Advancing materials science: Translating innovative research to commercial prospects

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Materials science is one of the disciplines characterised by steady research and development (R&D) efforts and technological innovation, being the backbone of many innovations in a wide range of industries from aerospace and automotive to healthcare.

Advances in material discovery, design, synthesis, characterisation and manufacturing have resulted in the development of newer materials, with each development contributing to technological progress in various industries and helping to overcome global challenges.

The field has witnessed an influx of research initiatives that have led to developing materials with unprecedented properties and expanding applications across various industrial domains. Developments related to nanomaterials, biomaterials, and smart and responsive materials contribute significantly to technological progress, meet industry-specific requirements, and address global challenges.

Nanomaterials have enhanced the performance of various components and devices due to their unique mechanical, electrical, and optical properties, and the development of various 2D materials beyond graphene is becoming important for next-generation communication, electronics, and optoelectronic devices. Biomaterials and biomimetic materials are increasingly adopted in coatings, healthcare, and personal care applications.

Sustainable materials are also being actively pursued in various industries, including textiles, building and construction, and automotive, in efforts to reduce carbon emissions. High entropy alloys and smart materials, which include responsive and adaptive materials, are being investigated in aerospace, defence, energy, and other industries where traditional materials face challenges.

With materials being key to advances in various industries, it’s evident that material development goes beyond just creating materials that meet application demands. It involves a holistic approach that considers the entire lifecycle of materials, from sourcing raw materials, their characterisation, design, and manufacturing to end-of-life disposal.

Innovations in materials discovery, design, synthesis, and characterisation

Research advances and integration of new methodologies in discovery, design, synthesis, and characterisation are accelerating the research pace and reducing the time to market. Still, they are also helping in the development of materials with tunable and new properties that are tailored for specific applications. The application of data-driven material discovery and design approaches, especially machine learning (ML) and (AI), has helped identify promising candidates for specific applications and predict material properties more efficiently than the traditional trial-and-error methods.

Initiatives such as the establishment of the Institute for AI-Enabled Materials, Discovery, Design, and Synthesis (AIMS), spearheaded by researchers from Penn State, MIT, and the University of Wisconsin-Madison to establish and nurture interdisciplinary collaborations to integrate AI advances and technologies in material development, develop frameworks, infrastructure, collaborative human-AI tools, etc., to accelerate material discovery.

High-throughput synthesis and characterisation methods are instrumental in accelerating material synthesis and characterisation. Integrating automation technologies and data analytics will help screen and analyse massive datasets and material samples, reducing the time needed to identify compounds with desirable properties. Efforts from institutes such as Pacific Northwest National Laboratory (PNNL), which has integrated ML and AI into synthesis and characterisation methods, including microscopy, to achieve both high throughput and precision in materials screening and Fraunhofer's Center for Material Characterization and Durability Analysis, which is focused on testing and measurement of different materials for varied applications including for solar energy utilisation, energy storage, and building energy technology, etc. opens new possibilities for materials discovery and design. These advances are also likely to reduce the reliance on rare or critical elements by providing cost-effective and sustainable alternatives.

Virtual simulation and modeling techniques, integration of ML with computational methods and advanced characterisation techniques, and autonomous experimentation platforms, such as the Scientific Autonomous Reasoning Agent (SARA), can help in parallel material synthesis, map reactions and transitions, and discover metastable materials. These methods can also predict material behaviours and properties and structure-property relationships of materials even at atomic and molecular scales, reducing R&D time and effort and providing detailed insights into materials interactions and behaviour under operational conditions.

Innovations in manufacturing processes

The material manufacturing landscape is currently characterised by deploying advanced processes that improve efficiency, enable precision, and help achieve required material properties. Thermal processes that raise metals above their boiling points, thermomechanical processes that combine thermal and mechanical processes to alter the microstructural properties of materials, additive manufacturing for layer-by-layer, on-demand manufacturing, deposition techniques that result in thin film coating or deposition onto various substrates to modify surface properties and improve performance. Surface treatment processes that modify a material's surface properties to enhance its characteristics, amongst others, have enabled material development with tailored properties for specific applications.

One of the major focus areas in material manufacturing is using energy-efficient processes and sustainable manufacturing. The development of sustainable materials has become a critical focus in materials science, as the materials industry is one of the carbon-intensive industries globally. As the industry aims to reduce environmental impact and promote resource efficiency, stakeholders actively explore bio-based, recyclable, and biodegradable materials to replace traditional, non-renewable ones. There is a significant shift towards integrating sustainability principles into materials development and manufacturing processes. For example, one of the focus areas of the Wallenberg Initiative Material Science for Sustainability is to research next-generation eco-friendly materials and manufacturing processes to develop future energy systems that are environmentally friendly.

Sustainable manufacturing: Gaining prominence

Manufacturing processes, especially high-temperature treatments like welding, cutting, and additive manufacturing, have traditionally been energy-intensive and environmentally taxing. Recent research focuses on making these processes more sustainable through energy efficiency and waste reduction. Advances in recycling and upcycling technologies have facilitated material recovery and reuse, contributing to a more circular economy.

Research initiatives such as that of the Max Planck Institute for Sustainable Materials explore the potential of various climate-neutral, resource-conserving approaches to manufacture and recycle essential materials, which can minimise waste and contribute to material circularity. Gaining interest in the use of sustainably derived materials and alternative feedstocks has resulted in customising various manufacturing processes, including additive manufacturing, to accommodate these materials, which can reduce the demand for virgin materials.

Using advanced computing and analytical techniques to optimise process parameters also helps minimise energy consumption and material wastage. Initiatives from institutes such as The Center for Sustainable Materials at Rutgers University undertake research and developmental activities related to renewable materials to reduce dependence on crude-derived sources. The use of green chemistry principles, solvent-free synthesis, and facilitating energy-efficient reaction and process conditions are helping to minimise the use of hazardous substances and reduce waste.

Integrating material characterisation methods to assess the environmental impact throughout the material lifecycle also helps design sustainable alternatives. A thorough understanding of the mechanisms that govern material properties, be it nanoscale or macroscale, helps design materials with specific functionalities and minimal environmental impact.

Multiscale modeling and simulation tools predict material behaviour across different scales, facilitating the design of high-performing and sustainable materials. For example, efforts from the Massachusetts Institute of Technology (MIT) have resulted in the development of computational models that can predict material properties based on atomic structure. Such models can be used to develop tailored, smart materials that consider environmental factors, thereby helping stakeholders achieve sustainability in material design.

What next for material development: Key action points

Advances in material development are to drive innovation in various industries. Continuous R&D and innovation are important to understand material properties and their interactions with various intrinsic and extrinsic factors at a molecular level, which is a prerequisite for developing next-gen, high-performance, and environmentally sustainable materials that meet industry-specific requirements. Continuous efforts from industrial stakeholders, academic researchers, and governmental bodies are essential to translate academic and fundamental research into practical solutions.

The complex and interlinked requirements from materials necessitate collaborative activities that cut across traditional developmental boundaries. There is an increasing need to involve interdisciplinary teams that combine expertise in physics, chemistry, manufacturing, materials science, data analytics, and advanced computing to tackle material developmental challenges and meet the ever-evolving needs of various industries. Interdisciplinary collaborations can also help develop integrated processes that minimise energy consumption, waste generation, and integrate recycled materials into manufacturing chains to promote circular and closed-loop systems.

Industry-academia collaborations can translate fundamental research into practical applications without minimal hassles. They can also facilitate the scaling up advanced and sustainable materials and processes and bridge the gap between laboratory research and commercial requirements. Continued access to funding and investment, not limited to specific stakeholders, can help develop holistic solutions for sustainable and smart material development.

Policies and regulatory support will go a long way in encouraging researchers and companies to develop advanced materials in their ongoing research initiatives. Incentivising sustainable practices can support sustainable material development and manufacturing and establish resilient and sustainable value chains.

Sources

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