Material Reports

Eleyon Publishers

2(1) (2019) 1 - 3

RESEARCH ARTICLE

OPEN ACCESS

Role of Artificial Intelligence in Material Science

Bogdan. D[1]

Abstract

The present study devoted to influence the emerging roles of artificial intelligences in modern fields of sciences such as Material science. In recent decades, the material science has been one of the important scientific domains with large number of applications being reported from scientific communities. Based on which, the present report was designed and present in the form of brief review.

Keywords: Material science, Artificial intelligence, Applications

Author Affiliation: [1]Moscow State University, Russia

Corresponding Author: Bogdan. D. Moscow State University, Russia, Email: Bogdanlist@mail.ru

How to cite this article: Bogdan, D, Role of Artificial Intelligence in Material Science. *Meterial Reports* 2(1), 1-3. Retrieved from http://mr.eleyon.org/index.php/mcrr/article/view/5

Source of support: Nil

Conflict of interest: None.

Received: 10 March 2019 **Revised:** 14 April 2019 **Accepted:** 16 April 2019

1. Introduction

Material science is an associative field including properties of the matter and their applications to a different field of engineering and sciences. It involves applied elements of chemistry and physics, as well as various engineering field chemical, civil, mechanical, and electrical engineering. Material science is exploring the relationship between process, structure, properties, and applications. New materials discovery plays a greater role in enhancing human society development. After the development of many centuries, a big amount of data has been collected in the material science area.[1-8] But the inherent restrictions of the human perception ability make this tough for humans to process and absorb the data products and massive literature every day. Artificial intelligence emergence with the materials science brings advancement. After more than 55 years of the development, from the easy perceptions to the typical multilayer neural networks. Artificial has been exhibited as a first algorithm infrastructure and a strong hardware base. ML (machine learning) is an essential branch of artificial intelligence that makes development rapidly in a few years; this is also a more promising application of artificial intelligence in material science research. The coming part addresses basic knowledge of machine learning; this is laid the foundation to address materials science research applications of artificial intelligence.

2. Role of the AI in Material Science

In current years artificial intelligence has pertained in many and more fields, and machine learning research in the area of the materials science is rapidly developing, especially in which it can combine advanced materials and predictive different chemical combinations.

2. Accelerated Simulation

The process of research for material science and computational chemistry has been up to date for the 3 rd generation.

The 1st generation refers to the calculation of structure performance; this mainly takes benefits of local optimization algorithm to predict the performance of materials from the structure.

The 2nd generation is "crystal structure prediction" this mainly acquires a global optimization algorithm to predict structure and performance from the component composition.

The 3rd generation identified as “statistically driven design", uses machine learning algorithms to forecast the structure, composition, and performance of the components form the chemical and physical data.[1] But, the theory imperfection has been also carried barriers to the discovery of the higher performance of the materials, and model parameters are not compatible with a practical condition like a mixed stage or boundary of grain. For example, the prediction of DFT of zirconium doped lithium tantalum silicate is 10^{-3} S cm^{-1}, where the subsequent experiment has been shown which its real conductivity is approximate 10^{-5} S^{cm-}, so finding methods to utilize machine learning to develop for simulation deficiencies is too essential.

2.2 Atom2vec

Atom2vec, an unsupervised machine learning program, again constructed periodic elements tables only a few hours. Atom2vec learns first to differentiate various atoms thorough analyzing the compounds list in the database online. Now, for this borrow the easy idea of natural language processing. The qualities of a word can be extracted from the other word around it. Elements of the chemical are gathered according to the chemical environment. At a similar time, the vectorized atomic descriptor can be utilized as the input of the many machine learning model because it brings a huge amount of information about elements periodic law, which gives an impacting innovation method to the quantitative representation of the material data in future.

2.3 Increasing simulation scale

In this, there are some continue repetitions in theoretical calculation of the atomic force field, when machine learning finds these repetitive patterns, corresponding force or energy field can be calculated fast. Hundreds of atoms movements in a few pico-seconds could be expanded to which of the millions of the atoms in few nanoseconds, that hugely increased the time and length range of calculation, simulation, and gets better outcomes. Complex type material structures like amorphous, polycrystalline, and chemical reactions like corrosion and interfacial reactions, etc. Must be simulated. In the large scale MDs, surface simulation and interfacial chemical process, reliable interatomic potentials of development is intimidating issues because of the wide range existence of atomic environment and too various type of bonds. In current years, the interatomic possible based on the artificial neural network (NNs) has been combined, that gives an unbiased way of the construction of possible energy surface of the system which is tough to explain by the traditional possible utilization of copper and zinc oxide as the references system to confirm the correctness and validity of interatomic potential of artificial neural network and explained CuZnO ternary combinations of the copper clusters.[2]

2.4 Computation amount reducing

Based on the massive combination space of the materials, this is typical to explore all the potential combinations in time by traditional calculation simulation. For example, the bimetallic configuration of the smallest sulfide nanocluster au15 (SR) 13 exceed 32000, and traversing all the possible structures is a big computational issue [5]. But, if the small part of data is utilized to train the machine learning model and model is utilized to forecast other combinations, computational complexity will be hugely removed, and filtering speed will be improved by the many order of the magnitude. A machine learning-based stochastic forest is way to forecast CO absorption energy of the nanocluster.

The 1st, DFT simulation data model for training of the Ag-alloyed Au25 nanocluster was utilized utilizing a two- step feature choosing procedure and feature engineering method, prediction of the absorption energy with accuracies of the 0.78 (R2) and 0.17 (RMSE). After explaining the key nodes of the random forest, find that distribution of the Ag atoms in the Au 25 had been the more essential impact on CO absorption sites. The machine learning model can be simply expanded to the other nanocluster based on the element Au. This model expected to be utilized as a screening tool of screen eligible material for future accurate analysis.

3 New Material Property Predictions

Researchers who done the material research normally hope that the required properties of the materials can be boosted, like conductivity of the electrolytes, the coefficient of Seebeck of the thermoelectric materials, and power conversion efficiency of the organic-inorganic hybrid pervo-skites. A big amount of trials and bugs experiments are based on theory base simulation or the chemical scientist instinct complex lead to dissatisfactory outcomes. Machine learning applications models can assist a lot through forecasting the structure and property of the materials with the acceptable correctness before synthesis. The machine learning model is developed in MATLAB to find out the small amount of the specific solid electrolytes in more than 12000 materials. Utilizing the well- known electrolytes set and their atomic structures for the training, they first untangle scientific literature and find approximate 40 solid crystalline materials. Cause of the small size data set this is essential to utilize the " intelligent" attribute which is based on the existing physical knowledge for the data representation.[2] So, the atomic structure of these 40 materials from the ICSD as the input, and also calculates 20 types of qualities based on the atomic position, electronegativity, atomic radius of the structure and mass of the atom, in this include the volume of the atom of each atom, lithium bond ionicity, and minimum anion- anion separation, number of the lithium adjacent elements and explains atomic local arrangement and chemical qualities of each crystal. Then 20 features are utilized as the input, values of the experiments of lithium-ion conductivity are utilized as results, and 40 known materials constitute a training set of the machine learning algorithm. After the adjustment of the constant parameter, the model can classify and screen the solid electrolyte. Then 317 materials candidates were forecasted. The outcome shows that the efficiency of recognizing possible new materials utilizing the modified MATLAB model is 3 times highest than which of the random guessing and 2 times higher than and compared the outcomes with DFT outcomes, the F1 score is about 50%.

3.1 Synthetic Route Planning

Organic synthesis contains a standard procedure that permits scientists to design computer programs to handle

synthetic issues. Scientists are concerned chemical reactions are data set which points out the relationship of the compound. The existence can be described as the data structure like network and graph. So artificial intelligence could handle structural data to lead the synthesis route.[4] An organic synthesis robot that involves an online spectral examination and response loop to done 6 experiments simultaneously. Its core elements include pressure pump and raw material tank assembled with the chemicals. These pumps are overseen for feeding the reactants into the 6 parallel operated reaction bottle. And the robot utilizes SVM way to automatically classify reactions mixture into the reactive or nonreactive mixture through real-time assessment of the reaction utilizing IR and NMR spectra copy. This way is faster than the manual experiments and can forecast the reactivity of the reagent combination. After gathering outcomes of about 10% of the experimental data set, the robot could forecast reactivity of approximately equal to 1000 reaction combinations with forecast correctness of across 80% and found 4 new reactions. For data, driven procedures also utilized the reaction rules to forecast the retrosynthesis analytic system and also made logic and knowledge-based search strategy to design the reaction route. So, the proposed retrosynthesis process can obtain based on the theory of a reasonable beginning material and a reaction route through analyzing the wanted compound. At present this technology has applied to synthesize new material and forecast different chemical synthesis.

3.2 Experimental Parameter Optimization

For the development of the traditional material, a huge number of parameters require to be examined and adjust manually in the processing, synthesis, and device assembly procedures. And the efficiency is too low and may not be capable to find out the optimal parameters. Machine learning has the powerful nonlinear regression capability to find out the best location concerning the huge parameter space. And this concept has been applied in the welding process. FSW (friction stir welding) is the new solid-state welding procedure that has been broadly utilized in the aerospace, automobile, shipbuilding, and other industries.[3] 108 independent experimental data is collected to train machine learning models, also including neural networks and decision trees, and also explored the original effects of welding parameters like temperature, shear stress on tool pins, strain rate, and torque and possible causative variables on the void development. The outcomes show that 2 algorithms can forecast the development of the defects well, and the highest forecast of accuracy is 96.6 %. In this model, the optimization parameters in welding procedures can be completed and the development of unfavorable factors like void development in FSW from machine learning can be avoided. The same example has applied to 3D printing. Aerosol jet printing (AJP) is noncontact 3D printing technology, which is generally to fabricate microelectronic devices on the flexible substrate. It has been deposition ability of the specific patterns, but the typical relationship between the main procedure's parameter is tough, and this will have a specific effect on printing quality. a new hybrid machine learning method is proposed to fix the best operating process window of the AJP procedures indifferent design spaces. This way contains classical machine learning methods, also including experimental sampling, a cluster of data, knowledge transfer, and classification. This method is based on a Latin hypercube sampling experiment design, and 2D design space is completely explored at a fixed printing speed. The effect of the sheath gas flow rate (SHGFR) and carrier gas flow rate (CGFR) on quality of the printing line was examined through the K-means clustering way, and the optimal operations procedures window was fixed by the support vector machine. For recognizing effectively more operations procedure windows at various printing speeds, the method of transfer learning is utilized to ensure the correlation between various operation procedures windows. So new printing speed, row samples are utilized in various numbers to recognize the new operation procedure window is greatly removed.[3] And finally to balanced typical relationship between CGFR, SHGFR, and printing speed and effective classification method is utilized to fix a 3 D operation procedure window.

4. Conclusion

The study reports the compilation of scientific reports on artificial intelligence and their applications in material sciences. In future much more research is awaited to explore the emerging roles of artificial intelligence in different domains

References

1. Tiwari, Artificial Intelligence And Machine Learning Empowering The Mass Medicine, Advanced Materials Letters, 10 (2019) 302-302.
2. R.Somashekara, S. Kusuma, Artificial intelligence in power systems, International Journal of Recent Trends in Engineering and Research, 4 (2018) 262-267.
3. Ade Maria Ulfa, Afandi Saputra, Yuswardi, Phong Thanh Nguyen, Role of artificial intelligence in pharma science, Journal of critical reviews, 7 (2020) 291-293.
4. M. Welling, Artificial Intelligence versus Intelligence Engineering, Harvard Data Science Review, 1(1) (2019).
5. R. R. Nadikattu, The emerging role of artificial intelligence in modern society, International Journal of Creative Research Thoughts, 4 (2016) 906-911.
6. R. R. Nadikattu, The Supremacy of Artificial intelligence and Neural Networks, International Journal of Creative Research Thoughts, 5 (2017) 950-954.
7. H.S. Rogers, Cheering Artificial Intelligence Leader: Creative Writing and Materializing Design Fiction, Leonardo, 53 (2020) 58-62.
8. R. Gawlik, Application of Artificial Intelligence Methods for Analysis of Material and Non-material Determinants of Functioning of Young Europeans in Times of Crisis in the Eurozone, Publisher: Warszawa: PWN, (2014).