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Application of Machine Learning Tools to Material Science: A Mini-Review

Orhadahwe TA[1]*, Oladunni AA[2] and Onadeko OO[1]

[1]Department of Mechanical Engineering, Ajayi Crowther University, Nigeria

[2]Department of Chemical Sciences, Ajayi Crowther University, Nigeria

***Corresponding author:** Thomas Aghogho Orhadahwe, Department of Mechanical Engineering, Ajayi Crowther University, Oyo, Nigeria; Email: thomasaghogho@gmail.com

Mini Review

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Abstract

Machine learning has become a global trend in artificial intelligence and computing. Its application cuts across different industrial verticals. The application of machine learning algorithms in material science and related fields is becoming a topic of interest to many researchers. However, unlike other fields such as health, sports, communication, and agriculture, the use of machine learning in material science is still in its ideation stage. This mini-review is designed to explore some of those machine learning tools that have been applied to material science, the importance of machine learning in material science, and the challenges limiting the implementation of machine learning techniques in material science. One of the major findings from this review is that the limited availability of material science data is a major challenge to the implementation of machine learning algorithms. A specialized material science data repository was recommended.

Keywords: Artificial Intelligence; Supervised Learning; Deep Learning; Convolution Neural Network; Material Processing

Abbreviations: ML: Machine Learning; CNN: Convolutional Neural Networks; ANN: Artificial Neural Network; DNN: Deep Neural Network; BMI: Body Mass Index; GB: Gradient Boosting; RF: Random Forest; SVR: Support Vector Regression; MCA: multi-component Alloys.

Introduction

Material science is a field of science that studies the relationship between the structure, properties, and applications of materials [1]. Professionals in this field are called material scientists. The importance of materials in engineering design and application cannot be overemphasized [2]. Engineering materials are needed to bring into reality various design concepts and ideas in the mind of engineers thereby turning them into useful products for the benefit of mankind and society by improving the standard of living and contributing to economic growth. In recent years, material science has become a growing field of study which is partly due to the high cost of materials and scarcity of certain materials due to global population growth and demand. These have necessitated material engineers to research alternatives by synthesizing new materials that are smart and more affordable than conventional materials. This can be achieved by altering the structures of materials through physical, thermal, or chemical treatments. The altered structure thereby presents new properties that are desired in specific operation conditions and service conditions [3,4].

During the design of engineering structures and machines, one of the design problems is material selection [5]. The engineer or scientist is faced with a wide range of materials and diverse properties to select from. Similarly, the availability of properties of different materials will further assist the material scientist with the necessary information required to synthesize new materials for new application areas. There are over 300,000 different materials on Earth comprising metals, non-metals, plastics, ceramics, and composites. A huge dataset will be required to capture all these materials and their properties. This has led material science researchers to diversify into the fields of data science and machine learning techniques in material science. The purpose of this review is to establish the extent of the work done, and the various machine learning tools and techniques that have been deployed in material science studies.

Machine Learning Tools and Techniques

Machine learning (ML) is a growing concept in the world of computing and artificial intelligence and has been viewed as one of the drivers for the actualization of Industry 4.0 [6]. The focus of ML is to develop computer systems that can learn from data. The process of machine learning begins with the development of an algorithm based on collected data, thereafter, the algorithm is trained to identify and understand relationships and patterns in the dataset. The algorithm or model is then tested with a similar dataset before it is finally deployed in the specific area of application. The process of training the model is referred to as the learning process. ML models can be broadly classified into four main groups based on how the models are trained or how the models learn as shown in Figure 1. The classifications are supervised learning, unsupervised learning, semi-supervised learning, and reinforcement learning [7].

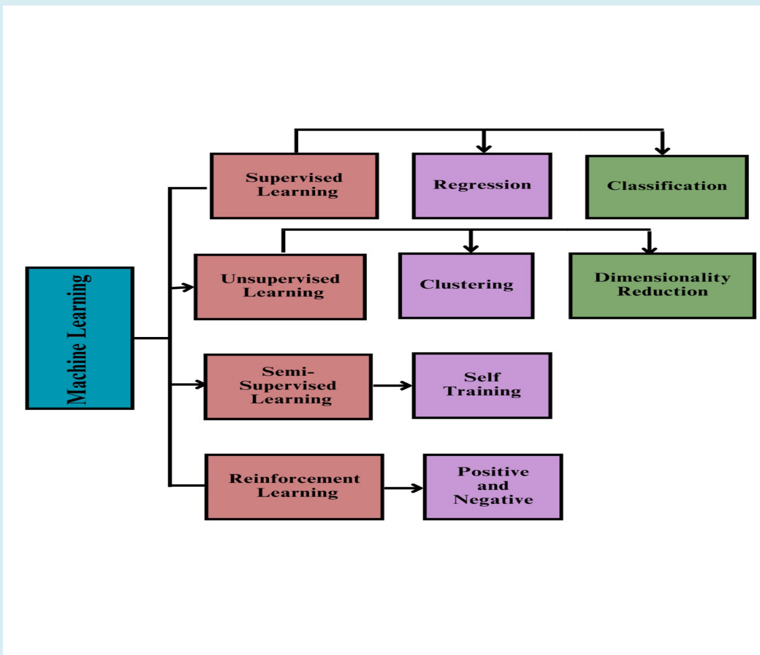

Figure 1: Classification of ML models [7].

In supervised learning, labelled datasets are used to train the model. This is done so that the model can recognize the relationship between the input and the outcome [8]. Examples of supervised learning include the use of regression models and classifications. Unsupervised learning is the use of unlabelled datasets in the training of the model or algorithm [9]. When both labelled and unlabelled datasets are used in training the model, it is called semi-supervised learning. The procedure for implementing semi-supervised learning is called self-training. It requires that the model be trained with a small labelled dataset and then be allowed to predict an unlabelled dataset. Meanwhile, reinforcement learning is based on a trial and error procedure that enables the algorithm to learn from the positive and negative feedback it gets from trying [10].

Some of the tools and techniques used in machine learning include Convolutional Neural Networks (CNN), Artificial Neural Network (ANN), and Deep Neural Network (DNN). ANN is an AI system trained to function like the human brain by using interconnected nodes in an organized structure just like the human brain. ANN process is often referred to as deep learning. CNN is an ANN framework designed to recognize and process images based on pretrained patterns. CNN models can find patterns in images for object recognition. DNN is a sophisticated ANN framework that contains some hidden layers to enhance the capability of the model to process very complex problems such as natural language processing and complicated image processing [11].

Data in ML Processes

Data is critical to the success of any ML model. Data identification is the first step in solving an ML problem. Over the years, machine learning models have been developed to handle different data types including; qualitative, quantitative, time series, controlled, and uncontrolled data. Qualitative data are either nominal (categorical) or ordinal (showing order) while quantitative data is based on set values such as body mass index (BMI). Furthermore, time series data is a type of data that is collected over some time with equal time intervals. Controlled data are data whose outcome can be determined by varying some sets of parameters while uncontrolled data is one whose outcome cannot be determined by any manual variation. Other types of data include historical data, experimental data, and simulated data [6]. Material science data are mainly quantitative but can be either controllable (such as the time of heat treatment) or uncontrollable (such as the depth of the impression of the indenter on a metal surface). It can also be experimental or simulated. The types of data generated in material science are presented in Table 1.

Data Name	Data Type
Hardness	Scalar (uncontrolled)
Temperature gradient	Time series
lattice structure	Categorical
SEM analysis	Image
Density	Uncontrolled
Thermogravimetric analysis	Time series
x-ray diffraction analysis	Spectral
Composition	Categorical
Fatigue strength	Scalar
Pyrometry	Time series
Melting point	Scalar

Table 1: Material Science data types [12].

Areas of Application of ML in Material Science

The use of machine learning and other computational techniques in material science has given rise to a sub-domain in material science called material informatics [13]. This becomes necessary because the analytical and experimental approach to material design is time-consuming, costly, and requires huge labour input. Several researchers have studied how ML tools and methods can be applied in material science. In this part of the review, several such works was highlighted.

Material Properties

Stergiou, et al. [7] reviewed how machine learning methods have been incorporated into material property prediction and optimization of processes. It was reported that ML methods can be used in predicting the thermal, mechanical, and optical properties of materials. Some of the techniques reported to have been used for thermal prediction include gradient boosting (GB) regression, Ridge regression, random forest (RF) regression, and support vector regression (SVR) techniques. Meanwhile, NN, ANN, and DNN techniques have been used to predict the mechanical properties of materials. Specifically, the study highlighted the use of the NN technique in determining the modulus of elasticity and rupture of wood with different moisture content [5,14].

Material Development

Picklum and Beetz [13] studied a novel machine-learning algorithm that was designed to assist material scientists in the design and development of new materials. The ML model called MATCALO enables users to generate queries on certain requirements that should be met by the new material and search the framework based on this query. The framework then generates a hypothesis. The hypothesis generated is a processing chain that indicates the step-by-step process required to synthesis the material with the desired properties as well as the parameters involved. The framework was designed to improve the turnaround time and reduce experimental costs associated with new material development.

Microstructure Identification

Microstructures are important pictographs in material science that are used to determine the phases present in a material. These phases are often associated with the material properties [15]. Oftentimes after microstructural examination, material scientists, most especially students may find it difficult to interpret the microstructure obtained. By training ML models with thousands of microstructural images, it is possible to use ML algorithms to interpret the phases present in a microstructural image. This was demonstrated in Figure 2 [16].

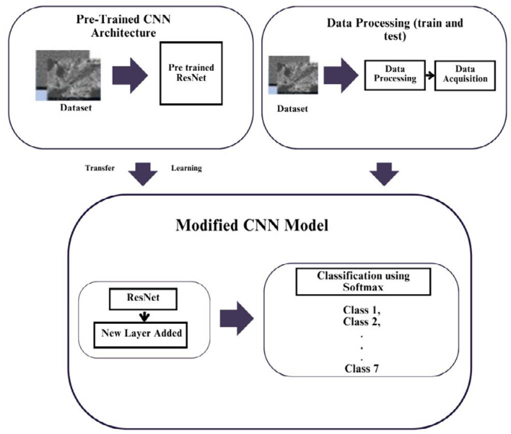

Figure 2: Phase classification in steel using CNN framework [16].

Formation of Multi-Component Alloys

The formation of multi-component alloys (MCA) is aimed at optimizing specific properties of the components of the alloys thereby making such alloys more suitable for specific areas of application. Usually, in conventional alloys, there is a trade-off in certain mechanical properties. For example, to improve the strength of mild steel, there might be a reduction in its ductility [17]. Conversely, MCAs have superior mechanical properties in comparison with the conventional alloy formation process. While the conventional alloy involves a solid solution, MCA can occur in different phases such that the target property is improved without negatively impacting other properties. Furthermore, the conventional method involves parametric phase selection, however, due to the complexity of MCA formation, parametric phase selection which is hinged on Hume-Rother rule may not be a perfect fit. Choudhury, et al. [16] reported the use of a CALPHAD model to predict phase formation for an MCA system. With this, it was posited that ML algorithms can be vital in developing multi-component alloys [18].

Other Areas

Several other areas of application of machine learning can be found in the literature. This includes; additive manufacturing process [19], material design [20,21], process optimization [22], prediction of material quality [23], metal forming processes [24], nanomaterials [25,26], and heavy production process.

Contemporary Studies

This section tabulates contemporary studies on the application of machine learning to material science as presented in Table 2.

Author	ML Technique	Area of application	Type of Study
Vasudevan, et al. [27]		Material design	Review
Sparks, et al. [18]	CALPHAD*	Structural materials	Review
Schmidt, et al. [28]	Support vector machine model	Solid-state materials	Review
Jennings, et al. [4]	Genetic algorithm	Material discovery	Experimental
Ramprasad, et al. [29]	Probabilistic models	Materials informatics	Review
Penumuru, et al. [30]	Support vector machine/ machine vision	Material classification	Experimental
Cruz, et al. [24]	ANN, FEM**	Process of metal bending	Experimental and simulation
Stoll and Benner [31]	Small punch test	Mechanical properties prediction	Experimental

Table 2: Previous works on the application of ML techniques in material science.
*Calculated Phase Diagram, **Finite element methodology

Challenges and Future Directions

Limited Data Availability: the backbone of machine learning is the availability of data. Training a model usually involves the use of a large dataset to enable the model to identify the pattern in the dataset and understand minute variations in the different data samples. This is to ensure that when new data is brought to the model to identify, the model can predict the outcome correctly. This becomes the main limitation of the application of machine learning to material science as there is no sufficient data on the over 300,000 materials known Sun, et al. [32]. Future works should focus on creating repositories for material scientists all over the world to archive data from various experimental works. The data can be kept in silos capturing various process points in material science. This data collated over time can be large enough to train models that can be helpful in material synthesis, processing, and characterization [33].

MCA-Based Models: as discussed earlier, several challenges have been identified in the synthesis of multi-component alloys despite their huge benefits in material science and engineering. One of which is the non-suitability of the use of parametric phase selection. The use of a machine learning algorithm which will be based on the material properties of the component elements can be a solution to the synthesis of MCAs. Further research can be conducted to develop deep learning models that can be used to predict the properties of MCAs based on those of their components.

Furthermore, more experimental and simulation-based studies on the application of machine learning to material science are needed as most of the reviewed works are reviews. Some of the studies have explained the theories that can assist in the development of machine learning models that can be used in material science. The actual development of such models is needed to affirm the benefits of machine learning to material science [29].

Conclusion

Machine learning is a growing field globally and has gained application across different industrial verticals including health, sports, agriculture, defense, and governance. The application of machine learning to material science will cut down the time, cost, and labour associated with laboratory experiments. Machine learning can be applied to all aspects of material science including material synthesis, processing, treatment, and characterization. However, the major pitfall is the insufficient availability of material science data that can enable the development of machine learning models. It is recommended that harmonization of experimental works by material scientists and archiving in data repositories can help forestall this shortcoming.

References

1. Callister WD, Rethwisch DG (2018) Materials Science and Engineering - An Introduction. 10th (Edn.), John Wiley & Sons, Inc, New Jersey, USA.
2. Anggraini L, Sugeng (2018) Analysis of Porosity Defects in Aluminium as Part Handle Motor Vehicle Lever Processed by High-Pressure Die Casting. IOP Conf Ser Mater Sci Eng 367: 012039.
3. Aweda JO, Orhadahwe TA, Ohijeagbon IO (2018) Rapid Cyclic Heating of Mild Steel and Its Effects on Microstructure and Mechanical Properties. IOP Conference Series: Materials Science and Engineering 413: 012016.
4. Jennings PC, Lysgaard S, Hummelshøj JS, Vegge T, Bligaard T (2019) Genetic Algorithms for Computational Materials Discovery Accelerated by Machine Learning. npj Computational Materials 5(1): 46.
5. Kai G, Yang Z, Yu CH, Buehler MJ (2021) Artificial Intelligence and Machine Learning in Design of Mechanical Materials. Materials Horizons 8(4): 1153-1172.
6. Weichert D, Link P, Stoll A, Rüping S, Ihlenfeldt S, WrobelS, et al. (2019) A Review of Machine Learning for the Optimization of Production Processes. International Journal of Advanced Manufacturing Technology 104(5-8): 1889-1902.
7. Stergioua K, Ntakoliab C, Varytisc P, Koumoulosc E, Karlssona P, et al. (2023) Enhancing Property Prediction and Process Optimization in Building Materials through Machine Learning: A Review. Computational Materials Science 220: 112031.
8. Tim M, Kusne AG, Ramprasad R (2016) Machine Learning in Materials Science: Recent Progress and Emerging Applications. In: Mueller T, et al. (Eds.), Reviews in Computational Chemistry 29.
9. Martinez DR, Nigam KDP, Sandoval LR (2021) Machine Learning on Sustainable Energy: A Review and Outlook on Renewable Energy Systems, Catalysis, Smart Grid and Energy Storage. Chemical Engineering Research and Design 174: 414-441.
10. Perera ATD, Kamalaruban P (2021) Applications of Reinforcement Learning in Energy Systems. Renewable and Sustainable Energy Reviews 137: 110618.
11. Liu Y, Niu C, Wang Z, Gan Y, Zhu, et al. (2020) Machine Learning in Materials Genome Initiative: A Review. J

Mater Sci Technol 57: 113-122.

12. Johnson NS, Vulimiri PS, To AC, Zhang X, Brice CA, et al. (2020) Machine Learning for Materials Developments in Metals Additive Manufacturing. Additive Manufacturing 36: 1-42.
13. Mareike P, Beetz M (2019) MATCALO: Knowledge-Enabled Machine Learning in Materials Science. Computational Materials Science 163: 50-62.
14. Kamal C, DeCost B, Chen C, Jain A, Tavazza F, et al. (2022) Recent Advances and Applications of Deep Learning Methods in Materials Science. NPJ Computational Materials 8(1): 59.
15. Durodola JF (2022) Machine Learning for Design, Phase Transformation and Mechanical Properties of Alloys. Progress in Materials Science 123: 100797.
16. Choudhury A (2020) The Role of Machine Learning Algorithms in Materials Science: A State of Art Review on Industry 4.0. IN: Archives of Computational Methods in Engineering 28(5): 3361-3381.
17. Orhadahwe TA, Akanni AA, Olayiwola AJ, Pelumi IP, Kolawole OJ (2020) Microstructural Image Analyses of Mild Carbon Steel Subjected to a Rapid Cyclic Treatment. Journal of Chemical Technology and Metallurgy 55(1): 198-209.
18. Sparks TD, Kauwe SK, Parry ME, Tehrani AM, Brgoch J (2020) Machine Learning for Structural Materials. Annual Review of Materials Research 50: 27-48.
19. DebRoy T, Mukherjee T, Wei HL, Elmer JW, Milewski JO (2021) Metallurgy, Mechanistic Models and Machine Learning in Metal Printing. Nature Reviews Materials 6(1): 48-68.
20. Frederic EB, Roland CA, Cyron CJ, Huber N, Kalidindi SR, et al. (2019) A Review of the Application of Machine Learning and Data Mining Approaches in Continuum Materials Mechanics. Frontiers in Materials 6: 1-23.
21. Zeqing J, Zhang Z, Demir K, Gu GX (2020) Machine Learning for Advanced Additive Manufacturing. Matter 3(5): 1541-1556.
22. Julia L, Antono E, Bajaj S, Paradiso S, Hutchinson M, et al. (2018) Machine Learning for Alloy Composition and Process Optimization. Proceedings of the ASME Turbo Expo 6: 1-10.
23. Parsa M, Wang ZJ (2016) Machine Learning for Quality Prediction in Abrasion-Resistant Material Manufacturing Process. Canadian Conference on Electrical and Computer Engineering, pp: 4-7.
24. Daniel JC, Barbosa MR, Santos AD, Miranda SS, Amaral RL (2021) Application of Machine Learning to Bend Processes and Material Identification. Metals 11(9): 1418.
25. Jiazhen C, Chu X, Xu K, Li H, Wei J (2020) Machine Learning-Driven New Material Discovery. Nanoscale Advances 2(8): 3115-3130.
26. Jing W, Chu X, Sun XY, Xu K, Deng HX, et al. (2019) Machine Learning in Materials Science. InfoMat 1(3): 338-358.
27. Rama V, Pilania G, Balachandran PV (2021) Machine Learning for Materials Design and Discovery. Journal of Applied Physics 129(7): 070401.
28. Jonathan S, Marques MRG, Botti S, Marques MAL (2019) Recent Advances and Applications of Machine Learning in Solid-State Materials Science. NPJ Computational Materials 5(1): 83.
29. Rampi R, Batra R, Pilania G, Arun MK, Kim C (2017) Machine Learning in Materials Informatics: Recent Applications and Prospects. NPJ Computational Materials 3(1): 54.
30. Penumuru DP, Sreekumar M, Karumbu P (2020) Identification and Classification of Materials Using Machine Vision and Machine Learning in the Context of Industry 4.0. Journal of Intelligent Manufacturing 31(5): 1229-1241.
31. Anke S, Benner P (2021) Machine Learning for Material Characterization with an Application for Predicting Mechanical Properties. GAMM Mitteilungen 44(1): 1-21.
32. Ning S, Kopper A, Karkare R, Paffenroth RC, Apelian D (2021) Machine Learning Pathway for Harnessing Knowledge and Data in Material Processing. International Journal of Metalcasting 15(2): 398-410.
33. Bhuvaneswari V, Priyadharshini M, Deepa C, Balaji D, Rajeshkumar L, et al. (2021) Deep Learning for Material Synthesis and Manufacturing Systems: A Review. Materials Today: Proceedings 46: 3263-3269.