Data-Driven Aerospace Equipment Based Materials Research Methods

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***Abstract*—Aiming to address the challenges faced by aerospace equipment encountering a series of problems such as high overload, high temperature, and susceptibility to oxidative corrosion, as well as the low efficiency of traditional experimental research and development methods during actual usage, this paper utilizes first-principle density functional theory calculations and machine learning technology to establish a material database and predict material properties. Through first-principle calculations, we can gather a large amount of material data to construct a comprehensive material database; the use of machine learning technology based on the material database to predict the materials we need to save a lot of R & D time. The results indicate that the predicted values are in line with the actual range of values.**

Keywords-Aerospace equipment; Aluminium alloy materials; First-principles calculations; Machine learning

I. INTRODUCTION

In the design of aerospace equipment, the selection of materials is crucial and directly related to the operational effectiveness of the overall system. Aluminum alloy is the preferred material due to its properties such as oxidation resistance, corrosion resistance, and lightweight, however, with the diversification of application scenarios and the improvement of technical requirements, the performance and stability of aluminum alloy materials have posed more stringent challenges. During large maneuvers, the equipment will be subjected to significant overload, which places higher demands on the strength and durability of the equipment. During high-speed flight, air friction causes heating of the carrier surface, impacting the thermal stability and reliability of the materials used in the equipment. Therefore, the materials for the equipment need to have a wide range of high-temperature applications and superior thermal conductivity and mechanical properties. During storage and transport, equipment may also be susceptible to corrosion in high-temperature and high-humidity environments, which presents a challenge to the long-term stability and reliability of the equipment. To address these issues, researchers have extensively explored the microstructure, macro-properties, and process design of aluminum alloys to enhance the overall performance of the equipment. It has been found that alloying is an effective method for enhancing material properties, and the careful selection and addition of alloying elements play a crucial role in determining the properties of aluminum alloys. Achieving the optimal alloy ratio, controlling the formation and interaction of alloy phases, and ensuring the fine and uniform distribution of the aluminum alloy organization are key factors in improving the comprehensive performance of aluminum alloys and exploring their potential. For a considerable period, the optimal design of aluminum alloy materials has primarily depended on experimental methods. However, traditional experimental methods have drawbacks such as lengthy research and development periods and high costs, particularly when conducting experimental research on a microscopic scale. In recent years, the rapid development of computer technology has led to the emergence of new research methods. The large amount of accumulated data generated by experiments and simulations can now play a significant role in driving the development of the field of materials science[1]. The introduction of first-principle computational methods and machine learning techniques offers a new perspective for the research and development as well as the design of aluminum alloy materials. Compared to traditional experimental methods, the new methods offer a shorter research cycle, greater feasibility, and relatively lower research costs.

First-principles calculations are based on quantum mechanics and are used to analyze the movement of electrons within a system. These calculations allow for the study of the material structure from the perspective of electron movement, ultimately yielding the wave function of electrons and their corresponding intrinsic energy. This information is then used to determine the total energy of the system, as well as its bonding, elasticity, stability, and other properties. First-principles calculations, which do not require any empirical parameters and offer unique accuracy, are increasingly favored by researchers among the many simulation methods. First-principles calculations have been widely utilized in the research and development of new aluminum alloys to accurately predict material properties and alloy phase interaction mechanisms. Domestic and international reports on the application of first principles in aluminum alloys primarily focus on the structural parameters, stability, and mechanical properties of aluminum alloy phases. The literature examined the impact of 13 solute atoms on the phase stability of aluminum alloys through first-principles calculations using a Gaussian-like distribution (GLD) model. The study revealed that strontium and yttrium are promising elements for the exploration and development of high-performance aluminum alloys with LPSO structures[2].

In today's rapidly developing field of artificial intelligence, data-driven machine learning (ML) techniques have demonstrated remarkable effectiveness in predicting material properties[3,4].In the field of materials, machine learning offers the opportunity for secondary development using experimental data which has emerged as a new method for predicting material properties and has been utilized to some extent[5–7]. Gao et al.[8] analyzed the data using machine learning techniques and methods such as feature engineering to predict the ferrite

content of 202 austenitic stainless steel welds. This study provided insights into machine learning-assisted material design. Fukuichi[9] utilized machine-learning techniques to relate the elemental physical properties and hardness of 3d, 4d, and 5d transition metal carbides. The study found that factors such as the number of valence electrons, electronegativity, and thermal properties of the material influence its hardness. Zhang et al.[10] developed a machine learning-based multivariate calibration model to predict trace elements in steel. Currently, machine learning techniques have been utilized as a novel approach to predict the performance of materials in service [11,12]. By utilizing the fundamental material data from previous experiments and the established database, researchers have initially achieved the prediction of material service properties.

This paper researches the impact of alloying elements on the structural stability and surface properties of aluminum alloys using the density functional theory-based first-principles calculation method. It accumulates a substantial amount of data and employs machine learning to predict material performance. The results demonstrate that the prediction model accurately aligns with the actual material performance.

II. Based on a Data-Driven Approach to the Study of Materials In General

A. Overall design framework

The desired materials can be extracted directly from the periodic table using first-principles computing, which enables the computation of large datasets, and machine learning, which predicts elemental combinations based on desired properties. In this paper, elements from the periodic table are chosen as the foundational components for the modeling process, enabling the construction of all possible combinations. For each constructed model, first-principles calculations are conducted to obtain data on properties such as lattice constants, densities, formation energies, magnetic moments, and bulk moduli, among other fundamental characteristics. The database created becomes the training data for support vector machines (SVMs), where various SVMs are created based on material properties and combinations. A trained support vector machine is utilized to predict material properties and aid in material selection based on the parameters provided by the inquirer. Based on the results, several predicted materials were tested and attempts were made to synthesize them in an experimental setting. Next, the synthesis of the desired materials is carried out based on the results of experimental investigations. In this paper, a material database and material prediction are created using density functional theory-based computation and machine learning techniques, respectively. We obtain a substantial amount of material data through first-principle calculations to build a comprehensive material database. Subsequently, we employ machine learning techniques to forecast the required materials from the database, thereby significantly reducing R&D time. The overall framework is depicted in Figure 1.

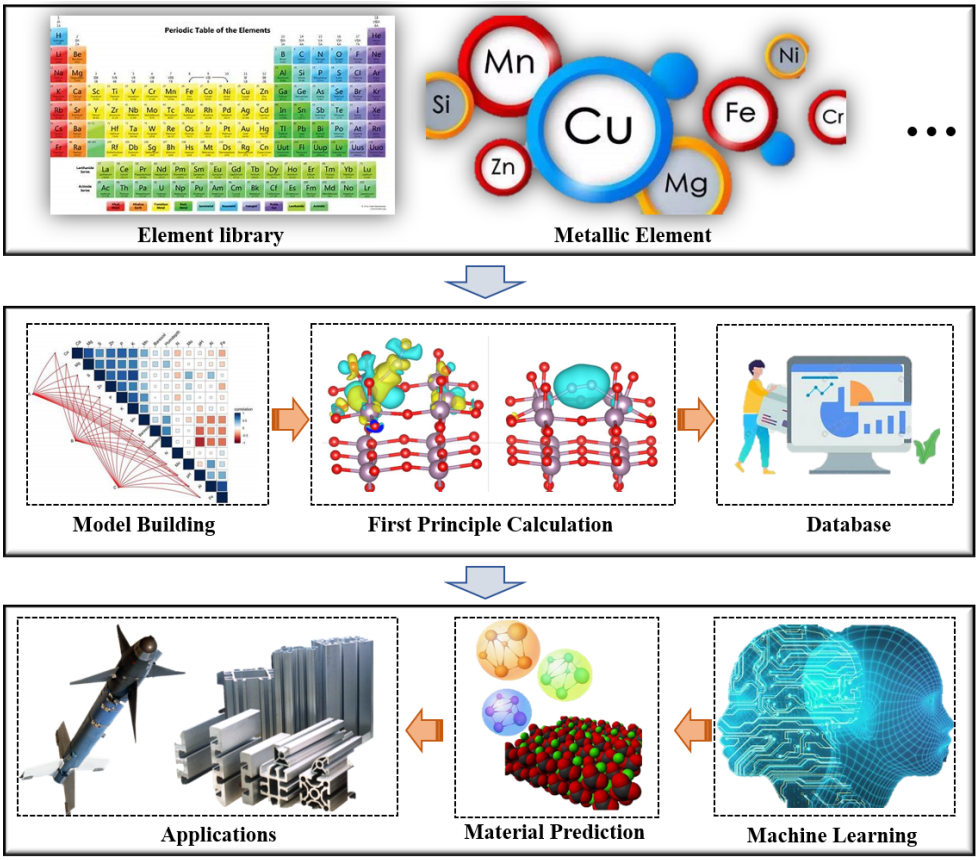

Figure 1. Overall Design Framework

B. Calculation method based on first principles of density functional theory

1) First Principle Calculations

First-principles calculations are essentially designed to solve the Schrödinger equation, in which five computational parameters are to achieve the integral solution for the electrons in the system.

First-principles calculations use only a few experimental parameters (m_0 , e , h , c , k_B) and do not depend on any empirical parameters. They are the preferred method for exploring and designing new materials.

The calculation method serves as a tool that can simulate the motion of electrons and accurately predict the natural states of matter. The first fundamental principle can be qualitatively described as the solution of the Schrödinger equation, which governs the motion of microscopic particles, through self-consistent calculations based on the adiabatic approximation and the single-electron approximation (illustrated in Figure 2) [13]:

$$-\left(h^2 / 2m\right)\Delta^2\phi + v(r)\phi = E\phi \tag{1}$$

In the given equation: h is the Planck constant; m is the particle mass; Δ is the operator; ϕ is the wave function; $v(r)$ is the potential energy of the particle in the force field; E is the intrinsic energy.

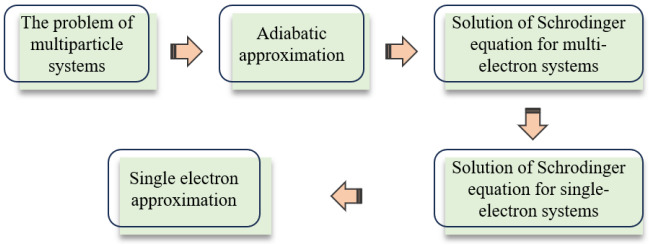

Figure 2. First Principles Research Ideas

2) Density functional

In materials simulation research and analysis, the focus of study typically involves a multi-electron system. However, the Schrödinger equation has limitations in accurately solving for the electronic structure of a single electron, and it is unable to calculate the complex structure of multiple electrons. Currently, the electronic properties and structural characteristics used to predict metals are typically based on density functional theory. This theory offers a theoretical foundation for understanding the interconversion between electronic singlet and poloidal problems, and it is one of the primary methods employed to investigate the ground state properties of multiparticle systems. The primary challenge in applying density functional theory to practical research is to accurately determine the exchange-correlation function. In this paper, two types of exchange-correlation functions are utilized in the research on density functional theory: the local density approximation (LDA) and the general gradient approximation (GGA).

a) Local Density Approximation (LDA)

In the exchange-correlation generalization, LDA was initially employed as the simplest and most effective approximation. It replaces the exchange-correlation energy density $\varepsilon_{xc}^{ham}\left[\rho(r)\right]$ of the uniform electron density in the system with the exchange-correlation energy density $\varepsilon_{xc}\left[\rho(r)\right]$ of the non-uniform electron density, i.e.:

$$E_{xc}[\rho(\vec{r})] = \int \varepsilon_{xc}[\rho(\vec{r})]\rho(\vec{r})dr \tag{2}$$

$$\varepsilon_{xc}[\rho(\vec{r})] = \varepsilon_{xc}^{ham}[\rho(\vec{r})] \tag{3}$$

The exchange-correlation potential is:

$$V_{xc}(\vec{r}) = \frac{\delta E_{xc}[\rho(\vec{r})]}{\delta\rho(\vec{r})} = \frac{\partial\left[\rho(\vec{r})\varepsilon_{xc}[\rho(\vec{r})]\right]}{\partial\rho(\vec{r})} \tag{4}$$

The LDA approximation applies to the multiparticle system of homogeneous electron gases. It does not depend on any empirical values and can be computed directly from the basic theory of quantum mechanics. This method can be used to compute a wide range of physical and chemical properties of materials.

b) Generalised Gradient Approximation Theory (GGA)

The GGA approximation takes into account the inhomogeneity of the charge density by introducing an electron density gradient term in $\varepsilon_{xc}\left[\rho(r)\right]$. The GGA approximation is based on the premise that the charge density is a function of spatial position. Assuming that the charge density $\rho(r)$ is a slowly varying function of spatial position, the exchange-correlation energy of the system can be expressed as:

$$E_{xc} = \int \rho(r)\varepsilon_{xc}\left[\rho(r)\right]dr \tag{5}$$

where $\varepsilon_{xc}\left[\rho(r)\right]$ is the exchange-correlation energy of any one electron, and the corresponding correlation equation can be expressed as

$$V_{xc}(r) = \frac{\delta E_{xc}}{\delta\rho(\mathrm{r})} = \varepsilon_{xc}[\rho] + \rho\frac{\delta\varepsilon_{xc}}{\delta\rho(r)} \tag{6}$$

C. Support vector machine algorithm model

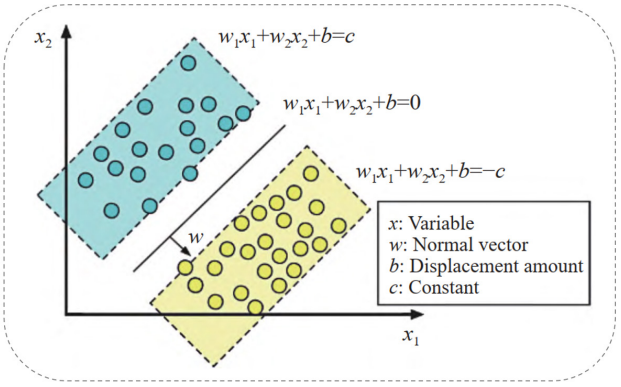

Figure 3. Support vector Machine Model

Support Vector Machines (SVMs) were initially employed for solving binary classification problems by identifying the optimal classification hyperplane to meet the classification criteria. A typical SVMs is shown in Figure 3. However, in real-world scenarios, the data is often not linearly separable. Therefore, it is necessary to transform the low-dimensional data into a high-dimensional space using a specific model and then identify the hyperplane. However, high-dimensional data leads to an increase in computational complexity, and to avoid dimensionality catastrophe, it is reasonable to use kernel functions instead of inner products. Support vector machines are capable of solving a variety of problems, including regression, pattern recognition, function simulation, and data classification. They are particularly advantageous in small sample, nonlinear, and high-dimensional pattern recognition scenarios. Compared to other similar methods, Support Vector Machines are characterized by their strong adaptability, generalization ability, and high training efficiency.

This paper discusses the use of a nonlinear support vector machine for predicting the behavior of aluminum alloy materials. There are several steps.

(1) Determine dataset $\mathrm{T}=\left\{\left(x_1,y_1\right),\left(x_2,y_2\right),\cdots,\left(x_\mathrm{n},y_\mathrm{n}\right)\right\}$, where $\mathrm{y}=\left\{-1,+1\right\},\mathrm{i}=1,2,\cdots\mathrm{N}$. Select the kernel function $\mathrm{K}\left(\mathrm{x},\mathrm{z}\right)$ and appropriate parameters C to build the optimal model for the solution.

$$\min_\alpha \frac{1}{2}\sum_{\mathrm{i}=1}^{\mathrm{N}}\sum_{\mathrm{j}=1}^{\mathrm{N}}\alpha_\mathrm{i}a_j y_i y_j K\left(x_i,x_j\right)-\sum_{\mathrm{i}=1}^{\mathrm{N}}\alpha_\mathrm{i} \tag{7}$$

$$s.t.\sum_{\mathrm{i}=1}^{\mathrm{N}}\alpha_\mathrm{i}\mathrm{y}_\mathrm{i}=0,0\le\alpha_\mathrm{i}\le\mathrm{C},\mathrm{i}=1,2,\ldots,N \tag{8}$$

Find the optimal solution, a^*, according to the equations. (7) and (8).

(2) The determinant chooses one of the positive components of a* and then calculates b*:

$$b^*=y_i-\sum_{\mathrm{i}=1}^{\mathrm{N}}a_i^*y_iK\left(x_i,y_j\right) \tag{9}$$

(3) Construct the decision function via f(x):

$$f(\mathrm{x})=sign\left(\sum_{\mathrm{i}=1}^{\mathrm{N}}a_i^*y_iK\left(x,x_i\right)+b^*\right) \tag{10}$$

III. Data-Driven Prediction of High-Performance Materials

The element aluminum is used as the base element, and the mixing ratio of aluminum to any other element is always 1:1. The arbitrary elements can be chosen from the following range: Fe, Cu, and Mn. Database A is created using the grid-based projection weighted wave (GPAW) method within the framework of density functional theory. This database stores both non-computational features and computational material properties of aluminum in combination with the elements Cu, Mn, Si, and Fe. These properties include body-centered cubic (BCC), face-centered cubic (FCC), and hexagonal closest-packed (HCP) structures. In this way, the support vector machine accurately identifies the pattern of change in the material's nature. In this paper, the support vector machine classification is trained using a variety of different datasets. Once the support vector machine is trained, it can predict categories based on user input. To predict material properties and material combinations, support vector machine classification from the sci-kit-learn library is utilized, and the weights are adjusted based on the frequency of the vector machine categories.

In this paper, five support vector machines were developed for predicting crystal structure, lattice constant, formation energy, magnetic moment, and bulk modulus. The data in database A is divided into a training set and a validation set. The training set includes element names, magnetic moments, formation energies, bulk moduli, etc., while the validation set is grouped based on specific labels for each support vector machine. The properties of Al-Fe, Al-Cu, and Al-Mn alloy materials have been removed from database A. The trained machine learning model predicted the material properties of these three alloys. Table 1 presents the predicted data for the crystal structure, lattice constants, formation energies, magnetic moments, and bulk modulus by the vector machine. It is evident from Table 1 that the machine learning model effectively predicted the material properties of these alloys.

Table 1. Material properties of aluminum-based alloys predicted by a support vector machine trained on Database A (actual values in parentheses)

	Structure	Lattice	Formation	Bulk	Magnetic
Al-Fe	FCC (FCC)	2.5-3.0 (2.85)	Exothermic (Exothermic)	100–200 (168)	0-1 (0.74)
Al-Cu	FCC (FCC)	2.5-3.0 (2.94)	Exothermic (Exothermic)	100–200 (173)	0-1 (0.65)
Al-Mn	BCC (BCC)	3.0-3.5 (3.21)	Exothermic (Exothermic)	100–200 (181)	1-2 (1.44)

The results demonstrate that predicting material properties is achievable. By expanding the content of the materials database, it will be possible to categorize materials not only by element name but also by crystal structure and element ratio. This extension will enable support vector machines to identify the precise combinations of elements, structures, and element ratios that will yield the desired material properties.

IV. Conclusion

Material synthesis and design can be accurately predicted using first-principles calculations and machine learning. In particular, material databases can be constructed based on first-principles calculations. The materials database is then utilized to train support vector machines in machine learning. The properties and combinations of materials were predicted using

a trained support vector machine, and the predictions were in good agreement with the experimental data. By manipulating the material database, it is possible to use machine learning to predict the desired materials.

Through a comprehensive examination of the microstructure and macroscopic properties of aluminum alloys, and with the aid of advanced computational methods, it is anticipated that the conventional R&D model will be surpassed, leading to the more efficient design of materials with superior performance.

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