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Progress in the Application of Mathematical Algorithms in Materials Science

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Abstract: As materials are the direct drive for scientific development and social progress, the research on their structure and properties has always been a research hotspot in materials science. At present, the discovery of new materials is mainly carried out by the researcher's intuitive judgment of materials and a large number of "trial and error" experiments, which is inefficient and difficult to effectively discover a large number of possible new material combinations. Materials science has long relied on two major means of experiment and calculation. The machine learning-based mathematical algorithms offers a new research method. This article systematically expounds the common mathematical algorithms and the basic processes of their calculation methods, details the application of mathematical algorithms in material performance prediction and new material design, and gives a summarization and outlook of the challenges and application prospects concerning their application in materials science.

1. Introduction

As one of the three pillars of the modern social development, materials play an important role in scientific development and social progress. Therefore, the development and application of high-performance materials has become an important topic in materials research. The research methods of materials can be roughly divided into experiment and calculation. Experimental research methods are mainly based on researchers' experience and intuition, but as often as not, there are problems such as high preparation costs, long R&D cycles, and low efficiency. Owing to their relatively accurate prediction, the commonly used computational simulations such as first-principles calculation, molecular dynamics, and finite element simulation have been widely used in semiconductor materials, luminescent materials, and new energy materials. However, the above-mentioned high-throughput calculation methods still face many limitations in terms of running time and computing power.

With the advent of the era of the "Fourth Industrial Revolution" led by artificial intelligence and big data, mathematical algorithms, a new branch of artificial intelligence, have been widely used in robot technologies, computer vision, data mining, and biomedicine, etc. Due to their efficient calculation and prediction capacity, mathematical algorithms have been gradually used in research of materials science. Based on sufficient experimental research and theoretical calculations, people can use mathematical algorithms to quickly complete data mining, learn useful information, reveal

the information and laws contained therein, and accurately predict material performance to screen target materials. Mathematical algorithms help researchers in carrying out theoretical calculations and experimental verification on a smaller scale, whereby the material research and development cycle is shortened.

2. Integration of Mathematics and Materials Science

The application of mathematical algorithms in the field of materials provides a new type of tool which allows discovering the law in high-dimensional data, helping reduce the amount of calculations to accelerate exploration of new materials. Feature extraction (feature engineering) is a key component of mathematical algorithms, and whether appropriate form is chosen for expression will directly affect the effect of the final model. In materials science, it is necessary to capture all relevant information to distinguish the environment of different atoms and crystals.[1]

Mathematical algorithms are critical to machine learning. Machine learning is mainly divided into supervised learning, semi-supervised learning and unsupervised learning by learning method, of which supervised learning is the most widely used. In supervised learning, a set of samples with known labels are used, and the parameters of mathematical algorithm model are adjusted to learn from the training data and make accurate predictions. The commonly used mathematical algorithms include support vector machines, decision trees, K-neighbors, artificial neural networks, and deep learning, etc. (As shown in table 1)

Table 1: Application of mathematical algorithms in materials science research

	Mathematical algorithms	**Materials science research**
1	Linear regression	Linear regression is suitable for simple regression problems, optimizing the error function in the form of least squares by gradient descent, with simple calculation and fast training.[2]
2	Logistic regression	Logistic regression is computationally fast when performing classification problems, and can be combined with regularization models to solve problems.[3]
3	K-Nearest neighbor	K-Nearest neighbor can be used for both regression and classification problems, and can be used for non-linear classification problems, but when the sample is not balanced, it may lead to inaccurate results. may lead to inaccurate results.[4]
4	Decision tree	Decision tree algorithm is suitable for dealing with samples containing missing attributes and can produce better results for large data sources in a short time.[5]

3. Data-driven Material Innovation and Change

Material innovation has always been the core of various disruptive technological revolutions. The conventional material research and development model mainly relies on “trial and error” or accidental discoveries, and takes as long as 10-20 years. To an extent, this has been unable to meet the demand for new materials in the future society. With the gradual maturity of mathematical algorithms and machine learning technology, researchers can apply algorithms to calculation of

materials theoretically, and obtain the relationship between key components, structure, process and the performance through known knowledge and calculation, thus accelerating research and development.

There are three R&D models in materials science:

The first mode is experiment-driven. Based on high-throughput synthesis and characterization experiments, materials are directly optimized and screened from piece by piece to batch by batch, leading to a transformation of quantitative into qualitative changes. A typical technology is the preparation of combined material chips. Inspired by circuit chips and gene chips, scientists integrate and fast characterize up to 10-108 components, structures, and phases with arbitrary element as the basic units, which greatly improves the experimental efficiency.

The second mode is calculation-driven. Based on theoretical computational simulation, the promising candidate materials are predicted to narrow the scope of the experiments, followed by verification with experiments finally. This mode is widely used, covering from atomic pole to continuum. The corresponding methods include first-principles method, molecular dynamics, mesoscopic method and continuum method.

The third model is data-driven. In the material informatics which is based on machine learning and data mining, models are established through a large amount of data and machine learning for predication of candidate materials and new materials. Compared with manual judgment of experienced chemists, the machine predication won out at a success rate of 89%:78%. This case fully demonstrates the power of machine learning methods, just like Alpha Go's impact on Go.[6]

The conventional R&D approaches the goal gradually. However, data-intensive data covers a wider parameter space, which results in fundamental changes in thinking. The way we understand the world has undergone experimental observation, theoretical deduction, and computational simulation successively. Now with the explosive growth of data volume and computing power like Moore's Law, scientific research has entered the fourth paradigm of “big data + artificial intelligence”. The experimental and computational drive is based on factual judgment or deduction of physical laws, without changing the original thinking mode or work routine. Comparatively, data-driven is truly revolutionary. The artificial intelligence is good at establishing incidence relation of data, being a complementation and extension of conventional recognition paradigm. Its comprehensive application will bring disruptive effects, and data-driven mode will become a development orientation of materials science in the future.

4. Application of Mathematical Algorithms in Materials Science

4.1 Material properties prediction

In recent years, mathematical algorithms have emerged in predicting material properties relying on their advantages such as strong generalization ability and fast calculation speed. They have been successfully applied to predicting various properties of materials including band gap, emission/excitation wavelength, glass formation ability, shear strength, luminous heat quenching temperature, work function, etc. The following is mainly an introduction of mathematical algorithms in predicting the properties of band gap, phosphor emission/excitation wavelength, glass formation ability, and shear strength, etc. (As shown in figure 1)

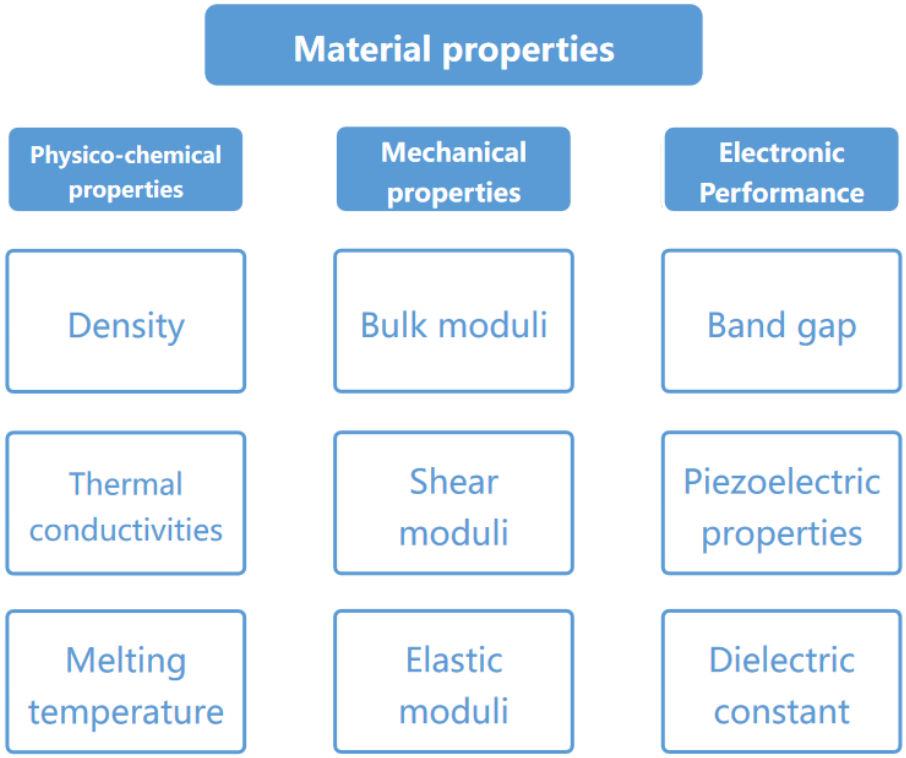

Figure 1: Material properties

4.1.1 Band gap

The band gap is the energy difference between the conduction band bottom and valence-band maximum of a semiconductor or insulator. The size of the band gap determines the energy band structure of the material and affects its electronic structure and optical property. In recent years, some domestic and foreign researchers have successfully predicted the band gap of various materials using mathematical algorithms.[7]

4.1.2 Phosphor emission/excitation wavelength

Phosphor materials have aroused materials scientists' research interest because of their wide application in solid-state lighting and display. In particular, Eu2+doped phosphors are characterized by narrow emission spectrum, high stability and high quantum yield. It is well-known that the emission wavelength of phosphor determines the color quality of display device. The mathematical algorithms are a brand-new method to study the emission wavelength of Eu2+doped phosphors, which helps with the optimization and design of novel phosphors.[8]

4.1.3 Glass formation ability

In recent years, the prediction of glass formation ability with mathematical algorithms has become a new research direction in glass physics. Where, the main focus is given to the glass formation ability of amorphous alloys. The critical cooling rate is the most reliable basis for measuring the glass formation ability, but it is often hardly available with conventional experiments. Experimenters often use the critical casting diameter (Dmax) to characterize the glass formation ability of bulk metal glass.[9]

4.1.4 Shear strength

Shear strength refers to the limit strength of a material when it is sheared off, which is an important indicator for describing the material's resistance to shear sliding. The use of mathematical algorithms to predict the shear strength of materials will greatly reduce the test cost and shorten the research cycle, which is of great significance to engineering applications, production and life. [10]

4.2 Discovery of new materials

Mathematical algorithms are not only widely used in predicting material properties, but also play an important role in the synthesis and design of new materials, which influences and promotes the development of materials science. For example, topological mathematics, as a powerful tool, can be used for quantitative analysis of data structures through changing scales. With the help of machine learning methods, high-precision material prediction machine learning models can be constructed for cluster structure analysis, cluster structure search, crystal structure energy prediction and the scientific research on many other material structure laws, which helps accelerate the discovery and application of materials. The following is a brief introduction of the application of mathematical algorithms in the fields such as rare earth fluorescent materials, perovskite materials, and catalytic materials.

4.2.1 Rare earth fluorescent materials

Fluorescent pigments are used in a wide range of applications. Fluorescent pigment products will automatically emit bright light in the dark and are mainly used to indicate signs and decorations. It can also be made into paints, lacquers, inks, plastic products, etc. Rare earth fluorescent materials have been used in multiple fields such as laser, lighting, display, and radiation detection because of high color quality, strong light absorption, high conversion efficiency, and stable physical and chemical properties. With the data-driven mathematical algorithms, a number of important research results have been achieved in discovery of new rare earth luminescent materials.

4.2.2 Perovskite materials

The development and application of high-performance perovskites have always been a research hotspot in materials science. Compared with conventional experimental methods and first-principles calculation methods, sufficient experimental and theoretical research show that mathematical algorithms play an important role in seeking high-performance perovskite materials.

4.2.3 Catalytic materials

Catalytic materials are essential in industrial production. The conventional experimental research methods are inefficient and costly, and require complex equipment, making it difficult to meet the evolving industrial demand. However, mathematical algorithms can help with fast mining of the relationship between the structure and activity of catalytic materials to discover new catalytic materials.

5. Conclusion

The application of mathematical algorithms in materials science is an in-depth integration of computer science and materials science. They are characterized by high flexibility, generalization, and accuracy in studying the correlation in complex data. At present, they have been widely used in the research of a variety of functional materials such as luminescent materials and catalytic

materials. It should be pointed out that the mathematical algorithms still have certain limitations. First, they are a data-driven approach and are highly dependently on data. In the research of materials science, however, it is costly to obtain a large amount of data and the data is not evenly distributed, either. The training of model with a small amount of data will result in overfitting which can directly affect the prediction effect. Furthermore, although mathematical algorithms have been applied to the prediction of material properties and discovery of new materials, the verification of the prediction result and in-depth research of the physical and chemical laws therein are still required. Although mathematical algorithms cannot substitute conventional computational and experimental research, the further improvement of theories and methods will promote wider and deeper application of mathematical algorithms in materials science, whereby new ideas and methods for materials science research will be provided.

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