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Review

Machine Learning in Enhancing Corrosion Resistance of Magnesium Alloys: A Comprehensive Review

Yanbing Guo [1,†], Mingze Sun [2,†], Wang Zhang [2] and Lvyuan Wang [3,*]

[1] Institute of Marine Materials Science and Engineering, College of Ocean Science and Engineering, Shanghai Maritime University, Shanghai 201306, China; yanbingg1984@126.com
[2] School of Mechanical Engineering, Shanghai Dianji University, Shanghai 201306, China; smz2000766@outlook.com (M.S.); zhangwang@sdju.edu.cn (W.Z.)
[3] School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, China
* Correspondence: lyuyuanwang@njust.edu.cn; Tel.: +86-02138284815
† These authors contributed equally to this work.

Abstract: While magnesium alloys have garnered attention for their lightweight properties across diverse applications, their susceptibility to corrosion presents a formidable challenge. Recent years have witnessed the emergence of machine learning (ML) as a formidable tool for predicting and augmenting material properties, notably corrosion resistance. This comprehensive review investigates the latest advancements and hurdles in utilizing ML techniques to investigate the corrosion behavior of magnesium alloys. This article delves into a spectrum of ML algorithms, encompassing artificial neural networks, support vector machines, and random forests, elucidating their roles in predicting corrosion rates, morphologies, and other corrosion-related characteristics in magnesium alloys. Furthermore, it underscores the pivotal challenges and opportunities within this field, such as data quality, model interpretability, and model transferability. Finally, it examines the potential of ML methods in the conception and enhancement of magnesium alloys endowed with superior corrosion resistance. This review aspires to offer valuable insights into harnessing ML's potential for optimizing magnesium alloy designs with heightened corrosion resistance, a facet of paramount importance across diverse industries, including the automotive, aerospace, and biomedical sectors. By addressing the challenges inherent in using ML to forecast corrosion rates, including data limitations and the intricacies of corrosion mechanisms, ML stands poised to emerge as a potent instrument for advancing the development of corrosion-resistant materials.

Keywords: machine learning; magnesium alloy; corrosion prediction; optimization; corrosion resistance

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1. Introduction

In recent years, with the widespread application of alloy metals such as titanium alloy and aluminum alloy in commercial and industrial fields, magnesium alloy has also attracted wide attention for its high strength-to-light weight ratio and its potential in various applications such as automotive, aerospace and biomedicine [1]. However, their poor corrosion resistance has been a major challenge limiting their widespread use in these applications. Therefore, the development of effective strategies to predict and optimize the corrosion performance of magnesium alloys is crucial for the successful implementation of these materials.

Magnesium alloys are a class of materials primarily composed of magnesium, with various alloying elements added to enhance their mechanical and physical properties [2]. Despite possessing appealing properties, magnesium alloys are extremely prone to corrosion, which can diminish their operational lifespan and undermine their structural integrity. The corrosion behavior of magnesium alloys is influenced by multiple factors, including alloy composition, corrosion environment, and exposure time. Therefore, comprehending

and forecasting the corrosion behavior of magnesium alloys are of paramount importance in designing and optimizing corrosion-resistant materials [3].

Machine learning (ML) is a rapidly developing field that has shown tremendous potential in predicting and optimizing material properties [4]. ML algorithms have the capability to analyze extensive and intricate datasets, recognizing patterns and relationships between input and output variables, thus enabling precise prediction of material properties. In recent years, ML has become a powerful tool for predicting and optimizing material corrosion resistance, including magnesium alloys [5]. ML methods can help overcome the challenges faced by traditional corrosion testing methods and can rapidly screen a large number of alloys and corrosion conditions. ML algorithms can additionally offer insights into potential mechanisms and influencing factors of corrosion behavior, fostering the design and optimization of corrosion-resistant materials [6].

Given the potential of machine learning (ML) in predicting and optimizing the corrosion resistance of magnesium alloys, this review comprehensively summarizes the latest developments and challenges in the application of ML techniques in this field. This article discusses various ML algorithms, including artificial neural networks, support vector machines, and random forests, and their applications in predicting the corrosion rate, corrosion morphology, and other corrosion-related properties of magnesium alloys [7,8]. Additionally, it underscores the challenges and opportunities in this domain, including data quality, model interpretability, and model transferability [9,10]. Finally, it discusses the potential of utilizing ML methods to design and optimize magnesium alloys with enhanced corrosion resistance [11–13].

Overall, this review aims to provide valuable resources for researchers and practitioners interested in the application of machine learning in the field of magnesium alloy corrosion by tackling the challenges in using machine learning to predict corrosion rates and emphasizing the opportunities for designing and optimizing corrosion-resistant materials. Therefore, this review of investigating the corrosion properties of magnesium alloys based on machine learning techniques can provide a new strategy to improve the corrosion resistance of magnesium alloys, thereby facilitating their broader utilization in various applications.

2. Machine Learning Algorithms for Predicting the Corrosion Performance of Magnesium Alloys

2.1. Artificial Neural Networks

Artificial neural networks (ANN) are highly useful modeling techniques based on statistical methods, and the principle of this model is to simulate the pattern recognition ability of the human brain [14,15]. The structure of artificial neural networks comprises three interconnected layers: the input layer, hidden layers, and the output layer. In the hidden layers, input data and output data are linked by processing elements (nodes or neurons) using a specific set of non-linear functions. The construction of an artificial neural network model follows these steps: data collection, training the neural network, during which the weights associated with each connection between neurons can be adjusted, and testing the trained model [16].

ANN models have been used to address multivariate issues in the field of corrosion. Sim et al. [17] developed a neural network for predicting the relationship between supercritical carbon dioxide corrosion and the environment. Malinov [18] used ANN to study the correlation between processing parameters and the mechanical properties and corrosion resistance of titanium alloys. To date, in the field of research based on magnesium alloys, there have been many studies on the application of ANN as tools for researching and predicting corrosion performance. Kirkland [19] used artificial neural networks to study Mg-Zn-Ca alloys for the development of customized absorbable implant alloys. Birbilis et al. [20] also used ANN to investigate the corrosion rate and yield strength of Mg-RE alloys with different alloying combinations.

Among them, there have been numerous studies using ANN to investigate the impact of compositional changes in multicomponent magnesium alloys on corrosion rates. Xia et al. [21] constructed an ANN model using JMP11 statistical software, with the model's inputs being alloy concentrations calculated in weight percentages, and the model's outputs were Vickers hardness values and corrosion rates, with corrosion rates represented in the form of corrosion current density (i_corr) from potentiostatic polarization experiments, as shown in Figure 1. Consequently, the corrosion rates predicted by the ANN were expressed in terms of corrosion current density (A/cm^2), as shown in Figure 2. Before training, they randomly selected 5 datasets for the final independent testing of the ANN model. Sixty-seven percent of the remaining datasets were used to train the ANN for microhardness and i_corr, and the rest were used for cross-validation.

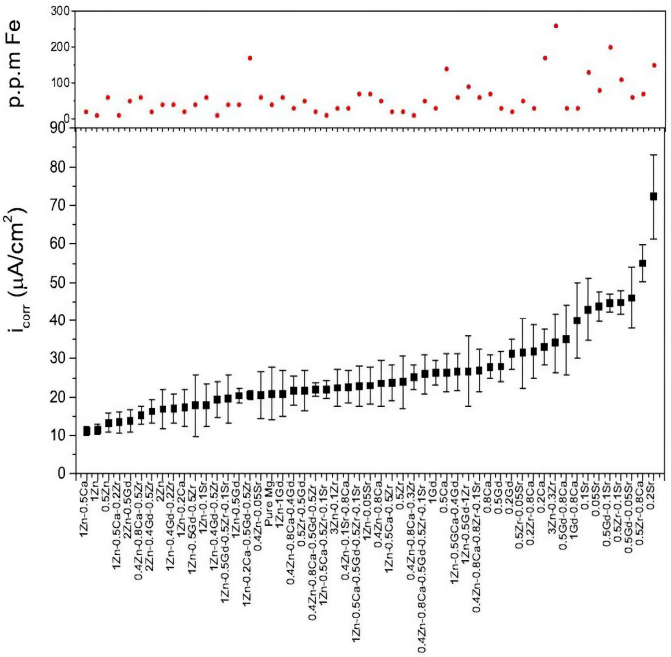

Figure 1. Corrosion rate in terms of corrosion current density (i_corr). Adapted with permission from Ref. [21]. Copyright 2016, Elsevier.

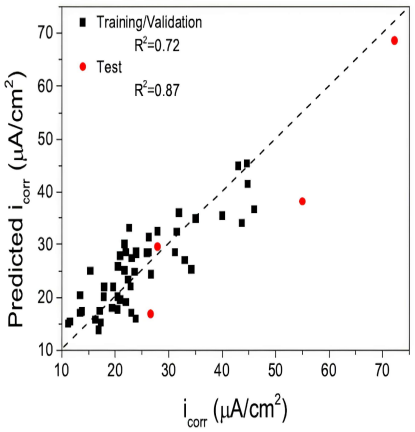

Figure 2. Correlation between predicted i_corr and observed i_corr. Adapted with permission from Ref. [21]. Copyright 2016, Elsevier.

From Figure 1, it can be observed that most alloy additives result in higher corrosion rates compared to pure Mg; the corrosion rate distribution spans a wide range, indicating that Mg is highly sensitive to the type and amount of alloying elements in terms of corrosion;

corrosion rates in binary and ternary alloys are higher than those in quaternary and quinary alloys; corrosion rates in quaternary and quinary alloys remain at similar levels within a certain range of compositions.

Among these, the accuracy of training/validation (R^2 = 0.72) and testing (R^2 = 0.87) is relatively lower compared to the accuracy of hardness. Nevertheless, due to the inherent chemical reactivity of Mg and the intricate interactions between alloy additives, this correlation is quite strong.

The impact of alloying elements on corrosion rates is depicted in Figure 3.

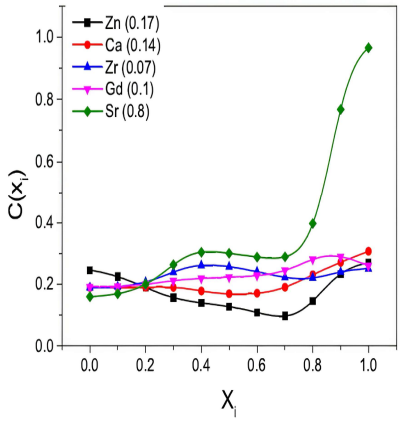

Figure 3. Fuzzy analysis chart of corrosion rate (i_corr). Adapted with permission from Ref. [21]. Copyright 2016, Elsevier.

From the graph, it can be seen that the range of each alloy addition is indicated in the legend. In contrast to the hardness, which has a monotonically positive effect with alloy additives, the influence on corrosion rate (i_corr) is complex. It can be observed that Sr has a much larger range (0.8) compared to other alloying elements, which is due to the relatively low solubility of Sr in Mg. The range of Zr is quite small, indicating that Zr has a relatively minor impact on corrosion in studies involving concentration and combinations. Ca and Gd exhibit relatively significant effects in determining corrosion rates. On the other hand, data collected from this study suggest that Zn is considered to have a certain positive influence on corrosion (in ternary alloys), with corrosion rates decreasing when Zn is added. This study suggests that ANN itself can provide mechanical details, and the model is capable of predicting corrosion rates (represented by corrosion current density i_corr) with satisfactory accuracy within the range of compositions used in this work.

2.2. Support Vector Machines

Support vector machines (SVMs) are based on two-class classification problems [22]. The application of support vector machines in regression problems is known as support vector machine regression, which is an important application branch of SVMs. Unlike support vector machine classification, in support vector machine regression, the sample points ultimately have only one type. Generally, input samples x are mapped to a high-dimensional feature space through non-linear mapping, where the regression function is estimated by establishing a linear model.

$$f(x, \omega) = \omega \cdot \Phi(x) + b \quad (1)$$

For the optimization function of support vector machine regression, it is defined as follows, where ω is the weight vector, and b is the threshold.

Wang [23] et al. used SVR to build a regression model to predict the Eads on the surface of binary Mg intermetallic compounds, and the cross-validation of the multidimensional feature SVR model is shown in Figure 4a, and the cross-validation of the optimal performance of the SVR model is shown in Figure 4b.

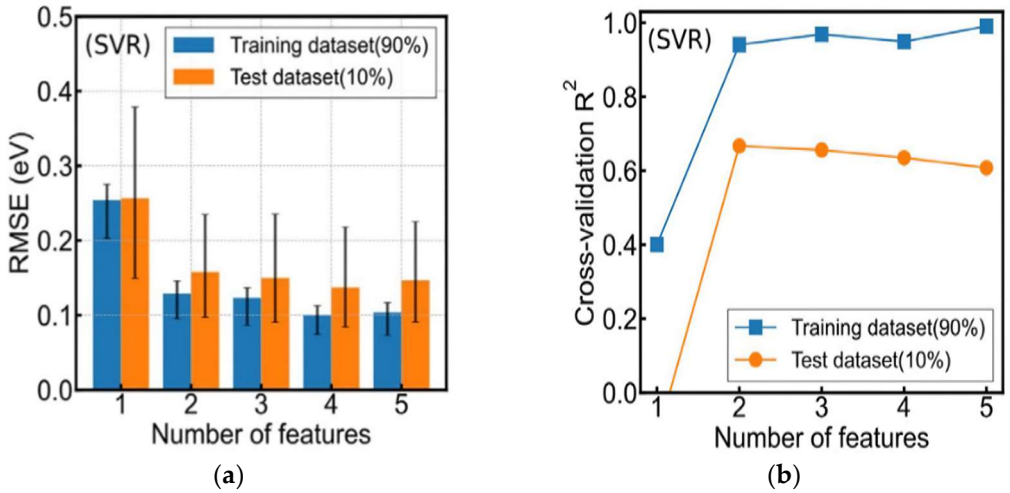

Figure 4. (**a**) The average RMSE of 500 random divisions for the training and test datasets of the multidimensional feature SVR model. (**b**) The cross-validation R^2 of the best-performing model of the SVR model [23].

From the figure, it can be seen that SVR reflects better predictive ability, but as the number of features utilized increases, the accuracy also increases initially, which indicates that more features will improve the predictive ability of the model, whereas a further increase in the number of features may result in overfitting, which reduces the accuracy of the prediction. Therefore, for the prediction of corrosion resistance of magnesium alloys, using support vector machines is more considerable, but special attention needs to be paid to exert control on the number of features to avoid a reduction in accuracy and overfitting.

2.3. Random Forest

The random forest regression model is an ensemble algorithm composed of decision trees [24]. The decision tree algorithm is a decision-making method based on a tree-like structure. With a given number of samples, a tree is constructed by branching on variables or features. Once the leaf nodes of the tree are determined, it can be used for decision making on new input data. Random forest regression combines classification and regression trees (CART). Using an exhaustive algorithm, it explores each feature and its values to select the best splitting variable and splitting point. The determination of the best splitting variable and splitting point is based on the impurity of the resulting nodes. Generally, there are four types of impurity functions: Gini impurity, information entropy, mean squared error (MSE), and mean absolute error (MAE). MSE is suitable for regression problems, and its formula is defined as:

$$H_{MSE}(X) = \frac{1}{N}\sum_{i \in N}(y - \overline{y})^2 \quad (2)$$

The y-average in this context represents the mean value of all target variable values within the current node. A training set is generated using the bootstrap sampling method, subsequently forming the respective decision tree. During prediction, it begins at the root node to establish the feature set of the input sample, determining whether the current node is a leaf node. If it is, the prediction is based on the average y-value at that leaf node. If not, it proceeds to evaluate the left and right child nodes until a leaf node is reached, at which point the average y-value is computed as the expected value [25].

Lu et al. [26] compiled corrosion data for magnesium alloys from previously published sources and utilized machine learning to formulate a model for predicting corrosion potential based on their chemical composition. Throughout the experimental process, they conducted a comparative analysis of four machine learning algorithms, with random forest (RF) yielding the most accurate forecasts. Figure 5 visualizes the prediction results of the

RF algorithm for corrosion potential and current density (blue circles represent the training dataset, while red circles represent the test dataset).

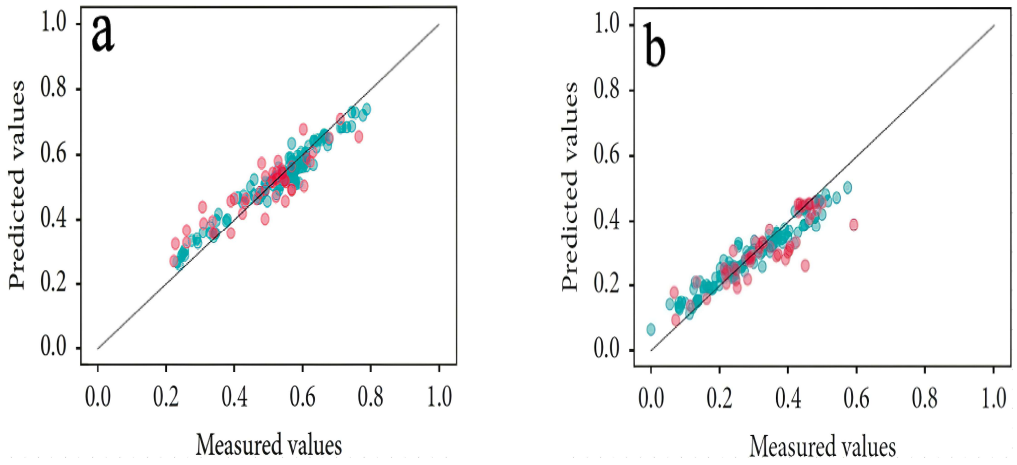

Figure 5. The prediction results of the corrosion potential and current density corresponding to the RF algorithm. (**a**) The corrosion potential prediction results of the RF algorithm. (**b**) The algorithm's predictions for the current corrosion [26].

The images obtained from measurement results are plotted as functions of measurement data, with all data points lying on the diagonal. The closer the data points are to the diagonal, the more accurate the predictions. The model suggests that the influence of different elements on the corrosion potential and current density of magnesium alloys is rather complex and cannot be represented by a simple linear relationship. The RF model, being an ensemble technique, can provide excellent fitting results.

The influence of various elements in multicomponent alloys on the overall corrosion performance of magnesium alloys is shown in Figure 6 (the impact is mainly reflected through the importance in the input features of corrosion potential or current prediction models).

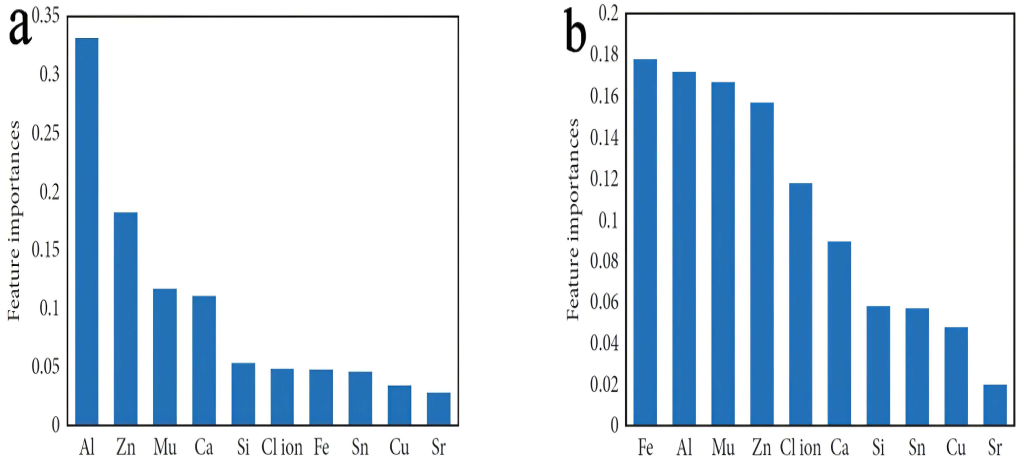

Figure 6. The importance of input features for corrosion potential (**a**) and corrosion current (**b**) prediction models [26].

The RF model assesses the importance of each feature by evaluating the influence of measured feature values on the target attributes. Based on the model's good fitting performance, the prediction model has captured the patterns of influence of each input on corrosion potential and corrosion current. For example, chloride ions are environmental factors that affect corrosion current. Chloride ions can dissolve the magnesium hydroxide

protective layer on magnesium alloys, converting it into magnesium chloride, making the surface more active and prone to corrosion [27]. Zn and Mn have significant impacts on corrosion potential and corrosion current. Zn forms Mg_xZn_y phases and serves as a local cathode within the Mg matrix. During this process, the cathodic reaction rate accelerates, leading to a higher corrosion rate [28,29]. Consequently, models with feature importance are considered reliable. The RF algorithm, even when confronted with the influence of environmental factors and varying chemical compositions, can visually depict the variations in corrosion potential and corrosion current. This highlights its exceptional practical value.

3. The Application of Machine Learning in Studying the Corrosion Behavior of Magnesium Alloys

3.1. Corrosion Rate Prediction

One of the main factors affecting the corrosion resistance of magnesium alloys is the alloy's composition, and the presence of impurities significantly exacerbates corrosion [30]. In the research progress of medical magnesium alloys, the content of impurity elements such as Fe, Ni, and Cu is a major factor directly leading to their corrosion resistance performance [31]. These elements have minimal solubility and often manifest active cathodic characteristics in magnesium alloys, consequently diminishing the corrosion resistance of magnesium alloys. The capacity limits of elements like Fe, Ni, and Cu in magnesium alloys are fixed [32]. For example, the capacity limits of Fe, Ni, and Cu in pure magnesium are 170, 5, and 1000 ppm, respectively [33]. The corrosion resistance of magnesium alloys is hardly affected when not exceeding the permissible capacity limits.

Therefore, using the mass fraction of impurities as features, we employed the high-performance random forest algorithm (RF) to test the mass percentages of different impurity elements such as Fe, Ni, and Cu, thus revealing the relationship between impurity element content and the corrosion rate of magnesium alloys: as the impurity content increases, the corrosion rate of magnesium alloys sharply decreases. This is because impurity elements in magnesium have very low solubility and tend to form compounds within the metal, establishing galvanic cells with the magnesium alloy matrix, consequently accelerating the corrosion of magnesium alloys [34,35].

3.2. Corrosion Morphology Prediction

3.2.1. Corrosion Surface

In atmospheric and aquatic environments, magnesium alloys can experience stress corrosion cracking (SCC) under the influence of mechanical stress, with cracks extending intermittently. When in an anodic solution, the cracks continue to propagate. These are two manifestations of stress corrosion cracking (SCC) in magnesium alloys. However, pure magnesium is not affected by this [36]. The detailed information on stress corrosion cracking (SCC) of AZ91 magnesium alloy at a strain rate of $3 \times 10^{-7} s^{-1}$ in double-distilled water is shown in Figure 7.

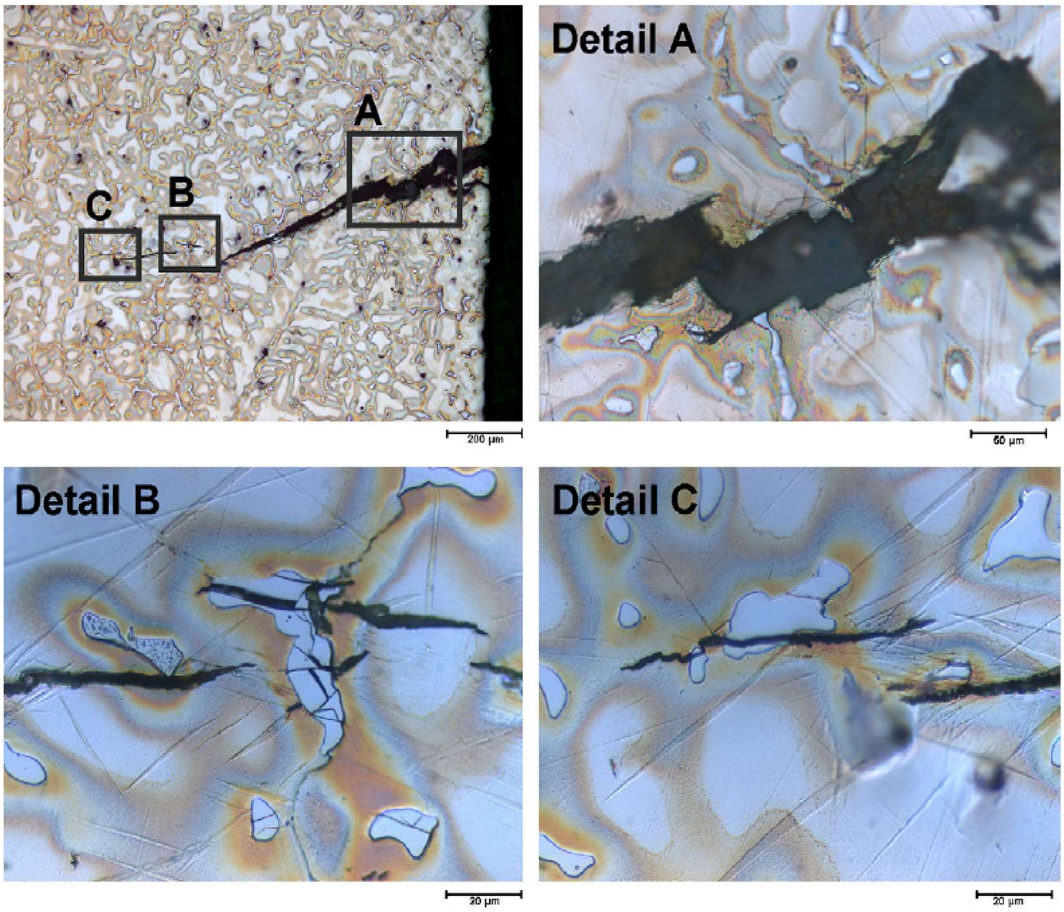

Figure 7. The detailed SCC of AZ91 in double-distilled water at a strain rate of $3 \times 10^{-7} s^{-1}$. Adapted with permission from Ref. [37]. Copyright 2008, Elsevier.

The content of certain metal elements can also influence the extent of stress corrosion cracking. Aluminum is one of the sensitive elements to stress corrosion cracking, and aluminum-containing magnesium alloys are most prone to stress corrosion cracking in air, distilled water, and chloride-containing solutions. As the aluminum content increases, the tendency for stress corrosion cracking also increases correspondingly. Therefore, magnesium alloys such as AZ61, AZ80, and AZ91, with aluminum content of 6%, 8%, and 9%, respectively, exhibit higher sensitivity to SCC, while AZ31 (3% aluminum alloy used in forging applications) is considered to have good resistance [38,39]. Zirconium and rare earth elements are only mildly sensitive, and magnesium alloys without aluminum or zinc are the most SCC-resistant, such as ZK60 and ZE41. By using the content of metal elements as parameters and considering the impact of different elements on the degree of stress corrosion in magnesium alloys, an ANN model can predict the corrosion performance of the cracking surface of magnesium alloys more intuitively, helping to identify appropriate measures for surface treatment.

Lu et al. [40] prepared Mg-Zn-Ca-based magnesium glass and evaluated it as an additive for PLLA. The degradation of crystalline Mg65Zn30Ca5 and amorphous Mg65Zn30Ca5 in Hank's solution was compared, and the surface morphology after soaking for 14 days in Hank's solution is shown in Figure 8. The surface of crystalline Mg65Zn30Ca5 exhibited numerous cracks and severe corrosion after corrosion, indicating poor corrosion resistance. Typically, the corrosion behavior of crystalline magnesium alloys is consistent with the phenomena described in the literature. Although corrosion products are present on the alloy surface after immersion, these corrosion products are mostly not dense enough to completely cover the alloy surface, isolating the corrosive medium, and thus cannot provide effective protection. On the other hand, for the corrosion products of amorphous

Mg65Zn30Ca5, as shown in Figure 8c,d, a dense layer resembling grass can be observed on the corroded surface, with no obvious cracks. This indicates that this dense oxide layer can provide long-term protection. Consequently, compared to crystalline magnesium alloys, amorphous magnesium alloys exhibit superior corrosion resistance. Therefore, the excellent corrosion resistance of amorphous magnesium alloys can help avoid a series of issues caused by rapid degradation of magnesium alloys, making them more promising for clinical applications.

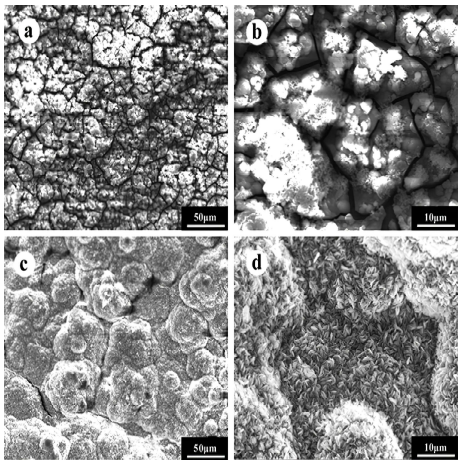

Figure 8. The SEM images of the striped surfaces after immersion in Hank's solution for 14 days: (**a**,**b**) crystalline Mg65Zn30Ca5; (**c**,**d**) amorphous Mg65Zn30Ca5 [40].

The evolution of pH over the first 14 days is shown in Figure 9a. Since both quenched and annealed strips were immersed in Hank's solution, for the annealed strips, the pH of Hank's solution increased sharply from 7.4 to 10.5 within the first 3 days due to the rapid degradation of the less corrosion-resistant annealed alloy. After 14 days, the low pH value indirectly indicates that the degradation of the quenched thin strips is very slow, demonstrating higher corrosion resistance, which is a typical characteristic of amorphous materials.

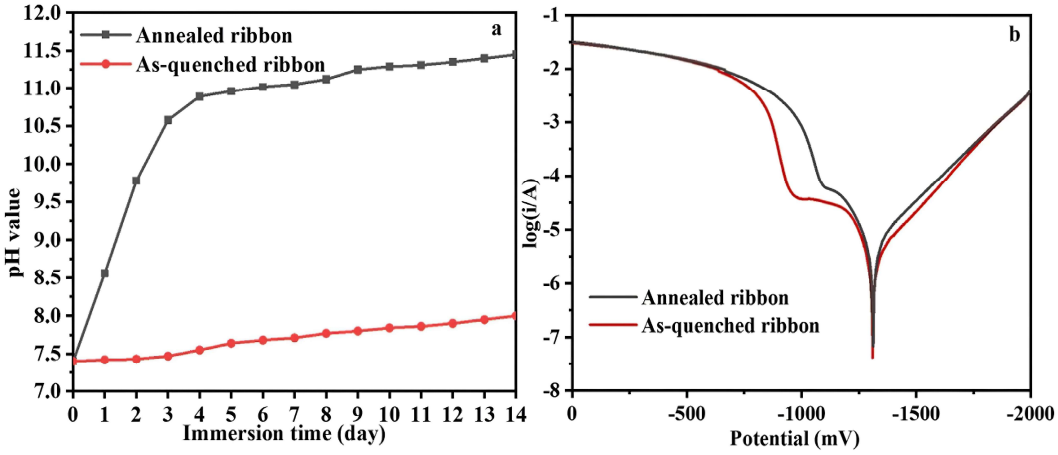

Figure 9. (**a**) The variation in pH of the Hank's solution containing quenched/annealed thin strips, and (**b**) the typical polarization curves of the quenched and annealed strips [40].

From Figure 9b, the typical polarization curves of the quenched and annealed strips can be observed. According to the Tafel extrapolation method, the corrosion potential (E corr) for both thin strips is 1.31 V, with a corrosion current density (i corr) of 3.56×10^{-5}A/cm^{-2} for the annealed thin strip and 1.10×10^{-5}A/cm^{-2} for the quenched thin strip, significantly

lower than that of the annealed thin strip. The lower i corr value for the quenched thin strip confirms that amorphous thin strips have better corrosion resistance than crystalline thin strips. Therefore, using a model to measure the relationship between the corrosion potential (E corr) and corrosion current (i corr) and predicting the corrosion performance of magnesium alloys based on information about corrosion products holds great promise.

3.2.2. Corrosion Products

Magnesium and its alloys exhibit excellent biocompatibility and chemical activity, and they can naturally degrade through corrosion in complex physiological environments. In the field of biomedicine, magnesium-based implants are hailed as highly promising implant materials. The corrosion products of magnesium-based implants mainly consist of four components: the corrosion surface of the implant, hydrogen gas, a significant amount of hydroxide ions and magnesium ions, and other alloying elements. Xin et al. [41] immersed AZ91 magnesium alloy in c-SBF, and the morphology after one day of immersion is shown in Figure 10. The white region contains a large amount of Ca and P, while the gray region also contains P but not Ca. The P concentration in the white region is much higher than in the gray region, and the surface layer thickness in the white region is significantly greater than in the gray region. Figure 11 displays cross-sectional images of the sample in Figure 10a. As discussed above, the formation of such non-uniform surface layers is suspected to result from localized corrosion. However, many other magnesium alloys exposed to simulated physiological environments often exhibit very uniform surface layers [42]. For example, in Hanks' solution, Mg-Zn-Mn alloys undergo uniform corrosion from the top, as shown in Figure 10b,c [43,44]. On calcium-rich magnesium alloy surfaces, a substantial accumulation of insoluble corrosion products can be observed [45]. In a 0.9 wt.% NaCl solution, the primary constituents of the surface layer are magnesium hydroxide and magnesium oxide [46]. Therefore, alloying elements may also be incorporated into the corrosion products.

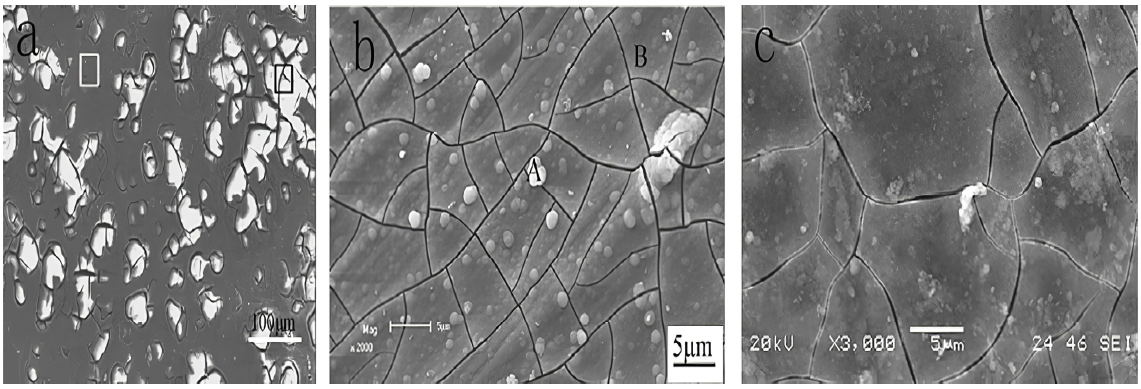

Figure 10. The corrosion morphology of magnesium alloys in simulated physiological environments: (**a**) AZ91 magnesium alloy exposed to c-SBF for 1 day; (**b**) Mg-Mn-Zn alloy exposed to Hanks' solution for 12 days; (**c**) pure magnesium after 30 days of exposed to c-SBF. Adapted with permission from Ref. [41]. Copyright 2011, Elsevier.

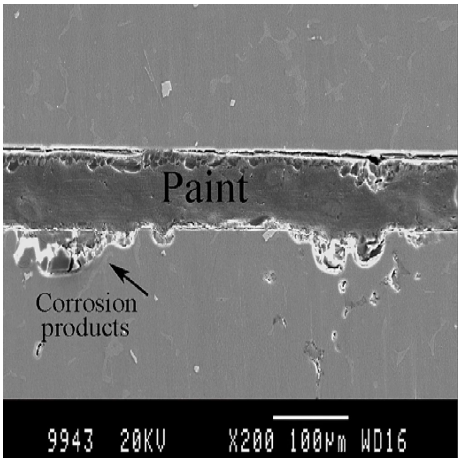

Figure 11. The cross-sectional image of AZ91 magnesium alloy exposed to c-SBF. Adapted with permission from Ref. [41]. Copyright 2011, Elsevier.

However, in some studies, solutions such as DMEM and PBS contain a significant amount of buffers like Tris-HCl, Q, R, which can consume hydroxide ions and control sudden changes in pH. Therefore, dissolved magnesium generally appears on the surface layer and in the solution. Li et al. [47] investigated the cytotoxicity and corrosion of magnesium in body fluids by immersing it in c-SBF, and after a period of time, most of the magnesium precipitated and adhered to the surface layer of pure magnesium. The composition of the corroded surface layer varies with the type of solution. Although some studies have indicated the presence of insoluble carbonate and phosphate crystals in the surface layer, it is difficult to accurately determine the specific components due to the amorphous nature of the substances in the surface layer [48]. Therefore, establishing a machine learning model based on the specific products of corrosion product surface layers would significantly reduce prediction accuracy. However, selecting the macroscopic main components of corrosion products as feature indicators can reduce errors caused by the uncertainty of substances and improve prediction accuracy.

3.3. General Corrosion and Pitting Corrosion

For the general corrosion and pitting corrosion of magnesium alloys, the presence of precipitates and various impurities can lead to the spontaneous formation of galvanic cells between the precipitates and the magnesium matrix, even if the magnesium alloy is not in contact with dissimilar materials, due to differences in electrochemical activity. This phenomenon results in galvanic corrosion [49]. Since the precipitate phases appear in the form of intermetallic compounds, and the electrode potential values of impurity elements distributed within them are higher than that of pure magnesium, the magnesium matrix becomes the anode. As a result, a typical large cathode and small anode structure is formed. Elements like Fe, Ni, Co, and others in the metal have very low hydrogen overpotentials, and they form a highly corrosive galvanic cell with the metal, leading to galvanic corrosion between the metals. Macroscopically, the galvanic corrosion formed between magnesium alloys and the second phase is known as general corrosion.

Magnesium does not undergo intergranular corrosion, as all grains opposite to grain boundaries are cathodic, preventing the occurrence of intergranular attack. Therefore, corrosion occurs at the anodic regions. Furthermore, corrosion is insensitive to differences in oxygen concentration, so crevice corrosion does not occur [50]. However, in non-oxidizing environments, when magnesium encounters chloride ions (Cl^-), its passive film is easily destroyed, leading to pitting corrosion at the self-corrosion potential E corr [51,52]. In the early stages of corrosion, due to local differences in oxygen concentration, the acidity in the corrosion environment increases, and the concentration of positive ions (cations) becomes higher. To maintain the electrical neutrality of the solution, negatively charged

chloride ions (Cl^-) react with positive ions (cations) in the film, forming water-soluble chlorides. This disrupts the film and creates small corrosion pits on the newly exposed metal surface, forming activation sites. During the formation of corrosion pits, the metal surface inside the pits undergoes active dissolution, resulting in a negative potential and behaving as the anode. In contrast, the metal surface outside the pits remains passive with a positive potential. This creates an activated microcell within and outside the corrosion pits. Therefore, by considering certain characteristics that appear during pitting corrosion, using machine learning algorithms to model the self-corrosion potential E corr as a metric, it is possible to predict the properties of magnesium alloys in terms of pitting corrosion with relatively good accuracy.

3.4. Corrosive Media

Magnesium alloys exhibit different corrosion characteristics in various corrosive media [53]. In dry environments, they tend to develop a gray protective film on the surface and are less prone to corrosion. In rural and industrial atmospheres, moderate corrosion occurs. In most diesel engine environments, corrosion is not a concern. The specific corrosion behavior in different corrosive media is as follows (Table 1):

Table 1. Corrosion state of magnesium in different corrosive media.

Medium	Corrosion Condition	Medium	Corrosion Condition
freshwater, seawater, humid atmosphere	corrosion damage	methyl ether, ethyl ether, acetone	non-corrosive
organic acids and their salts	severe corrosion damage	petroleum, gasoline, kerosene	non-corrosive
inorganic acids and their salts	severe corrosion damage	sodium hydroxide solution	non-corrosive
ammonia solution	severe corrosion damage	dry air	non-corrosive
formaldehyde, acetaldehyde	corrosion damage	anhydrous ethanol	non-corrosive

From the information in the table, it can be inferred that testing magnesium alloys directly is impossible because magnesium exhibits similar corrosion behavior in some different media. However, by considering the differences in the corrosion behavior of different alloy elements in various media, selecting the corrosive medium directly as a feature for predicting the corrosion of magnesium alloys, and using machine learning models to analyze the intensity of reactions corresponding to each medium, it is possible to predict the corrosion of magnesium alloys.

4. Challenges and Opportunities in Studying the Corrosion Behavior of Magnesium Alloys Using Machine Learning

4.1. Data Quality

High-quality data are a prerequisite for analyzing and using big data. The use and analysis of big data must be based on accurate and high-quality data, which is a necessary condition for generating value from big data. The biggest challenge in using machine learning to predict the maximum corrosion rate of magnesium alloys is undoubtedly the limited availability of reliable and high-quality data. Therefore, the question of how to obtain a large quantity of high-quality data covering different corrosion environments and exposure times, and how to assess it, is a topic that needs to be discussed repeatedly.

Existing research primarily focuses on two aspects: one is the study of network data quality, and the other is domain-specific research in fields such as biology, medicine, geophysics, telecommunications, and scientific data. With the increasing number of data sources, diverse data types, and complex data structures, the challenge of data integration also grows. In machine learning, raw data are typically not in a suitable form for learning. Variables and features need to be identified and extracted from raw data. Although features

are often domain-specific, there is still a need to establish general patterns to assist in feature identification. Poor data quality is manifested as missing data, duplicate data, highly correlated variables, a large number of variables, and outliers. Poor-quality data can pose serious issues for constructing ML models and big data applications. Zhou [54] et al. cited three different groups to identify corn ears based on fixed criteria and assessed their accuracy and quality metrics in performing the task. The flowchart of the program is shown in Figure 12.

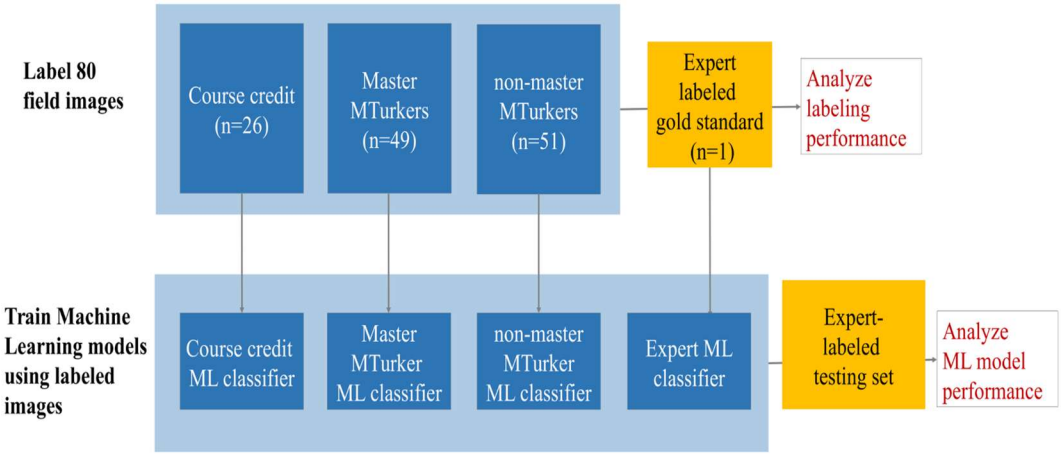

Figure 12. The general workflow diagram [54].

As shown, the first group is the Curriculum Studies subgroup, the second is the Robotics Masters group, and the third is the Non-Compensation Robotics Masters group. All labeled ears of corn are in a set of 80 images. One of the first steps is to evaluate the labeling performance against the gold standard, then analyze the performance of the experimental groups based on the results of the evaluation, match the ML classifiers used for training in each experimental group, and, finally, test each ML classifier against the expert-labeled test set. In this, each training method is tested against a separate expert-labeled training set to assess how differently the ML methods perform on different training sets. In addition, each set is also closely linked to each other, helping to determine the relative impact of large amounts of missing and duplicated data on data quality, thus answering the question of what improvements can be made in relation to data quality, allowing for more accurate measurements and assessments. Therefore, using the process structure described above as a basis for investigating the prediction of magnesium alloy corrosion performance, this will not only improve the prediction of corrosion rates, but will also maximize the benefits of the machine learning algorithm itself.

4.2. Model Transferability

When using machine learning to predict corrosion rates, the model's transferability is a topic that requires in-depth discussion. Machine learning models trained under one set of conditions may perform poorly when applied to different conditions, such as varying corrosion environments or materials. Therefore, it is crucial to assess their generalization ability before applying machine learning models to new conditions.

Sobehy et al. [55] compared the generalization ability of KNN and MLP NN methods. They evaluated the models' interpolation and extrapolation capabilities using two different approaches: test set selection and the sum of squares and sequences. This assessment was carried out because models with strong generalization abilities typically excel in both interpolation and extrapolation tasks. When selecting the test set, samples were chosen from within a square-shaped region. By adjusting the size of the square, they ensured that the test set's size was approximately 10% of the training set, as illustrated in Figure 13.

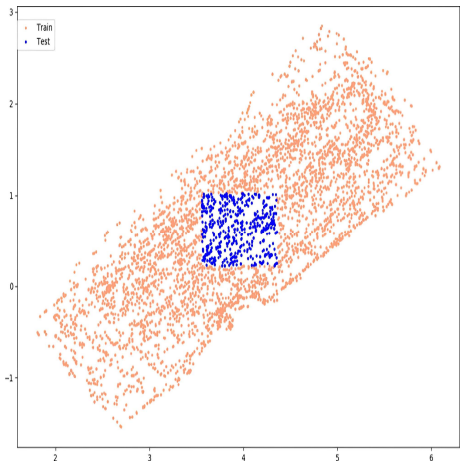

Figure 13. The distribution of the training and test sets. Adapted with permission from Ref. [55]. Copyright 2022, Springer Nature.

As shown in the figure, the square represents a blind spot region where the model must make predictions without any prior information, thus testing its extrapolation capability. Figure 14 displays the error analysis.

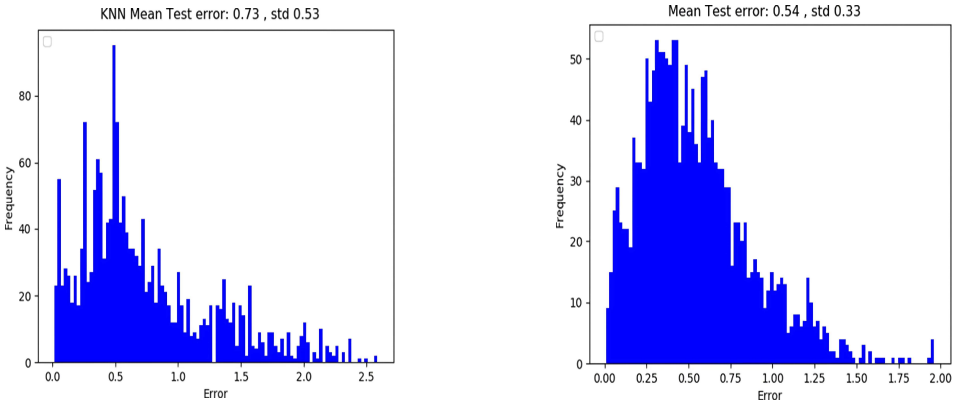

Figure 14. The error distribution of KNN and MLP neural networks on the square test set. Adapted with permission from Ref. [55]. Copyright 2022, Springer Nature.

As shown in Figure 14, the average error for KNN is 0.73 m, with a standard deviation of 0.53 m. This significant error indicates a complete failure of the model, as the error is only 0.023 m when randomly selecting test set samples. Although MLP NN has average error and standard deviation values smaller than KNN, at 0.54 m and 0.33 m, respectively, its error is still much larger than that of randomly selected test samples. Despite the error distribution appearing to be more structured than KNN's, it is challenging to conclude that a model with such substantial errors possesses decent extrapolation capability.

During sequential test set selection, since samples are chosen in a standard order, the likelihood of complete overlap is very low. It is improbable to select the same location twice, Therefore, in this selection method, the test set samples are dispersed along the feature space, with non-overlapping positions. The prediction task appears to be easier compared to square selection. The model needs to be capable of establishing correlations between the test set samples and nearby training samples, and then interpolate to estimate the test sample positions. The error analysis of KNN and MLPNN is shown in Figure 15.

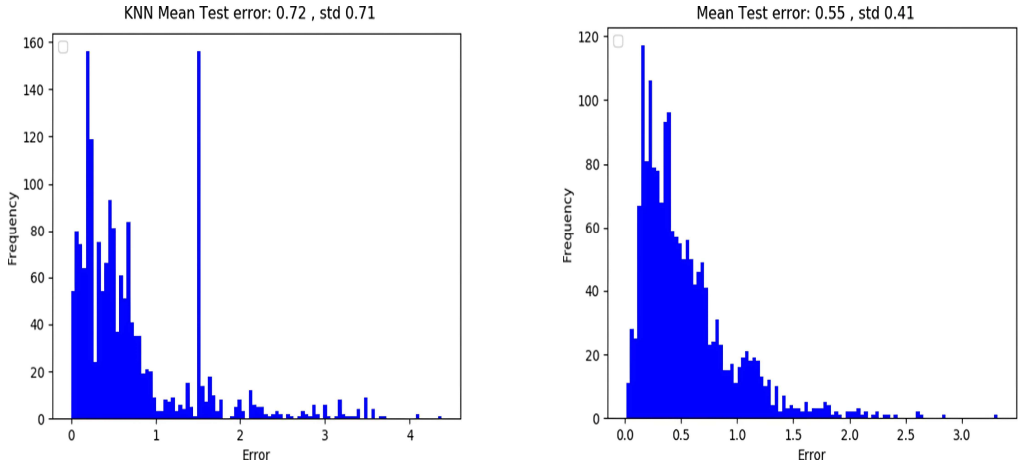

Figure 15. The error distribution of KNN and MLP NN on the sequential test set. Adapted with permission from Ref. [55]. Copyright 2022, Springer Nature.

As shown in Figure 15, the error for the KNN model is as large as that of the square test selection. When repeating the experiment with MLP NN, even the MLP neural network cannot perform well on the sequential test. However, the errors are as high as the experiments with square test selection, making it difficult to conclude that it has better generalization capabilities. The sparsity of measurements, focusing solely on labeled datasets, is a significant obstacle for both learning models.

When using machine learning to predict corrosion rates, experimental data on corrosion rates are often limited in quantity, and it can be challenging to obtain a substantial amount of data covering various corrosion environments and exposure times. Predicting magnesium alloy corrosion rates using the methods described above does not offer significant assistance in terms of model transferability. Therefore, using machine learning to predict magnesium alloy corrosion rates presents a significant challenge in terms of model transferability.

4.3. Feature Selection and Representation

Feature selection and representation are crucial for the performance of machine learning models. However, in corrosion research, choosing appropriate features can be challenging because many factors can influence corrosion rates, such as material composition, environmental conditions, and surface morphology. For magnesium and magnesium alloys, their chemical properties are unstable, and it is difficult to control the rate of change in their chemical reactivity in various corrosion environments. Therefore, selecting suitable features and transforming chemical properties into simple and favorable features for model predictions is a necessary research approach.

Diao et al. [56] proposed two methods for feature generation: transforming chemical property features into atomic property features and physical property features. This approach allows feature creation models to no longer be limited to materials with specific chemical compositions. Therefore, they incorporated atomic and physical property features in addition to the chemical composition and environmental factors for low-alloy steel. As a result, the machine learning corrosion rate prediction model exhibited a high level of accuracy in predicting corrosion rates.

Firstly, in the selection of machine learning algorithms, they compared the performance of various machine learning algorithms, as shown in Figure 16. They divided the original dataset into training and test sets, with the former used for optimization and the latter for accuracy assessment. The training set was split from 40% to 90%, with the remaining portion reserved for the test set.

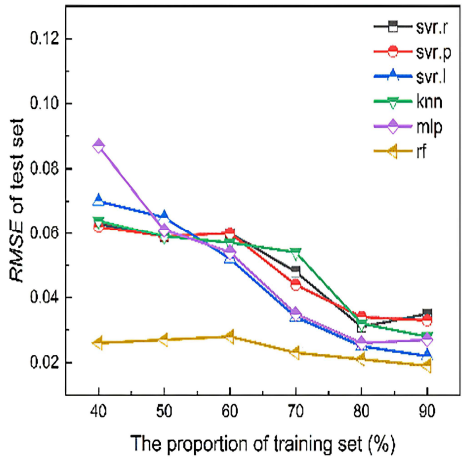

Figure 16. The different proportions of training and test set splits. Adapted with permission from Ref. [56]. Copyright 2021, Elsevier.

As shown in the figure, it can be observed that the random forest model provides the best prediction accuracy on the test set across various training data split ratios. Generally, increasing the dataset size tends to improve algorithm prediction accuracy as the amount of data is positively correlated with the information it contains. However, as seen in the graph, when the training set ratio exceeds 80%, algorithms like svr.r and mlp experience a slight drop in accuracy. This could be due to overfitting with these algorithms, leading to a significant reduction in model generalization capability [57]. Therefore, the random forest algorithm was chosen for use in this study.

Secondly, when investigating the influence of corrosion rate, they discussed the impact of temperature and alloy elements on the accuracy of corrosion rate predictions, and the results are shown in Figure 17.

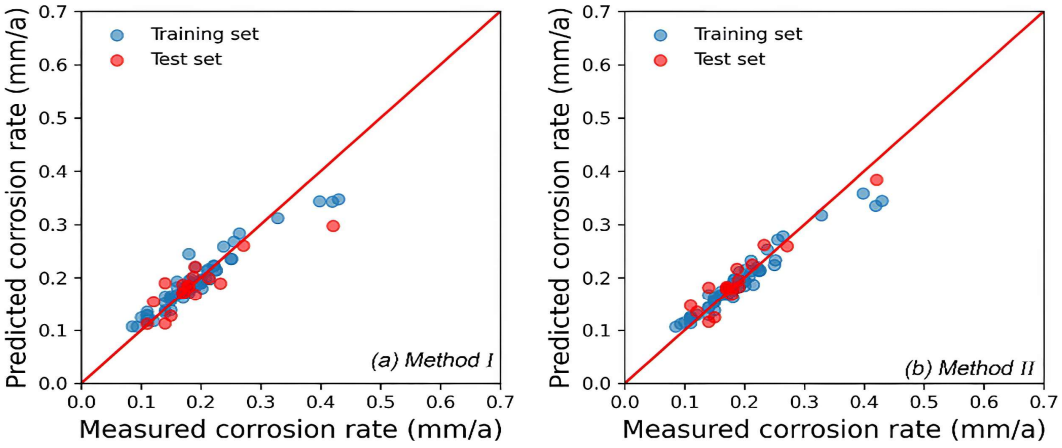

Figure 17. The prediction accuracy of corrosion rate prediction models based on input features derived from feature generation method I and feature generation method II. Adapted with permission from Ref. [56]. Copyright 2021, Elsevier.

As shown in the figure, the accuracy of Method II is very close to the GBDT and Kendall correlation-based methods it studied. If we consider the contributions of both metallic and non-metallic elements to the corresponding atomic and physical parameters individually, Method II appears to better reflect the differences in steel's chemical composition.

Finally, based on the conclusions drawn from the aforementioned research, they collected new experimental corrosion data as a validation set. These samples contained nickel, and the data were used to test the model's generalization capability. Using feature generation method II to convert their chemical composition into predefined atomic and physical

parameters, they predicted the corrosion rates for each sample. As shown in Figure 18, the corrosion rate prediction model still exhibited a high level of prediction accuracy.

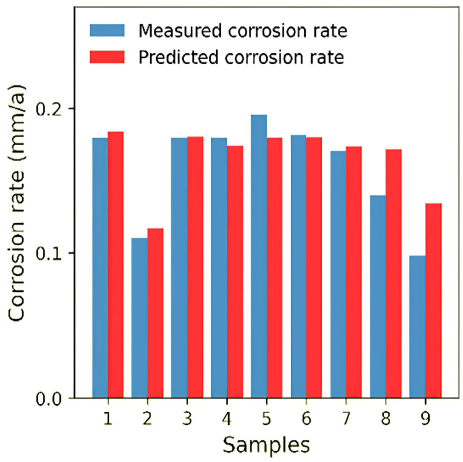

Figure 18. The comparison between the corrosion rates measured through immersion experiments and the corrosion rates predicted by the machine learning model. Adapted with permission from Ref. [56]. Copyright 2021, Elsevier.

Based on these results, applying the feature selection methods described above to the study of machine learning for magnesium alloy corrosion rates would provide a new and effective means of utilizing corrosion data. It could become a valuable tool in corrosion research.

Studying the corrosion behavior of magnesium alloys is indeed a challenging endeavor, as their properties, characteristics, environmental factors, and more present unprecedented issues and challenges. Addressing these problems and challenges requires interdisciplinary collaboration between materials scientists, corrosion engineers, and computer scientists. Developing new experimental techniques to generate high-quality and diverse data, selecting appropriate machine learning algorithms and features, and enhancing the interpretability and transferability of machine learning models are important research directions to advance the application of machine learning in corrosion research. This collaborative approach and ongoing research will contribute to a deeper understanding of corrosion mechanisms, more accurate corrosion rate predictions, and improved corrosion mitigation strategies in the field of materials science and engineering.

5. Machine Learning Potential in Designing and Optimizing Corrosion-Resistant Magnesium Alloys

5.1. Material Design and Optimization Using Machine Learning Methods

The complex evolution of materials relies on data, and with the significant growth in computational methods and experimental data, the rapid development of materials informatics, the establishment of models becomes increasingly crucial [58]. Moreover, there often exists a complex relationship between the inputs and outputs of material properties, making it challenging for conventional linear and non-linear correlation methods to handle them. However, with the continuous advancement of machine learning technology, people have been able to effectively model such complex relationships [59]. Machine learning (ML) is a branch of artificial intelligence (AI) used to construct models trained from past data and contexts [60]. This method does not require a deep understanding of the underlying physical mechanisms but can extract patterns from extensive experimental data and apply them to the development and design of new materials. ML takes a different approach: it does not rely on principles or physical insights but rather trains models with flexibility and often highly non-linear forms solely from available data. In materials science, the structure and properties of materials are often interconnected. Conventional correlation

analysis methods struggle to effectively address this issue. Consequently, ML methods have become an essential tool for predicting material properties and for material selection and optimization design [61]. Figure 19 illustrates the workflow of materials discovery and design based on machine learning.

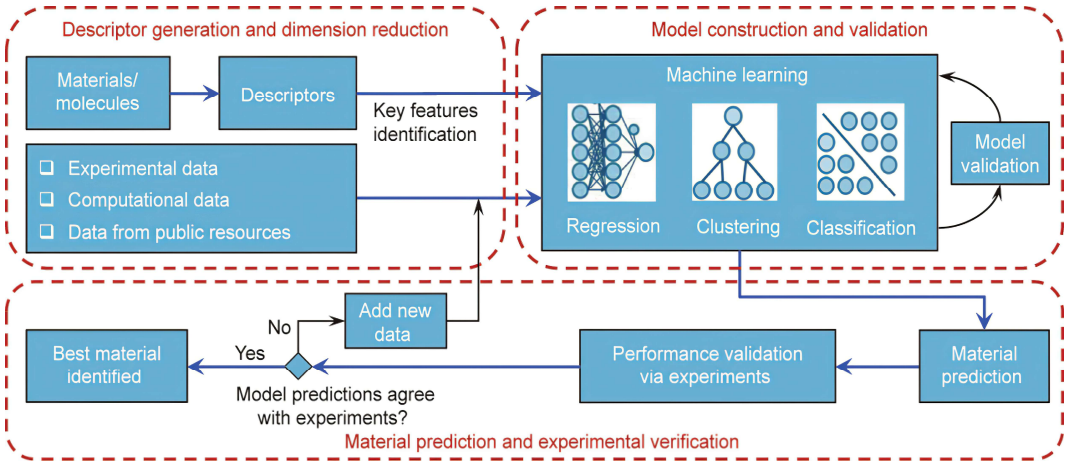

Figure 19. The general workflow of material discovery and design based on machine learning [61].

The process is divided into three main parts, namely: descriptor generation and dimensionality reduction, model construction and validation, and material prediction and experimental verification. The first step involves using descriptors to represent the content within a dataset, or using feature symbols to express it. This step requires a certain level of understanding of the types and applications of materials. The second step is to match descriptors with target characteristics and performance based on existing reference data. During the modeling process, a range of machine learning methods, from simple to complex, can be chosen. The final step involves reverse engineering to discover new materials and build ML models based on the required performance. Subsequently, experimental validation is performed to confirm the real properties or performance of the generated candidates.

Typically, the properties of each material depend on the preceding feature selection. Therefore, identifying critical features closely associated with enhancing the corrosion performance of magnesium alloys is a crucial preliminary step before employing machine learning modeling. For example, parameters such as the self-corrosion potential (E_corr), corrosion current density (i_corr), pH value variations, corrosion products, the impact of different elements on the corrosion of magnesium alloys, and the presence of a medium, among others, can serve as primary features for studying their performance. Using these features in lieu of directly matching magnesium alloys with their corresponding chemical properties can streamline the process and yield more intuitive and comprehensible results.

Characteristics of optimization-based methods often involve selecting materials that are more experimental in nature, rather than those that do not align with spatial design. In the study of magnesium alloy corrosion performance, random algorithms or deterministic algorithms can be employed as means to address the optimization problem of predicting their performance [62,63]. Once feasible operations are determined using this approach, the corrosion performance of magnesium alloys can be predicted. If the conclusions closely align with the predicted values, it can demonstrate the feasibility of optimization. Otherwise, algorithm selection and model development may need to be revisited.

5.2. Multiscale Modeling

The primary objective of multiscale modeling is to model and predict the corrosion process across multiple scales, from the microscopic to the macroscopic, to gain a better understanding of the mechanisms and behavior of magnesium alloy corrosion. Generally, it

is divided into three modeling approaches: microscopic-scale modeling, intermediate-scale modeling and macroscopic-scale modeling. Microscopic-scale modeling focuses on the influence of microscopic factors such as crystal structure, grain boundaries, and defects on the corrosion behavior of magnesium alloys. Intermediate-scale modeling serves as a bridge connecting the microscopic and macroscopic scales and is used to study local defects and the macroscopic behavior of materials. Macroscopic-scale modeling focuses on the corrosion behavior and performance changes in the entire magnesium alloy material.

Lei et al. [64] conducted virtual and homogenization tests on various microstructures in different research scenarios following a multiscale simulation chain, as illustrated in Figure 20.

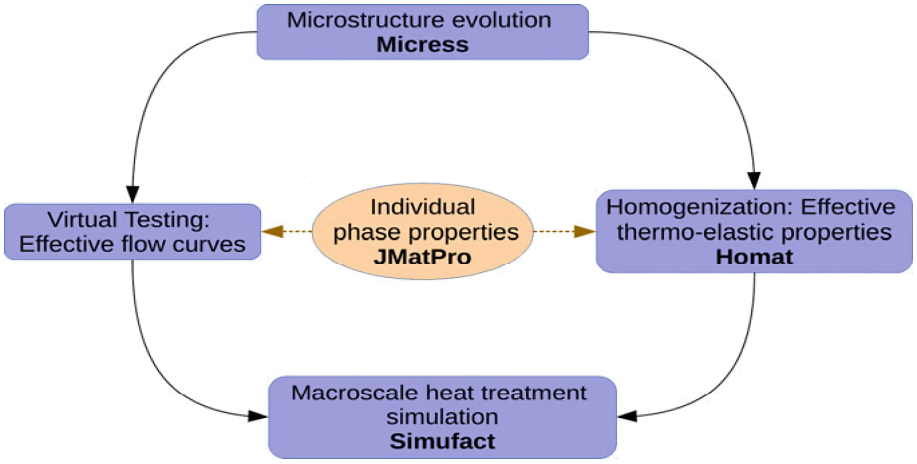

Figure 20. The multiscale simulation workflow. Adapted with permission from Ref. [64]. Copyright 2023, AIP Publishing.

As shown in the figure, they feed the calculated effective macroscopic performance into the macroscopic heat treatment simulation in Simufact. They initiate phase-field simulations using tracking point data from Simufact to obtain the microstructure evolution at tracking points during the macroscopic heat treatment process. Through this method, they calculate the evolution of microstructures across geometric shapes at different points and obtain corresponding effective macroscopic material properties. Subsequently, the obtained effective properties are transferred to macroscopic-scale heat treatment simulations, thus completing the multiscale simulation workflow.

Combining this approach with machine learning methods and selecting appropriate machine learning techniques for multiscale modeling based on the different characteristics of different samples is an indispensable and unique method in today's machine learning-based research for comprehensive analysis and prediction of research objectives at both microscopic and macroscopic levels.

5.3. Hybrid Modeling

Nguyen Lei et al. [65] employed a hybrid modeling approach in their study of landslide susceptibility mapping, as depicted in Figure 21.

As shown in the figure, the first step involved generating training and testing sets using data from the study area, comprising 70% and 30%, respectively. Next, a hybrid model was used to build predictions related to landslides. This was achieved by combining the RF ensemble and BDFT classifier to create RFBDFT. Additionally, particle swarm optimization algorithm was combined with the ANFIS classifier to create PSOANFIS, and with the ANN classifier to create PSOANN. Then, several criteria were set to conduct hybrid validation. The training set was used to assess the model's goodness of fit, and the testing set was used to validate the model's predictive capabilities. Finally, each landslide image within the study area was generated using the hybrid model. The use of hybrid

modeling allowed for a more comprehensive analysis of various study areas, resulting in more substantial outcomes.

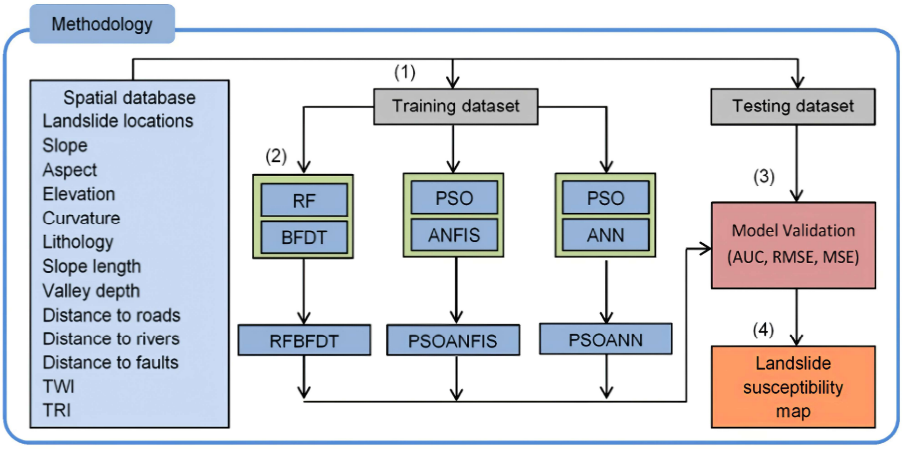

Figure 21. The method flowchart [65].

In the study of magnesium alloy corrosion, hybrid modeling methods can combine physical models with machine learning to fully leverage the strengths of both approaches. For example, this involves organically integrating the physical laws of a physical model with the data-driven capabilities of machine learning. This includes using the physical model to guide the training and predictions of machine learning models, as well as utilizing machine learning models to calibrate and optimize the parameters of the physical model. This approach enhances researchers' confidence in model predictions and provides more reliable decision-making support for engineering applications. However, hybrid modeling methods require the integration of various types of data, including experimental data, simulation data, and field monitoring data, among others. Attempting to perform hybrid modeling with a single type of data can significantly limit the model's capabilities. Therefore, it is advisable to test the model's effectiveness with different combinations of conditional factors to further enhance the potential for improvements in hybrid models.

6. Conclusions and Summary

Machine learning is a highly influential technology, and its strong appeal is gradually driving its application to more complex tasks and environments, especially in applications that could have a significant impact on research objectives. This article has provided an overview and outlook on the use of machine learning for predicting magnesium alloy corrosion properties. It discussed various machine learning algorithms for predicting magnesium alloy corrosion properties, such as artificial neural network algorithms, random forest algorithms, and support vector machines. Different criteria, such as corrosion current density i corr, mass fraction of alloying elements at the same magnesium content, RF corrosion potential, and RF corrosion current, were selected for predicting the corrosion properties of magnesium alloys. This aids readers in gaining a clear understanding of research in this domain. In current research, the incorporation of machine learning methods has made it possible to monitor various challenging corrosion behaviors to a significant extent. This not only reduces costs in materials but also minimizes the substantial time investment. With the advent of the Fourth Paradigm era, dealing with complex and voluminous data has become an inevitable challenge. However, with the vigorous growth of machine learning, it will play a crucial role in the field of alloy research. From the perspective of magnesium alloy research, the development of machine learning is boundless. However, various opportunities and challenges exist within it: challenges related to data quality, model interpretability, model transferability, feature selection, and representation continually demand that machine learning enhance its rapid responsiveness and processing capabilities to address increasingly complex domain problems that may arise in the future.

In conclusion, using machine learning methods for predicting the corrosion properties of magnesium alloys is a highly significant research topic. The subsequent research and practice can learn from the techniques and methods mentioned in the literature, in order to find the most suitable measures with the largest room for progress, and it is bound to become an integral component of numerous research domains in the future.

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Conflicts of Interest: The authors declare no conflict of interest.

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