic Tile Inspection	1. Accurate Glaze Thickness Measurement 2. Detection of Microscopic Cracks 3. Variation in Surface Texture Analysis
2	Alumina Ceramics	1. Semiconductor Manufacturing 2. Wear-Resistant Components 3. High-Temperature Furnace Insulation	1. Precise Dimension Measurement 2. Surface Roughness Analysis 3. Contaminant Detection
3	Zirconia Ceramics	1. Dental Prosthetics 2. Aerospace Components3. Biomedical Implants	1. Color and Transparency Analysis 2. Detection of Grain Boundaries 3. Structural Defect Identification
4	Silicon Carbide Ceramics	1. Automotive Components 2. Armor Inserts 3. High-Temperature Electronics	1. Microcrack Detection2. Crystallographic Structure Analysis3. Surface Contamination Identification

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5	Ferrite Ceramics	1. Magnetic Components in Electronics 2. Microwave Devices 3. Inductors and Transformers	1. Detection of Magnetic Anomalies 2. Measurement of Magnetic Properties 3. Impurity Identification
6	Magnesium Oxide Ceramics	1. Electrical Insulation 2. Refractory Linings 3. Catalyst Supports	1. Purity Analysis 2. Thermal Conductivity Measurement 3. Surface Defect Identification
7	Carbon-Carbon Composites	1. Aerospace Thermal Protection Systems 2. Brake Disks 3. High-Temperature Structural Components	1. Delamination Detection 2. Microstructure Analysis 3. Surface Defect Characterization

Vision Transformers in Composite Material

Composite materials are engineered materials created by combining two or more constituent materials with markedly different physical or chemical properties. This fusion results in a material with characteristics distinct from its components. These versatile materials are widely used in various industries, including aerospace, automotive, construction, and electronics, due to their lightweight nature, impressive strength-to-weight ratio, and durability [29-34]. As technology advances, there is a growing demand for efficient methods to design, analyze, and manufacture composite materials. In recent years, artificial intelligence (AI) and machine learning (ML) techniques, including computer vision, have emerged as powerful tools for enhancing the development and understanding of composite materials [35-37]. One of the innovative approaches in this domain is the application of Vision Transformers (ViTs), a type of deep learning architecture that has demonstrated remarkable success in image recognition tasks [38,39]. Composite materials comprise a matrix material that binds together reinforcements, resulting in materials with superior properties. The matrix can be a polymer, metal, or ceramic, while reinforcements can be fibres, particles, or other forms. Common types of composite materials include:

Polymer matrix composites (PMCs)

PMCs consist of a polymer matrix reinforced with fibres like glass, carbon, or aramid. They are lightweight and exhibit excellent corrosion resistance, making them ideal for aerospace and automotive applications [38].

Metal matrix composites (MMCs)

MMCs involve a metal matrix reinforced with ceramic or metal fibres. They offer high strength at elevated temperatures, rendering them suitable for aerospace and automotive components [39].

Ceramic matrix composites (CMCs)

CMCs consist of a ceramic matrix reinforced with ceramic fibres. They possess high-temperature resistance and are used in gas turbine engines, nuclear reactors, and aerospace applications [40].

The role of vision transformers in composite materials

Image-based characterization of composite materials

Characterizing composite materials often requires microscopic analysis to understand the distribution and orientation of fibres or particles within the matrix. Traditional image processing techniques have limitations in handling complex patterns and large datasets. ViTs, with their ability to capture intricate patterns in images, offer a solution to these challenges [38,39].

Detection and classification of defects

Detecting defects in composite materials is crucial for ensuring their structural integrity. ViTs can be trained to identify defects like voids, delaminations, or fibre misalignments in microscopic images, enabling rapid and accurate quality control during manufacturing [39,40].

Predictive modelling and simulation

Predictive modelling of composite materials involves understanding their behaviour under various conditions. ViTs can assist in simulating material responses based on microstructural features, aiding engineers in optimizing composite designs for specific applications [40].

Applications of vision transformers in different types of composite materials

Polymer matrix composites (PMCs)

Fibre orientation analysis

ViTs can analyze microscopic images of PMC samples to determine the fiber orientation distribution within the matrix. This information is vital for predicting material properties like stiffness and strength, enabling manufacturers to tailor composites for specific applications [41].

Defect detection and repair

ViTs can automate the inspection process for PMC components, identifying defects in real time during manufacturing. Furthermore, ViTs can guide robotic systems in performing precision repairs on detected defects, enhancing the overall quality and reliability of PMC products [42].

Metal matrix composites (MMCs)

Reinforcement distribution analysis

ViTs can analyze scanning electron microscopy (SEM) images of MMC samples to quantify the distribution of reinforcing particles. This analysis helps researchers and engineers understand the relationship between particle distribution and material properties, facilitating the development of high-performance MMCs [41].

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Fatigue analysis

ViTs can assist in analyzing microscopic images of MMC samples subjected to fatigue testing. By recognizing microstructural changes indicative of fatigue damage, ViTs can aid in understanding the material's fatigue behaviour, leading to the development of MMCs with improved fatigue resistance [43].

Ceramic matrix composites (CMCs)

Microstructure-based modelling

ViTs can analyze high-resolution images of CMC microstructures and extract valuable data for computational models. By integrating this data into finite element simulations, engineers can accurately predict the thermal and mechanical behaviour of CMC components, enabling the design of CMCs for high-temperature applications [40,42].

Creep and thermal analysis

ViTs can be employed to analyze SEM images taken before and after high-temperature creep tests on CMC samples. This analysis helps in understanding microstructural changes and deformation mechanisms, allowing researchers to optimize CMC compositions for enhanced creep resistance and thermal stability [43].

Vision Transformers in Energy Materials

The convergence of artificial intelligence (AI) and material science has ushered in a new era of innovative solutions across diverse fields, particularly in the realm of energy materials [40-42]. A significant breakthrough in AI, specifically in the domain of computer vision, is the emergence of Vision Transformers (ViTs). These ViTs, a type of deep learning model, have demonstrated exceptional prowess in image recognition tasks [43-45]. Their unique approach to images as sequences of tokens, as opposed to conventional patch-based processing, allows ViTs to discern intricate patterns and long-range relationships within images, rendering them highly effective for various visual tasks [44,45]. Table 3 shows the role and challenges of vision transformers in magnetic materials.

Role of vision transformers in energy materials research

Materials discovery and optimization

Energy materials research often involves delving into intricate material compositions to enhance energy storage, conversion, and efficiency. ViTs significantly expedite this process by analyzing extensive databases of material structures and properties. Their ability to discern subtle patterns in materials expedites the discovery and optimization of novel materials for energy applications. By processing images of crystal structures, defects, and material compositions, ViTs assist scientists in pinpointing promising candidates for batteries, solar cells, and other energy devices [45].

Characterization of nanomaterials

Nanomaterials play a pivotal role in energy applications due to their unique properties at the nanoscale. ViTs aid in characterizing nanomaterials by analyzing high-resolution imaging data from techniques such as transmission electron microscopy (TEM) and scanning tunnelling microscopy (STM). By interpreting these images, ViTs help researchers comprehend the morphology, size, and surface features of nanoparticles. This knowledge is instrumental in designing nanomaterials tailored for specific energy-related tasks, including catalysis and energy storage [46].

Monitoring and quality control

In the production of energy devices, ensuring the quality and consistency of materials is paramount. ViTs, equipped with machine vision capabilities, can monitor manufacturing processes and conduct real-time quality control. By analyzing images of materials during production, ViTs can identify defects, impurities, or inconsistencies that might affect the performance and durability of energy devices. This application not only enhances the overall quality of energy materials but also reduces waste in the manufacturing process [47].

Predictive modeling and simulation

Predictive modelling is crucial for comprehending the behaviour of materials under diverse conditions. ViTs analyze images generated from simulations and experiments to provide insights into the structural changes and interactions within materials. By processing visual data, ViTs contribute to the development of precise computational models for predicting the performance of energy materials. These models are invaluable for researchers and engineers engaged in the design and optimization of energy devices such as fuel cells and supercapacitors [48].

Applications of vision transformers in various energy materials

Battery technologies

A. Electrode microstructure analysis

ViTs can scrutinize the microstructure of battery electrodes, encompassing parameters such as particle size, distribution, and connectivity. This analysis aids in optimizing electrode designs for enhanced energy storage and faster charge-discharge rates. ViTs' capacity to process vast amounts of electrode microstructure images expedites the development of high-performance batteries for electric vehicles and renewable energy storage systems [46-48].

B. Solid-state batteries

Solid-state batteries, with their improved safety and energy density, present promising alternatives to traditional lithium-ion batteries. ViTs contribute to solid-state battery research by analyzing images of solid electrolyte materials and electrode interfaces. These analyses help researchers identify suitable materials and optimize interfaces for efficient ion transport, culminating in the development of safer and more reliable solid-state battery technologies [49].

Solar cell technologies

A. Thin-film solar cells

Thin-film solar cells, prized for their lightweight and flexibility, find applications in wearable devices and building-integrated photovoltaics. ViTs assist in the analysis of thin-film materials such as organic polymers and perovskites by processing images of film morphology and composition. This analysis guides researchers in optimizing fabrication processes, leading to the production of efficient and cost-effective thin-film solar cells [50].

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B. Multijunction solar cells

Multijunction solar cells, comprising multiple semiconductor layers, achieve high efficiency by capturing a broader spectrum of sunlight. ViTs aid in characterizing each semiconductor layer by analyzing images obtained from techniques like scanning electron microscopy (SEM) and atomic force microscopy (AFM). By comprehending the morphology and quality of individual layers, researchers can design multijunction solar cells with improved efficiency and stability, crucial for concentrated solar power and space applications [48,50].

Catalyst materials for fuel cells

Fuel cells, acting as electrochemical devices converting chemical energy into electrical energy, have applications ranging from stationary power generation to fuel cell vehicles. ViTs play a pivotal role in analyzing catalyst materials, including platinum group metals and metal oxides, used in fuel cells. By processing images of catalyst nanoparticles and their interactions with electrolytes, ViTs assist in optimizing catalyst designs for enhanced catalytic activity and durability. This optimization is pivotal for advancing fuel cell technologies and promoting their widespread adoption as clean energy sources [49].

Supercapacitors and energy storage devices

A. Electrode nanostructure analysis

Supercapacitors, or ultracapacitors, store energy through electrostatic charge separation at the electrode-electrolyte interface. ViTs aid in analyzing the nanostructure of supercapacitor electrodes, including parameters like pore size, surface area, and electrode morphology. By optimizing these parameters based on ViTs' analyses, researchers can enhance the energy and power density of supercapacitors, rendering them suitable for high-performance energy storage applications in renewable energy systems and portable electronics [50].

B. Electrolyte characterization

The choice of electrolyte profoundly influences the performance and stability of energy storage devices. ViTs can analyze images of electrolyte materials, encompassing ionic liquids and polymers, to assess their purity, composition, and homogeneity. This analysis ensures the development of high-quality electrolytes, leading to improved energy storage device performance, lower internal resistance, and longer cycle life [48,49].

Table 3. Role and challenges of vision transformers in magnetic materials.

S/N.	Energy Material	Roles of Vision Transformers	Challenges
1	Solar Cells	- Detecting and classifying defects in solar panels. - Enabling predictive maintenance for solar power plants. - Assessing solar resources through satellite imagery analysis.	- Managing large-scale satellite imagery datasets. - Ensuring real-time analysis for timely maintenance. - Addressing environmental factors such as cloud cover affecting image analysis.
2	Battery Materials	- Analyzing microstructures to enhance battery performance. - Ensuring quality control in battery manufacturing processes. - Predicting battery degradation and remaining lifespan.	- Interpreting complex microstructures accurately. - Limited availability of high-quality labeled data for training models. - Addressing privacy concerns in manufacturing facilities.
3	Wind Energy	- Monitoring and inspecting wind turbine blades. - Analyzing wind patterns for energy output prediction. - Detecting and preventing wildlife collisions.	- Maintaining image clarity in adverse weather conditions. - Integrating vision systems in dynamic environments. - Ensuring safety for technicians and wildlife during inspections.
4	Nuclear Energy	- Inspecting nuclear reactors for safety. - Detecting and analyzing radiation leaks. - Automating routine maintenance tasks.	- Ensuring accurate a nd reliable radiation detection. - Adhering to strict safety protocols during inspections. - Addressing ethical concerns related to nuclear energy.
5	Hydropower	- Monitoring dam structural integrity. - Predicting water flow for energy optimization. - Assessing environmental impact through aquatic life monitoring.	- Managing varying water levels affecting image quality. - Developing algorithms for real-time flow prediction. - Balancing energy optimization with environmental conservation.
6	Photovoltaic Materials	- Analyzing surface morphology for enhanced light absorption. - Identifying defects and impurities to improve efficiency. - Predicting material behavior under different conditions.	- Interpreting nanoscale features for material optimization. - Handling variations in material composition affecting imaging results. - Integrating machine learning models with experimental research.
7	Carbon Capture and Storage (CCS)	- Monitoring facilities for leaks and structural integrity. - Analyzing geological formations for secure CO2 storage. - Automating gas sample analysis.	- Ensuring continuous and precise monitoring to prevent CO2 leaks. - Addressing security concerns related to underground storage sites. - Developing real-time gas composition analysis algorithms.

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8	Bioenergy	- Analyzing biomass feedstock quality and composition. - Monitoring fermentation processes in biofuel production. - Automating bioenergy crop inspections.	- Identifying diverse biomass sources and their properties. - Ensuring consistency in fermentation processes. - Adapting vision systems to varying field conditions.

Vision Transformers in Electronics and Photonic Materials

Vision Transformers (ViTs) have emerged as potent deep learning models in the realm of computer vision, originally tailored for image classification tasks [4,5]. Their impact extends far beyond their initial design, demonstrating significant potential across diverse fields, including electronics and photonic materials research [5,9,10]. ViTs' distinctive ability to interpret images as sequences of tokens, thereby capturing intricate long-range relationships, has ushered in groundbreaking applications within material science [3,5].

ViTs in electronics and photonic materials

Material recognition and classification:

ViTs play a pivotal role in the identification and categorization of materials in electronics and photonic research. By processing images of materials such as electronic circuits or photonic devices, ViTs accurately classify them based on composition, structure, or other defining properties. This capability expedites the work of researchers and engineers, aiding in the swift identification and categorization of diverse substances and their variations [50].

Material property prediction:

ViTs also excel in predicting various material properties like electrical conductivity, refractive index, or bandgap energy. Through training ViTs on material images alongside their corresponding properties, researchers can create models capable of estimating these properties for new or unknown materials. This predictive ability proves invaluable in material design, enabling scientists to explore novel materials tailored for specific electronic or photonic applications [48,49].

Image-based quality control:

ViTs are instrumental in automating quality control processes in electronics manufacturing. By analyzing images of electronic circuits, photonic devices, or material surfaces, ViTs identify defects, inconsistencies, or imperfections. This automation enhances efficiency, reduces costs, and elevates the overall reliability of electronic and photonic products [51].

Simulation and virtual prototyping:

In the domain of electronics and photonics, ViTs are applied in simulating and virtually prototyping circuits and devices. Processing images of circuit layouts or device designs, ViTs offer insights into performance characteristics and signal propagation. This information empowers engineers and researchers to optimize designs before physical prototypes are developed, saving time and resources in the development process [52].

Material discovery and exploration:

ViTs accelerate the discovery of new materials with unique electronic or photonic properties. By analyzing extensive datasets of material images, ViTs uncover patterns, correlations, and novel structures that might elude human researchers. This data-driven approach expedites the discovery of groundbreaking materials, fostering innovation in various technological applications [51].

Vision Transformers in Materials Synthesis

The fusion of artificial intelligence (AI) and machine learning techniques with materials synthesis has ushered in a new era of scientific and technological progress [46,47]. At the heart of this transformation lies the innovative application of Vision Transformers (ViTs) in deciphering complex material structures and properties. In the domain of organic materials, essential in electronics, energy, and healthcare, ViTs excel at comprehending intricate molecular configurations. By analyzing vast databases of organic compounds, ViTs unveil relationships between molecular structures and material characteristics, expediting the creation of tailored materials for flexible electronics, efficient organic photovoltaics, and biocompatible polymers used in medical applications [48-50]. Inorganic materials, the backbone of aerospace engineering, renewable energy, and catalysis, also benefit significantly from ViTs' capabilities. ViTs dissect subtle structural nuances, enabling researchers to predict inorganic materials' behaviour under diverse conditions. Through the analysis of crystal structures and electronic configurations, ViTs optimize synthesis parameters, foresee phase transitions, and design materials boasting superior mechanical, thermal, and electrical properties. This proficiency extends to the development of high-strength lightweight alloys and the creation of efficient catalysts for sustainable chemical processes [48].

Nanomaterials, characterized by size-dependent properties, have reshaped fields like medicine, electronics, and environmental science. ViTs have enhanced the synthesis and characterization of these materials by discerning intricate nanoscale patterns [49]. Utilizing ViTs, researchers can decode data from advanced imaging techniques such as Transmission Electron Microscopy (TEM) and Atomic Force Microscopy (AFM). ViTs aid in identifying nanoparticle morphologies, crystal structures, and surface properties, enabling precise control of nanoparticle synthesis for applications like targeted drug delivery, quantum dot-based electronics, and efficient water purification technologies [46-48].

Furthermore, ViTs have a crucial role in optimizing composite materials, blending two or more distinct components to create synergistic properties. In aerospace engineering, ViTs assist in designing lightweight yet robust composites, ensuring structural integrity and improving fuel efficiency. Similarly, in biomaterials, ViTs facilitate the development of biocompatible composites for medical implants, harmonizing mechanical strength with biological compatibility. The marriage of ViTs

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with materials synthesis not only accelerates scientific discovery but also paves the way for groundbreaking innovations across diverse industries [51].

Vision Transformers in Polymers

Polymer materials, integral components of our daily lives, serve a wide range of purposes in fields spanning from healthcare to electronics, shaping the contemporary industrial landscape and driving innovation. In the era of artificial intelligence (AI) and machine learning (ML), new horizons emerge for augmenting the comprehension, design, and production of polymer materials [51,52]. Among these cutting-edge AI techniques, Vision Transformers (ViTs) stand as a promising tool poised to revolutionize the exploration and application of polymer materials [53-55].

Material discovery and design:

ViTs expedite the swift exploration of expansive chemical compound spaces, empowering researchers to unearth novel polymers tailored to specific properties. By training ViTs using images of molecular structures and their associated attributes, researchers can forecast material behaviour predicated on visual patterns. This approach expedites the discovery of polymers attuned to applications such as lightweight composites, flexible electronics, and biodegradable materials [52].

Microstructure analysis:

Grasping the microstructure of polymers holds paramount significance in predicting material characteristics. ViTs proficiently scrutinize microscopic images of polymer specimens, capturing nuanced features that might prove challenging for conventional image processing techniques. By recognizing patterns in the arrangement of polymer chains, ViTs contribute to characterizing crystallinity, defects, and morphological variations, thereby offering invaluable insights for material optimization [53].

Quality control and defect detection:

In the domain of polymer manufacturing, ensuring product quality assumes utmost importance. ViTs excel in quality control tasks by inspecting polymer surfaces for anomalies, irregularities, or contaminants. Through training ViTs with images of both ideal and defective polymer samples, manufacturers can implement automated inspection systems, significantly boosting production efficiency and reducing wastage [51,52].

Predictive modelling and simulation:

ViTs play an instrumental role in predictive modelling by scrutinizing images obtained from simulations or experiments. By discerning the intricate associations between polymer structures and properties, ViTs aid in the formulation of precise predictive models. These models empower researchers to simulate polymer behaviour under diverse conditions, facilitating the design of materials with enhanced performance and durability [50].

Polymer recycling and sustainability:

In an era of growing environmental consciousness, polymer recycling and sustainable material development have ascended in importance. ViTs prove invaluable in the recognition and categorization of polymer materials in recycling facilities. Additionally, ViTs can evaluate images of recycled polymer blends, guiding the development of sustainable materials by unravelling the impact of various additives and processing techniques on material properties [52].

Biomedical applications:

Polymers occupy a pivotal role in biomedical applications, encompassing drug delivery systems and tissue engineering. ViTs contribute to the analysis of images related to biomaterials, enabling researchers to optimize polymer scaffolds for tissue regeneration. ViTs also facilitate the comprehension of the interplay between polymers and biological entities, fostering the development of biocompatible materials for medical devices [53].

Utilizing vision transformers (ViTs) for polymer morphology analysis

The characteristics of polymers, such as crystallinity, grain size, and phase distribution, profoundly impact their properties. ViTs excel in analyzing microscopy images to delve into polymer morphology. For instance, in semi-crystalline polymers like polyethylene, ViTs accurately discern and quantify crystalline and amorphous regions. This precision offers valuable insights into mechanical and thermal properties. Likewise, in polymer blends, ViTs differentiate between phases, aiding the development of tailored blends for specific applications [51,53].

Harnessing ViTs for polymer property prediction

Understanding and predicting polymer properties are crucial for customizing materials for specific uses. ViTs, with their capacity to discern intricate patterns in vast datasets, can predict properties like mechanical strength, thermal conductivity, and optical transparency. For example, ViTs trained on images of stressed polymer samples can predict mechanical properties based on deformation patterns, enabling swift and precise assessments without physical tests. This acceleration in the materials discovery process leads to the creation of innovative polymers for advanced applications [54].

Integrating ViTs into polymer processing monitoring

Polymer processing methods, such as extrusion and injection moulding, significantly influence final material properties. Real-time monitoring of these processes is vital for ensuring product quality. ViTs incorporated into monitoring systems can analyze video feeds from processing lines. By identifying patterns and anomalies, ViTs facilitate early defect detection, ensuring only high-quality polymer products reach the market. This real-time monitoring enhances efficiency, reduces waste, and elevates overall production quality [55].

Automating polymer recycling with ViTs

Polymer recycling is pivotal in mitigating environmental impact. ViTs assist in automating sorting and recycling processes. By analyzing images of mixed polymer waste, ViTs efficiently classify and sort materials. This automation not only boosts recycling rates but also ensures recycled polymers meet quality standards. ViTs contribute to fostering a circular economy by promoting sustainable practices in polymer material usage [52,54].

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Enhancing polymer nanocomposite development through ViTs

Polymer nanocomposites, where polymers are reinforced with nanoparticles, exhibit superior properties. ViTs play a crucial role in their development by analyzing images from transmission electron microscopy (TEM) and scanning electron microscopy (SEM). ViTs identify nanoparticle dispersion, size, and orientation within the polymer matrix. This in-depth analysis assists researchers in optimizing nanocomposite formulations for exceptional mechanical, electrical, and thermal properties, driving innovations in fields such as electronics and aerospace [54].

Table 4. Roles and challenges of vision transformers in nanomaterial research.

S/N.	Nanomaterial Type	Roles of Vision Transformers	Challenges
1	Nanoparticles	1. Characterization: Analyzing electron microscope images to determine size, shape, and surface properties.	1. Resolution: Achieving high-resolution images for accurate characterization.
		2. Quality Control: Detecting defects and ensuring consistency in production.	2. Data Variability: Managing variations in imaging conditions affecting analysis.
2	Nanotubes	1. Structural Analysis: Identifying nanotube structures, including chirality and defects.	1. Complex Structures: Developing algorithms for analyzing complex multi-walled nanotube structures.
		2. Functionalization Monitoring: Observing changes in surface properties during functionalization.	2. Limited Training Data: Insufficient labelled data for nanotube-specific models.
3	Nanocomposites	1. Phase Distribution: Analyzing images to ensure uniform distribution of components.	1. Image Noise: Managing noise interference in microscopic images.
		2. Performance Evaluation: Evaluating mechanical, electrical, or thermal properties through images.	2. Integration Challenges: Integrating Vision Transformers with other analytical techniques.
4	Nanowires	1. Composition Analysis: Identifying elemental composition based on images.	1. Sample Artifacts: Addressing artifacts introduced during sample preparation.
		2. Integration in Devices: Assisting in precise integration into various devices.	2. Real-time Analysis: Developing fast real-time image processing algorithms.
5	Quantum Dots	1. Size and Shape Analysis: Analyzing images for uniformity in size and shape.	1. Fluorescence Variability: Managing variations in quantum dot fluorescence.
		2. Bioimaging Support: Enhancing analysis for bioimaging applications.	2. Biological Context: Incorporating nanomaterial analysis in complex biological systems.
6	Nanorods	1. Optical Properties: Understanding optical properties for sensor and imaging applications.	1. Interparticle Interactions: Analyzing interactions in clustered nanorods.
		2. Surface Modification Monitoring: Observing surface modification processes.	2. Sensitivity: Ensuring detection of subtle surface changes.

Vision Transformers in Nanomaterials

Nanomaterials, with their distinctive properties derived from their minuscule scale, have ushered in groundbreaking advancements across diverse fields, including electronics, medicine, energy, and catalysis [56-58]. Understanding these materials at the nanoscale is vital to grasp their behaviour and unlock their full potential. Conventional methods such as electron microscopy and X-ray diffraction have been pivotal in this pursuit. However, the advent of artificial intelligence (AI) and machine learning, specifically Vision Transformers (ViTs), has transformed nanomaterials science [57,58]. Table 4 shows the roles and challenges of vision transformers in nanomaterial research.

Nanoparticles:

Nanoparticles, ranging from 1 to 100 nanometers, exhibit distinct optical, magnetic, and catalytic properties compared to

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bulk materials. ViTs can analyze high-resolution transmission electron microscopy (HRTEM) images of nanoparticles. By training ViTs on extensive HRTEM datasets, researchers can develop models adept at precisely identifying nanoparticle size, shape, and crystal structure. This information is indispensable for tailoring nanoparticles for applications in drug delivery, imaging, and sensing [59].

Nanocomposites:

Nanocomposites, formed by integrating nanoscale materials into a matrix, find utility in lightweight materials, automotive components, and aerospace structures. ViTs can analyze scanning electron microscopy (SEM) images of nanocomposite surfaces. Through semantic segmentation, ViTs differentiate nanoscale filler particles from the matrix material, offering insights into nanoparticle dispersion and alignment within the composite. This comprehension is pivotal for optimizing the mechanical, thermal, and electrical properties of nanocomposites [60].

Nanowires and nanotubes:

Nanowires and nanotubes boast exceptional electrical and thermal conductivity, making them ideal for nanoelectronics and energy storage devices. ViTs can process transmission electron microscopy (TEM) images of these materials, identifying crystallographic defects, stacking arrangements, and surface modifications. By analyzing these features, researchers can design nanowires and nanotubes with enhanced performance for applications in batteries, sensors, and flexible electronics [61].

Quantum dots:

Quantum dots, semiconductor nanoparticles with quantum mechanical properties, exhibit size-dependent optical and electronic behaviors. ViTs can analyze fluorescence microscopy images of quantum dots, extracting details about their size distribution, emission spectra, and surface chemistry. This meticulous characterization is indispensable for developing quantum dot-based technologies, including displays, solar cells, and biological imaging probes [62].

Nanocatalysts:

Nanocatalysts, owing to their extensive surface area and unique surface reactivity, are pivotal in catalysis and environmental remediation. ViTs can analyze high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images of nanocatalysts, providing insights into particle size, shape, and composition. By correlating these structural features with catalytic activity, researchers can design efficient nanocatalysts for applications in hydrogen production, pollutant degradation, and chemical synthesis [63].

Conclusion

This study thoroughly explored the applications, obstacles, and prospects of employing Vision Transformers across various Material Science domains, including Biomaterials, Ceramic Materials, Composite Materials, Energy Materials, Magnetic Materials, Electronics and Photonic Materials, Materials Synthesis, Polymers, and Nanomaterials. Navigating through these diverse arenas has shed light on the transformative potential of Vision Transformers, offering a profound glimpse into the future of Material Science research and innovation. One of the standout findings from this investigation is the diverse array of applications that Vision Transformers offer across different material types. In the realm of Biomaterials, these AI-driven models assist in developing biocompatible materials, optimizing their properties for medical implants and tissue engineering. In Ceramic Materials, Vision Transformers aid in understanding material microstructures, enabling the design of advanced ceramics for various industrial applications. Composite Materials, crucial in aerospace and automotive industries, benefit from AI algorithms that enhance the structural integrity and performance of these materials. Furthermore, in Energy Materials, Vision Transformers can significantly enhance the efficiency of solar cells and energy storage devices, paving the way for sustainable energy solutions.

Nevertheless, challenges persist in the integration of Vision Transformers in Material Science. The scarcity of high-quality labeled data, a perennial AI challenge, hampers the training of accurate models. Overcoming this hurdle requires collaborative efforts between material scientists and data scientists to curate extensive datasets. Additionally, the interpretability of AI-driven models remains a concern, particularly in fields where understanding material behavior is as crucial as the predictions themselves. Striking a balance between predictive power and interpretability is essential to ensure the trust and acceptance of these AI technologies in the scientific community. Despite these challenges, the future outlook for Vision Transformers in Material Science is exceptionally promising. Ongoing advancements in AI, especially in self-supervised learning and few-shot learning, hold the key to addressing the data scarcity issue. Collaborative initiatives involving research institutions, industry partners, and AI developers can lead to the creation of comprehensive material databases, fueling the development of robust Vision Transformer models. Moreover, incorporating domain-specific knowledge into AI algorithms can enhance the interpretability of these models, making them invaluable tools for material scientists.

In the years to come, the convergence of Vision Transformers and Material Science is set to revolutionize various industries. The ability to expedite the material discovery, optimize material properties, and predict material behaviour with unprecedented accuracy will catalyze innovation and drive economic growth. Furthermore, the sustainable practices enabled by AI-driven material design will play a pivotal role in addressing global challenges such as climate change and resource scarcity. The integration of Vision Transformers in Material Science marks a paradigm shift in how materials are researched, designed, and utilized. This research journey has illuminated the vast potential of AI in enhancing our understanding of materials and accelerating the development of groundbreaking technologies. As we move into this AI-driven future, collaboration, innovation, and a profound understanding of both material science and artificial intelligence will be the driving forces propelling us toward a new era of scientific discovery and technological advancement.

Disclosure statement

No potential conflict of interest was reported by the author.

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