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PROSPECTIVE REVISIONS ON THE USE OF MACHINE LEARNING IN THE ALUMINUM ALLOY DEVELOPMENT: A REVIEW ON TECHNIQUES AND FUTURE APPLICATIONS

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ABSTRACT: *Alloy design is the major driving force of next-generation materials technology. Traditionally alloy design has relied on empirical rules and iterative trial-and-error experimentation, with the process of identifying novel compositions being time-consuming, costly, and inefficient. The landscape has recently been revolutionized by advances in machine learning (ML) that enable data-driven methods to improve the efficiency of sophisticated alloy design, selection, and property prediction. ML algorithms can learn effectively the relationships between composition, processing, structure, and properties from existing data, and thus guide the discovery of novel alloys with target properties. In this review, a survey of ML approaches employed in alloy design is provided, including supervised and unsupervised learning, feature engineering, and combination with physical modeling frameworks, such as CALPHAD.*

KEYWORDS: Alloy Design, Empirical Rules, Machine Learning (ML), Data-driven Methods, Property Prediction, CALPHAD, Materials Discovery, Aluminum Alloys, Materials Informatics.

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INTRODUCTION

Mechanical behavior in alloys is determined by their microstructures, and these in turn are determined by chemical composition and fabricating processes. Standard metallurgical-property prediction therefore uses a two-step process. In step one, the microstructure is either simulated or predicted from processes/compositions, and in step two, the material property is related to the microstructure. Mingwei *et al.* (2021) in their work, Prediction of Mechanical Properties of Wrought Aluminum Alloys Using Feature Engineering Assisted Machine Learning Approach, pointed out that there were many empirical, physical metallurgy models that were used to simulate strengthening mechanisms and strength contributions. Many models have been put in place to ascertain the strengthening mechanism, such as representative models, which include the grain boundary effect described by the Hall-Petch relation, solid-solution strengthening described by the Fleischer equation, dislocation strengthening described by the Bailey-Hirsch relation, precipitation strengthening governed by the Orowan equation or dislocation shearing mechanism. These constitutive models quantitatively connect the microstructure of polycrystalline metallic alloys with a certain strengthening mechanism, which can be utilized to estimate the alloy strength by linear summation.

Pure metals are rarely used in their unadulterated form because their inherent properties often do not align with the specific demands of a product. However, introducing even small amounts of a second or third element can drastically alter a metal's characteristics, leading to the creation of alloys with significantly enhanced properties.

Industries such as aerospace, automotive, and structural engineering require materials that offer both excellent mechanical tolerance and low weight. As Rajat (2024) highlighted, the efficiency of well-designed alloys, particularly aluminum alloys, is evident in their extensive use in electric vehicle (EV) body structures, chassis, and battery housings. These alloys provide superior mechanical properties and their low weight contributes to reduced overall vehicle mass, leading to improved cost-effectiveness, enhanced corrosion resistance, and better acceleration.

Aluminum alloys are second only to steels in their widespread use as structural metals. Aluminum's density is a mere 2.7 g/cm^3, roughly one-third that of steel (7.83 g/cm^3). The exceptional qualities of aluminum alloy, including its outstanding corrosion resistance, lightweight nature, high specific strength, good low temperature resistance, and ease of extrusion molding, have been widely acknowledged by researchers like Chen *et al*. (2022), Zhou *et al*. (2023), Zhou and Young (2018), Yan *et al*. (2022). These attributes make aluminum alloys a preferred material across diverse sectors, including explosion-proof applications, marine environments, bridge construction, large-span roofing, and curtain wall systems. The integration of machine learning (ML) with computational methods, such as calculation of phase diagram (CALPHAD) and density functional theory (DFT) has further advanced the development and understanding of these crucial materials.

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LITERATURE REVIEW

Overview of Aluminum Alloys

Aluminum alloys can be broadly classified into two categories: wrought alloys and cast alloys, which are further divided into heat-treatable and non-heat-treatable groups. Common alloying elements include Cu, Mg, Si, Zn, Mn, and Li, which influence the alloy's mechanical, thermal, and corrosion properties (Jinliang *et al*., 2019), whereas the notable series include:

a. 2xxx: Al-Cu, high strength, used in aerospace

b. 6xxx: Al-Mg-Si, good formability, widely used in automotive

c. 7xxx: Al-Zn-Mg, very high strength, but more prone to corrosion

Understanding the influence of composition and processing routes on final performance is a key challenge in optimizing these alloys; this is where machine learning has shown increasing promise. Liu *et al*. (2023) applied a genetic algorithm guided by ML property predictors to design Al-Mg-Si-Cu alloys with improved corrosion resistance.

Applications of ML in Aluminum Alloy Development

Machine Learning (ML) models depend heavily on the quality and quantity of data. Several studies by Yi *et al*. (2021) have constructed datasets from literature and experimental databases, CALPHAD-based Simulations (Thermo-Calc, JMatPro), and Open-source Repositories, while features typically include: Composition (%wt of elements), Processing Parameters (annealing temperature, aging time) and Microstructure Features (grain size, phase fractions). Traditionally, the design, selection, and development of aluminum alloys have relied so much on empirical, trial-and-error methods. This approach is problematic, as solidification defects like porosity and oxide films in aluminum castings can significantly reduce fatigue life by acting as crack initiation sites, leading to failure (Ahmad *et al*., 2020). To address these challenges, the deployment of ML prediction, leveraging available datasets and different machine learning algorithms, such as supervised and unsupervised learning, has become crucial for alloy selection and design (Gus, 2021; Huu-tai, 2022).

According to the researcher of unsupervised learning and pattern recognition in alloy design, Bhat *et al*. (2024) emphasized that supervised learning algorithms are ideally adapted to predictive problems wherein historical data can be learned to predict future outcomes. The models learn from labeled datasets, wherein input features are associated with known outputs, such that material properties can be inferred from compositional and processing variables. This predictive capability is also very valuable in alloy design and nanomaterials. By systematic exploration of the correlation between input parameters and material properties, supervised ML models can guide the development of new materials with enhanced properties.

Unsupervised learning, on the other hand, uncovers hidden patterns in data, regardless of the target properties, and can offer guidance on new research direction and investment well in advance of applications. Although unsupervised learning is used throughout materials informatics, this is a relatively untapped area of metal alloy design with huge potential to extract latent information contained within high dimensional combinatorial data. Examples are limited but include nanoalloys, high entropy alloys, and commercial Al and Mg alloys.

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As the demand for advanced materials with tailored properties continues to grow, there is an increasing need for more efficient and predictive design strategies that can effectively narrow down candidate options prior to building structure property models. Traditional alloy development methods are often slow, costly, and resource intensive, prompting researchers to explore data-driven approaches as a means to overcome these limitations.

In this context, unsupervised learning techniques have emerged as valuable tools for analyzing the complex, high-dimensional datasets commonly encountered in materials science without the requirement of pre-labelled property data. The primary goal of unsupervised learning is to detect patterns within unlabeled data, where physicochemical property information is not available. Key tasks in this domain include cluster analysis and dimensionality reduction (DR). Cluster analysis groups individual structures based on similarities or dissimilarities in a high-dimensional space, using distance metrics to identify representative prototypes at cluster centroids. DR techniques, on the other hand, help to create simplified, lower-dimensional representations of data, either by reducing the number of features describing each alloy or by selecting the most influential alloys from a larger set. This not only streamlines model training but also enhances generalizability.

These approaches enable researchers to reveal hidden trends, simplify complex datasets, and identify potential outliers that may represent novel or previously unexplored materials. Despite their potential, applications of unsupervised learning in alloy design remain relatively limited, highlighting significant opportunities for future research to address key challenges in this field.

Supervised Learning Approaches

Supervised learning is the most commonly used ML approach in alloy design. Algorithms such as linear regression, support vector machines (SVM), decision trees, random forests, and artificial neural networks (ANNs) are trained on labeled datasets to predict target properties.

Yi *et al.* (2021), Wem *et al.* (2020) and Liu *et al.* (2021), emphasized in their research that regression models such as Random Forests, Support Vector Machines (SVM), Gradient Boosting Machines (GBM), and Deep Neural Networks (DNN) have been employed to predict properties such as Elongation, Fatigue life, Yield strength, (UTS) and Corrosion resistance. For example, Liu *et al*. (2021) used ensemble learning (XGBoost) to predict yield strength and elongation of 7xxx-series aluminum alloys, achieving high accuracy and interpretability through SHAP analysis. Numerous studies have demonstrated the successful prediction of mechanical properties of aluminum alloys using ML. Zhou *et al*. (2021) also used ensemble models to predict yield strength and elongation of 7xxx-series alloys with over 90% accuracy, while Yin *et al*. (2020) implemented a deep learning model to estimate hardness based on composition and heat treatment parameters.

Udesh *et al*. (2020) highlighted that ML, as a data-driven method, can accurately predict optimal compositions from large datasets, attracting significant interest in novel alloy development due to its high accuracy. They emphasized the importance of identifying the desired combinations of mechanical properties when considering alloy development. Further research by Udesh *et al*. (2022) on ML-guided design of high-temperature NiTiHf shape memory alloys revealed that traditional alloy development is a time-consuming process with low accuracy, resulting in a 68% failure rate for NiTiHf alloys. The complexity of phase transformations and their sensitivity to composition have made traditional alloy design a laborious trial-and-error endeavor, especially for optimizing alloy composition and heat

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treatment mechanisms in multicomponent aluminum alloys for improved mechanical properties. This process is both time-consuming and challenging to execute accurately and efficiently.

In response to these limitations, the rapid advancements in computer technology have paved the way for computational alloy design approaches based on theoretical modeling and prediction. These methods can significantly accelerate the design of alloy compositions, heat treatment mechanisms, and even manufacturing processes. Yi *et al*. (2021) further supported this, concluding that the traditional trial-and-error method is highly inefficient for developing novel casting aluminum alloys. They demonstrated that computational thermodynamics (CT), particularly within the CALPHAD framework, data-driven ML techniques, and their synergistic combinations, are effective approaches for the design of casting aluminum alloys.

Unsupervised Learning Approaches

Ninad *et al.* (2024) in their research on unsupervised learning and pattern recognition in alloy design noted that, while unsupervised learning is yet in its early stages in the domain of alloy design, it offers new ways to investigate high-dimensional alloy data to uncover structures and correlations that are difficult to see using traditional tools. With unsupervised learning, researchers can identify specific subsets within alloy data sets that are more than just metal composition partitions, and help optimize and design new alloys with specified properties. Combining these data science strategies into alloy design speeds up the process of discovery and reveals new relationships that were not previously known, with profound effects on materials innovation in science. In this review, scientific progress and future applications to using unsupervised machine learning in alloy design are outlined. Unsupervised learning (UL) uses only the unlabeled feature set in order to learn unseen patterns in the data regardless of the properties. In contrast to SL, there are no studies with UL in the design of metallic alloys.

METHODOLOGY

Bhat *et al.* (2023), in their research of unsupervised machine learning discovery classes in aluminium alloys, highlighted that, Iterative label spreading (ILS), an unsupervised machine learning approach, was used to identify the different classes of Al alloys, drawing from a specifically curated dataset of 1154 Al alloys (including alloy composition and processing conditions). Using ILS, eight classes of Al alloys were identified based on a comprehensive feature set under two descriptors. Further, a decision tree classifier (DTC) was used to validate the separation of classes. The DTC was used to determine if the clusters are separable classes, using the cluster number as labels.

The classifier obtained a test R2 score of 1 and a fivefold cross-validation score of 0.994 ± 0.009. Table 1 shows the high precision, recall and f1-score of the DTC. The matrix, known as the “Confusion Matrix” in Figure 1, confirms that the clusters are classes.

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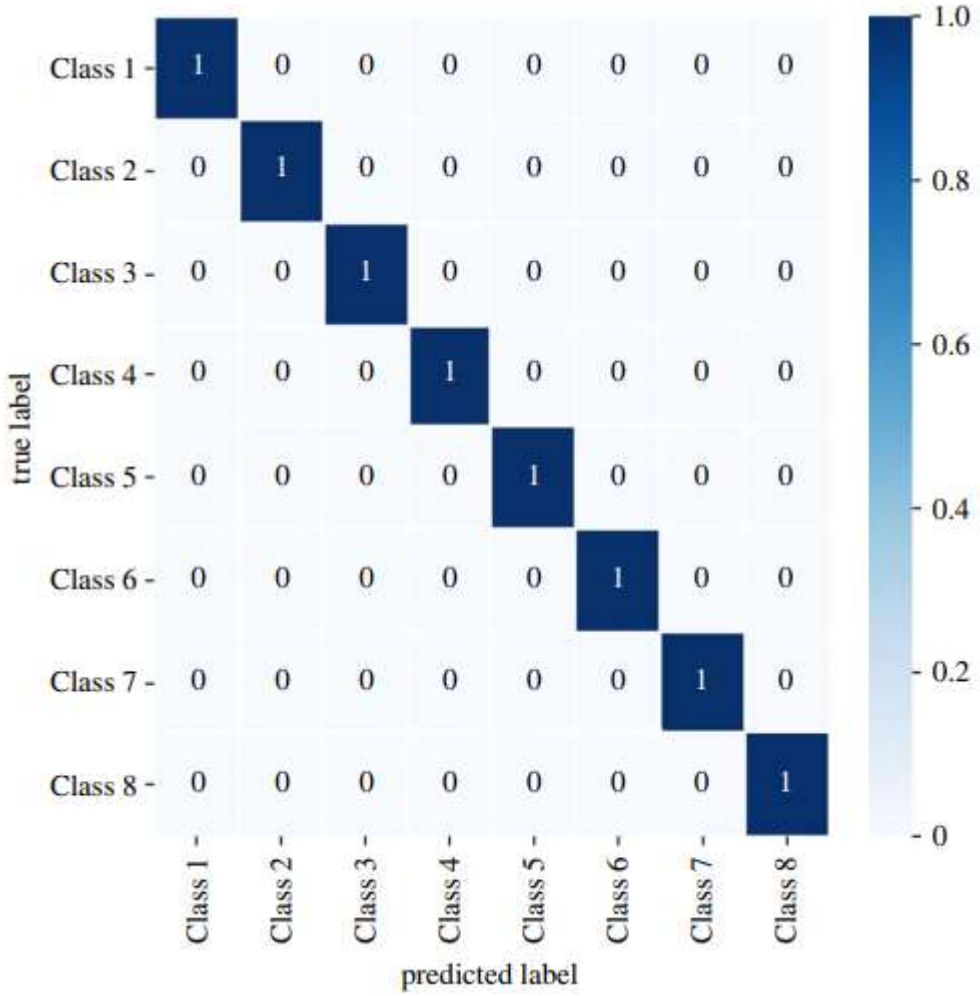
Table 1: High precision, recall and f1-score of the DTC.

	precision	recall	F1-score
Class 1	1.0	1.0	1.0
Class 2	1.0	1.0	1.0
Class 3	1.0	1.0	1.0
Class 4	1.0	1.0	1.0
Class 5	1.0	1.0	1.0
Class 6	1.0	1.0	1.0
Class 7	1.0	1.0	1.0
Class 8	1.0	1.0	1.0

Table X shows the high precision, recall and f1-score of the DTC.

Fig. 1: Confusion matrix showing true positive, true negative, false positive and false negative of DTC classes.



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RESULT AND DISCUSSION

This review shows that unsupervised clustering algorithms can be used to classify separable classes merely on the basis of similarity in features. Unsupervised ML was successfully used to detect the underlying hidden patterns and classify alloys, thereby respectively into classes. The prediction of the different classes of Al alloys from a dataset of 1154 Al alloys included alloy composition and processing parameters. Through the use of the ILS technique, eight distinct clusters of Al alloys were obtained using the feature set of 34 dimensions. By using a DTC, these clusters were recognizable classes. It was discovered that 11 features were responsible for classifying classes using recursive feature elimination with a DTC. The feature importance profiles recognized processing conditions and key combinations of major alloying factors as largely separating the eight classes. The approach was shown to recover Al-alloy class information that is understandable and which well discriminated some of the important commercial alloy classes in a rational manner. Based on the work here, the classes can serve as a point of reference for rational, data-considerate Al-alloy design in future models that focus on optimizing alloy design using ML.

One such positive affirmation is the study of Zhang *et al*. (2019). Unsupervised discovery of solid-state lithium-ion conductors which positively asserted that, unlike supervised learning models, which require nicely labeled training data, unsupervised learning is readily applicable to large datasets regardless of whether any properties or labels exist. As a technique to deduce from data characteristics without specific labeled attributes, unsupervised learning has been applied in materials science for feature extraction, pattern recognition, clustering, and phase mapping. Utilizing unsupervised learning for the direct discovery of new materials with optimized properties has been rarely explored. Unsupervised learning, through training across a broad range of materials, can identify boundaries between good and poor examples, selecting out candidates that look like good examples, and later be verified by more accurate first-principles calculations. In their study, a colorful method was employed to illustrate the outline of the unsupervised discovery of solid-state Li-ion conductors (SSLCs) materials, as shown in Fig. 2.

For training the unsupervised model, a quantitative representation of the complex materials structure (Fig. 2a) is required as input. Instead of using a set of hand-chosen features, digital diffraction patterns of the crystal structure were used. Specifically, a representation for each crystal structure was built up based on Bragg's law to convert the three-dimensional periodic crystal lattice to a set of X-ray diffraction intensities at a specified set of 2θ values. Here, considering only the anion lattice of the crystal structure, based on the premise that anion arrangement and Li+-anion interactions have a strong effect on Li sites, diffusion channels, and the energy landscape of Li migration, the anionic lattice was pinned to S anion and resized to the same atomistic volume, so that the representation was invariant to lattice parameter or the chemical constituent. The resulting representation, termed modified X-ray diffraction (mXRD), is uniquely determined for every anion lattice (Fig. 2b), fully encoding the anionic crystal structure information. Here, we performed our unsupervised discovery over 2986 compounds that contain lithium but not transition metals. Since some compounds have the same structure, one representative structure was selected. 528 representative anionic structures and their mXRDs were conducted for the unsupervised learning.

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Fig. 2a

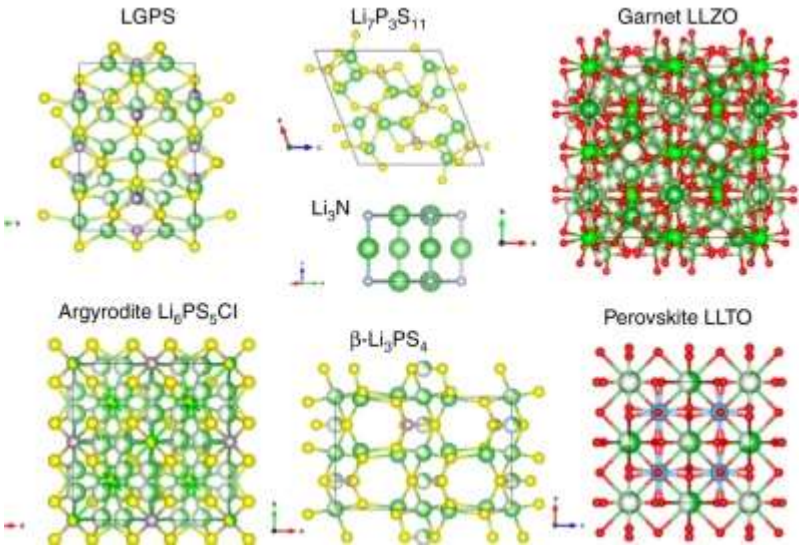
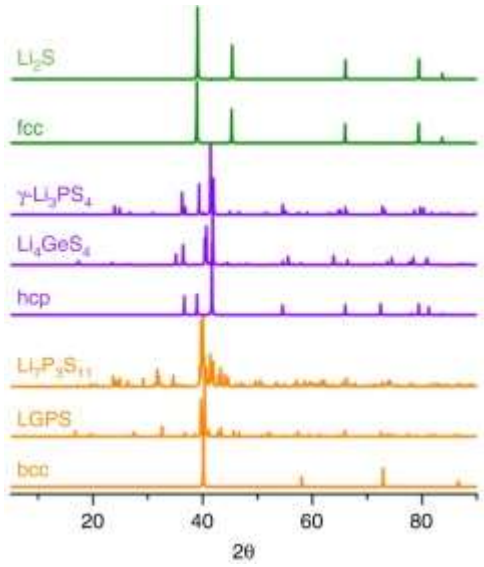


Fig. 2b



Integration of ML with computational methods (e.g., CALPHAD, DFT).

ML models are being used to complement DFT and CALPHAD simulations. Seko *et al*. (2019) demonstrated the use of ML to accelerate DFT calculations in high-throughput alloy screening. Huang *et al*. (2021) used ML to interpolate CALPHAD results across unexplored compositions.

Yi *et al*. (2021) in their work on boosting for concept design of casting aluminum alloys driven by combining computational thermodynamics and machine learning techniques deduced that Computational Thermodynamics (CT), machine learning, and hybrid approaches have been employed in alloy development. CT, which integrates phase equilibrium and thermochemistry through computational methods, has advanced to include kinetic simulations alongside thermodynamic calculations. This evolution has made CT a robust tool for material design. It

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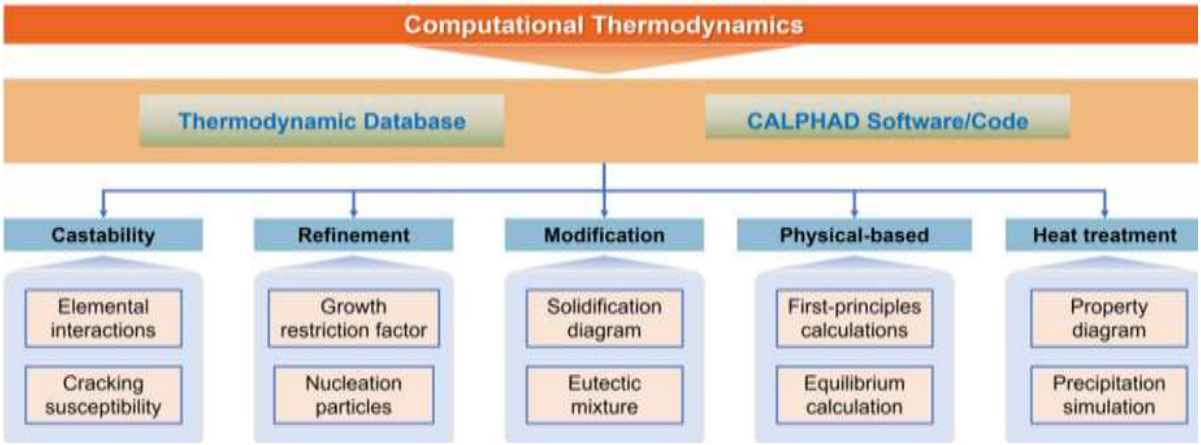
accurately predicts factors crucial to casting aluminum alloys, such as castability, cracking susceptibility, grain refinement, microstructure modifications, and fundamental physical properties. These predictions enable the optimization of alloy composition, heat treatment processes, and manufacturing techniques through a multi-objective design strategy.

The CALPHAD technique, utilizing accurate thermodynamic databases within the CT approach, has proven effective in predicting critical factors for the as-cast microstructure of alloys. These factors include castability, crack susceptibility index, and growth restriction factor, all of which are vital for efficient alloy design. Furthermore, CT-derived property diagrams have facilitated the optimization of solid solution and aging temperatures for specific casting alloys, such as the Sc-enhanced Al-Si-Mg series. The figure below shows the strategic workflow for alloy design approach driven by computational thermodynamics as a tool for Yi *et al.* (2021)'s success.

Fig. 3: Strategic workflow for alloy design approach driven by computational thermodynamics.



Result and Discussion of the Synergistic Approaches: Combining CT and ML

This review strongly advocates for integrating CT and ML to quantitatively establish the "Composition, Process, Microstructure and Properties" relationships in casting aluminum alloys. Additionally, using ML to train a "Microstructure-Properties" matrix could offer deeper insights into the strengthening and toughening mechanisms of casting aluminum alloys. Ultimately, the work concludes that combining CT and ML significantly accelerates the conceptual design of cast aluminum alloys for diverse industrial applications.

ML-Guided Phase Design for High-Entropy Alloys

Ziqing *et al*. (2019)'s research on ML-guided phase design for high-entropy alloys (HEAs) demonstrated that Artificial Neural Networks (ANNs), one-dimensional Convolutional Neural Networks (CNNs), and Support Vector Machines (SVMs) can effectively evaluate existing phase design rules and explore new ones. These three ML algorithms are well-suited for supervised classification problems. ANNs, for instance, utilize a feed-forward structure with input, hidden, and output layers.

In addition, ML models can predict phase stability and microstructure evolution, as confirmed by Chen *et al*. (2020), combined ML with CALPHAD data, to forecast phase diagrams and

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solidification behavior. Another literature by Zhang et al. (2022) trained CNNs to classify grain morphology from microstructure images of aluminum-silicon alloys.

Experimental verification of ML modeling, including casting, melt spinning, and co-sputtering, for a new Fe-Cr-Ni-Zr-Cu HEA system generally aligned with ML predictions. However, the experiments also revealed that the phases in the ML-designed HEAs were cooling rate dependent. This observation is sensible, as amorphous (AM) phases are metastable, and even solid solution (SS) phases in some HEAs can be cooling-rate sensitive.

CONCLUSION

Machine learning has emerged as a cornerstone technology in the modern development of aluminum alloys, enabling rapid prediction, optimization, and discovery. This review encapsulates the vast progress in ML-assisted design, outlines the key challenges, and highlights the importance of interdisciplinary collaboration in advancing this domain. As tools and datasets evolve, ML promises to unlock next-generation lightweight, high-performance alloys tailored for structural, aerospace, and sustainable applications.

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