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A short review of machine learning in materials engineering: state of art, recent trends

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ABSTRACT

This paper summarizes the developments in machine learning in material science. It begins with an overview of basic machines learning methods and describes their application in important fields of material science such as discovery of new materials, prediction of material properties and optimization of their performance. It notes recent trends in the field such as the growth of big data, the appearance of explainable AI as well as improvements in numerical techniques. The objective of this paper is to give an overview of how machine learning helps accelerate the process of making discoveries in the sphere of materials science.

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1. Introduction

It is important to acknowledge that advancements in materials science not only influence our everyday lives but also drive development. Materials have become essential to progress, making the quest for new materials a vital and modern topic in the field. To enhance the discovery and design of innovative materials, a variety of computational methods have been developed alongside experimental techniques [1]. The integration of machine learning (ML) and artificial intelligence (AI) is profoundly transforming the field of materials engineering, significantly accelerating the discovery and development of novel functional materials [2, 3]. Machine learning offers powerful, data-driven modeling. It provides new insights that go beyond traditional methods [4]. Materials engineering has traditionally developed alongside advances in characterization and synthesis techniques and computational capabilities. In recent years, AI has been added to this ever-developing toolbox [5, 6], and may help overcome challenges in the discovery of new materials [7] for particularly important applications, including renewable energy, quantum computing, and clean water. Although there seems to be promise associated with these AI developments, there is still much ambiguity to researcher's intended use of these tools, the skill sets needed to effectively utilize these technologies, and how they will change research practices among materials engineers. AI innovations may lead to considerable progress, such as the creation of room-temperature superconductors, fundamentally altering industries and scientific paradigms. While ML has similarities with traditional statistics, it's critical to recognize that AI has advanced so rapidly that we are moving into an area, or way of thinking, that was once considered science fiction. In this regard, it is important to understand that researchers will need to adapt their skills and methods to flourish in an AI-enabled future [8-12].

This mini-review introduces the concept of the machine learning in the realm of materials engineering. Moreover, the potential of machine learning to accelerate discovery, enhance material performance, and drive technological progress is emphasized. The application of machine learning in materials science is characterized by the specific data types and features relevant to the field, such as Chemical, thermal, and electrical properties.

1.1. Machine Learning in Materials Engineering

The process of creating new materials with the desired characteristics usually takes a lot of time in research to collect enough information about certain materials. Although new experimental and computational technologies have been developing fast and producing a large amount of data, people are still limited in how they perceive and utilize this information. Therefore, it is necessary to come up with some new techniques to speed up the process of developing new materials [13, 14]. The enormous

influence that machine learning (ML) has made on this process can be seen in the ability it gave researchers to create predictive models, which helped significantly reduce the time needed for making materials. Moreover, ML technologies help researchers acquire new knowledge about materials, which enables faster development and design of materials. Lastly, ML may also be utilized in the processing of images, which helps to identify and classify the objects and create images; it has also proved to have the ability to process atomic-scale data [2]. The field of machine learning makes it possible for learning to occur using limited experimental data with the ability to create models involving complicated and non-linear relationships with multiple inputs. This is particularly applicable when estimating composite materials produced by many factors including material properties, processing conditions, and the relationships in the final product. By using machine learning for this purpose, material designers will reduce the number of experiments needed for determining certain relationships between properties and ultimately create better models [5].

Fig. 1 illustrates the human AI interaction in a coordinated setup with a central AI, using an LLM interface that accesses scientific literature, physics, math engines, internet, databases, and controls robotic experiments [8].

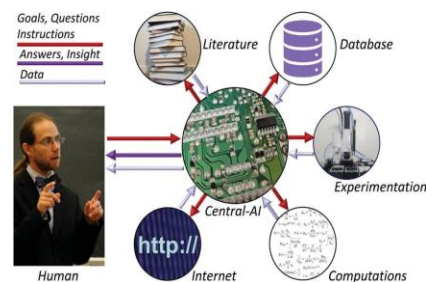


Fig. 1. Illustration of the human AI interaction in a coordinated setup with a central AI, using an LLM interface that accesses scientific literature, physics, math engines, internet, databases, and controls robotic experiments [8].

1.2. Importance and Impact

By automating mundane processes, expediting experimental cycles, and improving decision making, machine learning and AI technology are revolutionizing materials research [15, 16]. The use of these technologies speeds up the process of finding and improving the characteristics of new materials while allowing scientists to work more productively rather than replacing them [6]. Advanced devices like large language models can assist in literature searches, formulating hypotheses, and designing experiments, thereby creating new possibilities for more effective research processes. The use of AI will require researchers to be more

adaptable and able to think strategically and creatively as it becomes more advanced and integrated into their workflows [8].

2. Machine Learning Techniques

Machine learning can be classified into various categories, including supervised learning, unsupervised learning, semi-supervised learning, reinforcement learning, transduction, as well as learning-to-learn [17]. On top of that, machine learning in the field of not only involves several different stages which are: 1) data collection and management, 2) selection of relevant features, 3) model evaluation and selection, 4) training of the model, and 5) tuning of hyperparameters [8, 18].

Beyond basic models, large language models use transformer architectures to comprehend complex scientific and language data. In the meantime, neural networks [19, 20], reinforcement learning [21, 22], clustering [23, 24], and physics-informed neural networks [25] are also applied in material science in order to process obtained data, ensure the optimization of the various processes, and all physical laws as well. All in all, different ML methods help to speed up discovery process as well as to cope with complex emerged problems [8].

3. State of the Art in Machine Learning Applications

In order to produce optimal, practical engineering solutions, thorough examinations of several parameters are required in many conditions. It can be hard to model the complex interaction of these parameters, requiring mathematical approaches. This has caused the research community to look for computational methods that can offer faster and cheaper solutions. With the emergence of machine learning, this area of science is undergoing a major change. The use of machine learning has already produced some promising results in the field of materials science [6]. Fig. 2 shows various machine learning applications [26].

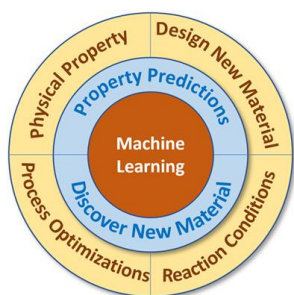


Fig. 2. Various machine learning applications [26].

3.1. Material Discovery and Design

Integrating artificial intelligence and machine learning into materials science has opened innovative ways to discover and optimize new materials [27]. A key advancement is Inverse Design, where AI and ML techniques predict the appropriate material composition or structure to fulfil particular specifications in terms of the desired properties, effectively reversing the conventional approach and speeding up the discovery process [28, 29].

In a research, Rickman et al. [30] developed a supervised learning method to screen high-entropy alloys by combining

regression analysis, canonical-correlation analysis, and genetic algorithms. This technique detected promising alloys with high hardness through properties prediction from existing data and validating predictions through experimental synthesis. In another research, Mannodi-Kanakkithodi et al. [31] demonstrated that curated materials data can be used to train models that promptly predict properties of new materials from simple fingerprints. By combining these models with genetic algorithms, polymers with desired dielectric properties were identified, offering a powerful tool for rapid polymer design and screening. However, this method was limited to specific building blocks and simple representations.

3.2. Predicting New Materials

Over recent years, ML has been employed effectively for predicting material behavior; however, widespread large-scale application of different algorithms remains limited. In particular, recent studies on polymer composites highlight ML's potential for applications such as prediction, optimization, uncertainty quantification, and sensitivity analysis—offering valuable insights into enhancing composite material performance [6].

In a study by Mansouri Tehrani et al. [32] ML was used to predict elastic moduli and guide the discovery of hard materials. By screening over 118,000 compounds, they synthesized a rhenium tungsten carbide and a molybdenum tungsten borocarbide, both of which closely matched the model's predictions, with less than 10% error. Microhardness tests showed both exceed 40 GPa, demonstrating the effectiveness of ML-driven materials development. In another study, Oliynyk et al. [33] trained a machine-learning model to identify Heusler compounds, intermetallics with versatile properties for thermoelectric and spintronic applications. The model can distinguish Heusler, inverse Heusler, and CsCl-type structures among over 400,000 candidates, achieving a true positive rate of 94%. It also assists in data validation. Applying it to AB₂C formulas, the model predicted 12 new gallides, which were confirmed experimentally, including TiRu₂Ga, showing clear Heusler order.

3.3. Mechanical, Thermal, and Electrical Properties

Machine learning has become an invaluable asset in the study of the physical, chemical, and mechanical properties of polymer composites because of their use in a wide spectrum of applications including the aerospace, automotive, marine, and civil sectors. Key applications of machine learning include predictions of properties and uncertainties as well as sensitivity analysis. Difficulties regarding dimensionality and overfitting can be solved with the help of modern algorithms, thus paving the way for advancements in research [4].

Machine learning models trained on material datasets can efficiently predict mechanical properties and identify optimal compositions or structures [10]. Deep neural networks have designed oxide glasses with properties like Young's modulus and shear modulus [34, 35]. Neural networks have also been used for designing strong copper alloys [36-38] and predicting fracture toughness, elasticity, and strength in diverse materials like composites and spider webs. Atomistic descriptors and convolutional neural networks (CNNs) excel in capturing structural-property relationships in nanostructured materials, polymers, and

more. ML methods are transforming mechanical property prediction and materials design [10].

In a study, Wu et al. [39] combined ML algorithms with laboratory synthesis and advanced measurements, resulting in the discovery of polymers with competitive thermal properties. This demonstrated the potential of ML in accelerating material discovery in polymer science. This work indicated the success of ML techniques on material innovation. In another study, Ducamp et al. [40] showed that ML can be employed to predict the thermal characteristics of siliceous zeolites based on some parameters such as geometry and topology. The authors developed machine learning algorithms trained on DFT data, which worked well especially when geometric descriptors were used. Their models can be applied for the large-scale investigation of structure databases like the PCOD2 zeolite database containing 600,000 structures. Moreover, Liang et al. [41] demonstrated that machine learning can optimize two-stage aging parameters in Cu-Ni-Si alloys, enhancing strength and conductivity through multi-objective optimization. The process achieved a tensile strength of 875 MPa and excellent electrical performance, thanks to the combined precipitation of DPs and CPs, offering new insights for alloy property improvement. Additionally, Kutsukake et al. [42] Showed how using an ML-based approach is possible to optimize two-stage aging in Cu-Ni-Si alloys, increasing their strength and conductivity through multi-objective optimization. The results included a tensile strength of 875 MPa and good electrical properties achieved with the aid of combined DPs and CPs precipitation.

Liu et al. [43] created a neural network to predict carrier recombination velocity at grain boundaries based on photoluminescence profiles. The network was created using 1800 noise-containing simulated profiles. The results showed that the predicted value was accurate (R^2 equals 0.97) and computation time was significantly reduced. In a study by Tawfik et al. demonstrated that machine learning can be used to successfully predict vibrational properties, such as entropy, capacity of heat, dielectric function, and a band gap based on quantum simulations, which allows performing fast screenings and facilitating material discovery [44]. Moreover, Tuan-Anh and Zalesny [45] used machine learning techniques in determining (hyper)polarizabilities of more than 50,000 molecules based on quantum chemical facts. The models obtained correlation coefficients above 0.9, however, analysis showed that diversity of linkers plays an important role in the selection of training sets.

3.4. Optimization Techniques

The Design of Experiments provides an opportunity for simultaneous testing and optimization of many variables. This is a fast way to discover new materials while saving time and resources. If coupled with machine learning, this method allows for a more complex view on optimization by moving from testing in isolation towards experimentation as a multidimensional process [46]. In a research, Ling et al. [47] suggested a data-based optimization technique in order to save time in finding new materials by connecting experimental results and predictive models that suggest what the next experiment should be. The key idea of the approach is that it operates with high-dimensional parameter spaces, and thus allows to combine explorative and exploitive approaches through uncertainty analysis. The results of the experiments showed a three-

time reduction of the number of experiments needed to get optimal candidates compared to the random sampling.

3.5. Active Learning and Surrogate Models

Hsu and Lin [48] propose a method known as ALBL, which is a pool-based active learning technique that employs intelligent machines to select efficient techniques. In ALBL, various strategies are selected based on their performance with the help of feedback. The idea uses the algorithm EXP4.P from the literature of multi-armed bandits and the computation of performance through importance-weighted accuracy. The experiments show that this method is very effective for making reasonable choices and sometimes surpasses other random or human techniques, thus proving to be very practical.

Guo et al. [49] The innovative technique for constructing surrogate models in input-output problems is to find important characteristics using principal components and then leverage active subspace techniques to generate low-dimensional models for those features. The main goal of the new adaptive learning mechanism is to achieve a balance between exploring unknown areas and improving pre-existing areas with high errors, leading to better accuracy of the model while transforming the newly created data back to the original high-dimensional space. The technique is applied in simulations of additive manufacturing that is characterized by complex distribution of residual stresses.

4. Recent Trends in Machine Learning for Materials Engineering

In recent years, materials informatics has progressed quickly with the implementation of machine learning (ML) and artificial intelligence (AI) in research. Some noteworthy directions are: validation by means of experiment or simulations; development of ML tools suited to the complicated heterogeneous structure of material data; improvement of high-throughput methods of data acquisition; enhancement of effectiveness of scientists by means of explainable and interpretable ML; introduction of the physics to ML techniques [50].

Nanotechnology materials are valuable in the area of catalysis or energy storage as well as in the field of biomedicine. However, how to control defects has been a challenge for technologies so far used. The use of artificial intelligence and machine learning is a magical and unprecedented opportunity for prediction and control of defect creation along with optimization of synthesis process [51].

Even though major strides have been made in big data machine learning recently, a number of important challenges remain to be addressed. Examples include the need to enhance preprocessing and rule-learning methods, cope with non-consistent message source interpretations where ontologies and semantic web tools can be applied, and strike a balance between the cost of training data and model efficiency. Furthermore, there is a growing interest in the integration of different approaches such as data mining and cloud computing as well as machine learning in a unified system. Moreover, working on the issue of data privacy in the analysis of information and the implementation of the research results are necessary pathways for future activities [52].

ML is transforming material science, especially for solving complex issues in polymer composites. Hybrid ML combines

algorithms to improve prediction accuracy, as seen in applications like stochastic impact mechanics and shear capacity estimation. Adaptive ML, using reinforcement learning, adjusts predictions based on feedback and is effective for multi-scale analyses and bridging molecular to continuum scales. Techniques like multi-fidelity modeling optimize diverse datasets for high accuracy. Recent advancements, including feature selection and adaptive learning, show ML's immense potential in polymer composite research, despite being in its early stages [4].

4.1. Integration of Big Data and Machine Learning

Big data is quickly growing across all fields of science and engineering. Although its potential is immense, fully understanding and utilizing these vast datasets demands new perspectives and innovative learning methods to tackle associated challenges. In this paper, we review recent developments in ML techniques for processing big data [52].

ML models improve with more data, but large-scale multi-omics analyses on a single computer are often impractical. Advances in optimization, parallelization, and cloud computing now make it feasible allowing, for example, deep neural networks to be trained in hours instead of days—greatly enhancing high-dimensional data analysis [53]. Fig. 3 Shows the standard flow path of ML towards data-based scientific discovery in materials science, from data production to classification or inference [54].

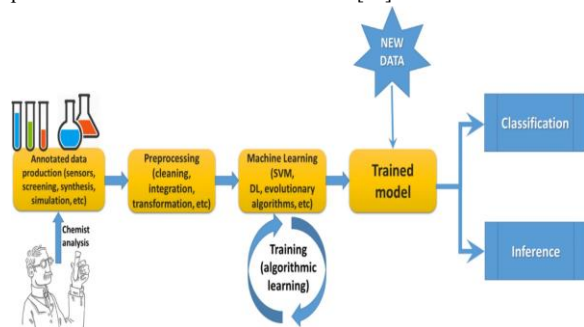


Fig. 3. The standard flow path of ML towards data-based scientific discovery in materials science, from data production to classification or inference [54].

4.2. Explainable Artificial Intelligence (XAI) in Materials Science

Machine learning has become a vital and powerful tool in materials research, especially as more data are generated through high-performance computing (HPC) and high-throughput experiments. While ML accelerates scientific discovery, its true potential relies on models that not only predict accurately but also offer explainability. Explainable Artificial Intelligence (XAI) in materials science is crucial for building trust, identifying model limitations, and uncovering scientific insights by making model decisions transparent and understandable [55].

Explainable models are those in which explanations for their predictions can be generated, either by directly inspecting the model (intrinsic interpretability) or through additional post-hoc methods (extrinsic explanations) [56, 57]. While technically any ML model's process can be fully reproduced, these are often complex and difficult to interpret within the relevant domain these are called

quasi-explanations, which rely on concepts beyond the model's application context. The key qualities of a good explanation are understandability how well it relates to domain concepts and completeness how fully it describes the model's underlying workings. There's often a trade-off between these qualities: a fully detailed explanation might be technically complete but hard to understand, while a simpler, domain-relevant explanation might sacrifice some completeness. Effective explanations should align with domain theories and be potentially actionable, helping users make informed decisions based on the model's insights [55].

XAI methods are vital in the context of materials science as they facilitate the development of models whose predictions can be understood. Some intrinsic methods like linear models or decision trees inherently provide clear explanations, while post-hoc methods examine complex models (e.g., neural networks) to find the features responsible for their prediction. The given explanations make it possible to gain trust in the predictions, point out the nature of the processes involved, and provide valuable insights into scientific discovery in materials science [58]. Fig. 4 Shows XAI process [56].

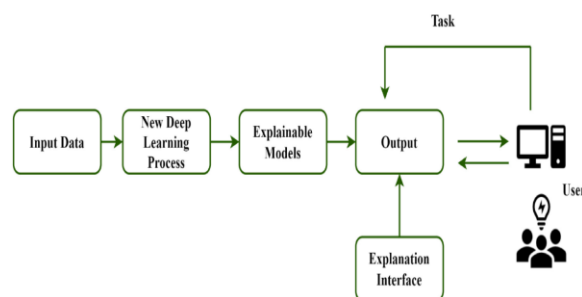


Fig. 4. Explainable AI process [56].

In machine learning, it is important to evaluate the quality of explanations in terms of fidelity and usefulness. Basic rules are to evaluate explanations for their applicability, reliability, sensitivity, and simplicity. The main challenges in materials science are the absence of known truths, the complexity of evaluating explanations, and the issues of model errors. Advanced training strategies like adversarial training increase the quality of explanations. The development of user-friendly tools for explainable artificial intelligence, the usage of domain knowledge in the XAI process, and the implementation of other approaches, including physics-informed models, are critical directions for the future work in the area of explainable AI [13]. Fig. 5 shows different scopes and aspects of explainability [13].

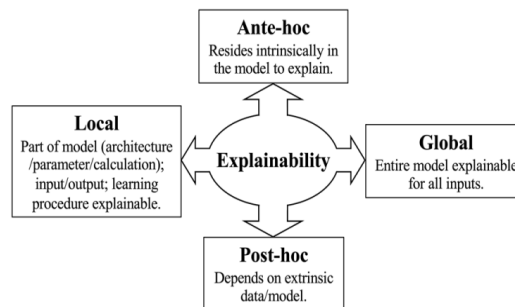


Fig. 5. Different scopes and aspects of explainability [13].

4.3. Advances in Computational Techniques

The recent breakthroughs in computational methods have provided significant impetus for a preferred use of the ML technology in materials engineering. Due to the application of different HPC systems, which include multi-core processors and extremely parallel processing systems, the scale and speed of simulations have improved tremendously. Multinode processing clusters have made it possible to deal with big datasets and complex models [59]. Besides, ML methods are often used for the creation of surrogate models, which allow saving funds on expensive simulations like DFT, MD, and CFD. The use of such models significantly quickens the material property prediction and provides the opportunity to make multi-scale modeling easier, thus contributing to a wider exploration of materials [60]. In addition, new technologies, like GANs and transformer-type models, are used for innovative materials. All of these developments in technology allow materials science to become faster, better, and scalable [9].

5. Conclusion

In the field of materials science, human expertise has always been an important factor in obtaining reliable results; however, limitations of human intellect make the process of prediction less efficient and precise. Even though new technologies have significantly improved the available methods and tools, getting new materials still takes time and effort. The processing rate of the human brain is very limited, which has led to the need for new techniques speeding up the materials development. AI development, especially related to machine learning, has already improved the field by allowing fast prediction of properties of materials, as well as formulation of materials and gaining insight in the working mechanisms. However, to achieve the desired results, it is also necessary to know how to preprocess information properly and how to choose the right model.

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Marziyeh Azad: Contributed to writing the original draft and reviewing and editing the manuscript.; **Bhekumuzi Sfundo Khanyileb:** Contributed to writing the original draft and reviewing and editing the manuscript.

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Conflict of Interest

The authors confirm that there are no conflicts of interest to declare.

Data Availability

No data are available for this study.

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