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Enhancing Tribological Performance of Aluminum Matrix Composites through Graphene Reinforcement: Insights from Machine Learning Regression Analysis

Swathi Harohalli Ramachari[1], K. Vimala Devi[2], Sathiya Priya Selvaraj[3], Vinay Hiralal Singh[4], Sumanth Ratna Kandavalli[5], Revathi Rallabandi[6] and Mayakannan Selvaraju[7*]

[1]*Department of Mathematics, Nitte Meenakshi Institute of Technology, Bengaluru, India*
[2]*School of Computer Science and Engineering, Vellore Institute of Technology, Vellore, India*
[3]*Department of Computer Science and Engineering, Vel Tech Rangarajan Dr. Sagunthala R and D Institute of Science and Technology, Tamil Nadu, India*
[4]*Department of Chemistry, Konkan Gyanpeeth Karjat College of ASC, Karjat Raigad Maharashtra, India*
[5]*Department of Mechanical Engineering, Tandon School of Engineering, New York University, Brooklyn, New York, USA*
[6]*Department of Electronics and Communication Engineering, Koneru Lakshmaiah Education Foundation, Guntur, India*
[7]*Department of Mechanical Engineering, Vidyaa Vikas College of Engineering and Technology, Tiruchengode, Namakkal, Tamil Nadu, India*

***Correspondence to:**
Mayakannan Selvaraju
Department of Mechanical Engineering,
Vidyaa Vikas College of Engineering and Technology,
Tiruchengode, Namakkal, Tamil Nadu, India.
E-mail: kannanarchieves@gmail.com

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Abstract

This research delves into the influence of graphene on friction and wear resistance in self-lubricating metal matrix composites (MMCs) based on aluminum. Experimental results from laboratory testing clearly demonstrate that the incorporation of graphene leads to a substantial improvement in the composites' resistance to both coefficient of friction (COF) and wear rate (WR). The study specifically investigates the friction and wear characteristics of aluminum matrix composites reinforced with graphene. To predict abrasion and friction rates accurately, the research utilizes five different machine learning (ML) regression models, shedding light on the potential of these materials for practical applications where enhanced wear resistance is essential. The findings from this research hold promising implications for industries and manufacturing processes, as graphene's incorporation into these MMCs offers the potential for improved the COF and WR performance. ML showed that the wear and friction behaviors of aluminum-graphene/graphite (Al-Gr) composites were significantly influenced by the percentage of graphene in the composite, the specific loading conditions, and the material hardness. Graphene has been highlighted as a promising component for improving the tribological characteristics of MMCs, which might lead to major advances in addressing wear and friction difficulties. Improved engineering materials may be created thanks to the insights gained from the ML models, which shed light on the complicated relationship between material composition and tribological performance.

Keywords

Machine learning, Self-lubrication, Aluminum, Graphene, Friction, Wear

Introduction

For many technical uses, MMCs are favored over standard alloys due to their superior material qualities. When it comes to tribological applications and sectors where saving weight is crucial, like the aerospace and automotive industries, aluminum MMCs are chosen over monolithic aluminum alloys [1]. However, these composites suffer from issues including increased brittleness and poor machinability due to the poorly dispersed ceramic particles in the aluminum matrix. Al-Gr composites have garnered a lot of attention as a low-cost, effective choice for minimizing seizing tendency, friction, and wear [2].

These MMCs are often processed via casting, spray deposition, or powder metallurgy. The hexagonal graphite structure has carbon atoms arranged in an unusual, layered pattern, which gives graphite its inherent lubricity [3]. Due to the presence of graphite particles, Al-Gr MMCs have superior tribological performance in sliding applications. Large graphite particles found in self-lubricating Al-Gr MMCs may alter their mechanical properties. Recent research on graphene-reinforced aluminum-matrix composites (MMCs) has shown that excellent tribological and mechanical characteristics may be attained simultaneously [4, 5].

Graphene is made of tightly packed sheets of a single atom of carbon and has a honeycomb shape in two dimensions. Graphene stands apart from other materials due to its exceptional friction and wear qualities. Graphene's ultrathin, atomically smooth surfaces make it useful for applications at the nanoscale and microscale. Graphene's strong mechanical strength is a contributing factor to its durability.

Using atomic force microscopy (AFM) nanoindentation, researchers demonstrated the extraordinary strength of graphene in monolayer graphene membranes. In addition to its remarkable Young's modulus (E) of 1 TPa, the tensile strength of defect-free monolayer graphene was measured at 130 GPa. Graphene's bilayer and Tri layer Young's moduli and tensile strengths were independently calculated to be 1.04 TPa and 0.98 TPa [6-9].

In matrix-reinforced composites, particularly in the case of matrix-matrix composites (MMCs), a unique synergy arises by combining the toughness and ductility of the matrix with the strength and modulus of the reinforcing material. Graphene, with its plate-like structure, demonstrates superior dispersibility compared to other carbon-based fillers such as graphite and CNT [10]. This characteristic makes graphene an appealing choice as a reinforcing agent in self-lubricating MMCs. Its cost-effectiveness, inherent shear capabilities, and remarkable mechanical properties further enhance its suitability for this application.

Several recent scientific studies detail the fabrication processes and associated mechanical features of graphene reinforced aluminum multi-material composites (GMCs). Adding graphene to an MMC's metal matrix increases the material's mechanical strength. The strengths may be negatively impacted if the particles are dispersed in an agglomerated manner. The tensile properties of an Al-Gr MMCs was found to be enhanced by 62% when compared to the tensile properties of the pure aluminum base alloy when graphene nano-sheets were used as the reinforcing phase.

Researchers shown that a significant barrier to progress in tribological research is the lack of mathematical derivations from basic principles [11]. The development of data-driven AI and ML techniques has allowed us to go beyond the 2-parameter level in our exploration of higher-order correlations. To find patterns in datasets and make accurate predictions, complex ML models like ANN and gradient boosting machines (GBMs) use a wide range of methods. Data-driven "Triboinformatics" may be used to examine tribological test parameters and mechanical/material aspects in the field of tribology. Al-Gr MMCs and aluminum alloys can considerably benefit from this technology for predicting wear and friction (MMCs) [12].

The tribological performance of Al-Gr MMCs under various lubrication conditions were studied by the authors [13, 14] using separate and combined models. This type of data analysis has great potential for elucidating the principles driving friction and wear in graphene-infused multi-material composites. It's a chance to learn more about the complex interactions at play in the tribological performance of these high-tech materials.

Researchers are investigating the effects of wear and friction on multi-material composites made of Al-Gr. Experimental data were used to train ML models for friction and wear predictions and trend identification in the tribological features of these materials.

Materials and Methods

This section provides a comprehensive discussion of the creation and improvement of ML models for forecasting friction and wear performance. Collecting data, processing it, creating models, and optimizing their parameters across several ML models are all covered here.

Data collection and its parameters

The precision of a model's predictions is directly proportional to the quality of the data used to train it. It is more probable that ML models will be generalizable and robust if they are trained on a large dataset that includes a variety of input-output interactions. Tribological testing requires extensive time and resources to prepare for, as it requires many testing sets and samples of diverse material quality. As can be seen in figure 1, the information was drawn on the tribological performance of Al-Gr composites taken from the published literature [15, 16].

As the sliding velocity changes, so does the intensity of the wear mechanism. Due to the completely functional graphene lubricating sheets, Al-Gr MMCs exhibit moderate wear at low sliding speeds.

In this ML study, COF and WR prediction models were built using datasets containing 442 and 380 sample data points, respectively. 15 tribological and material parameters were tested to create accurate regression models. Several variables were considered, such as the mechanical and physical characteristics of graphene, aluminum, silicon carbide,

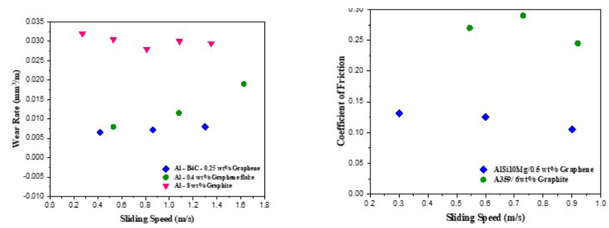

Figure 1: Impact of sliding speed on **(a)** WR **(b)** COF.

graphene itself, graphene manufacturing methods, graphene heat treatment, graphene density, and graphene ductility. The tribological study considered the sliding distance, normal load, velocity, counter face, and testing technique. Quantitative variables included everything but the kind of graphene, production technique, heat treatment, counter face, and tribo-testing protocol [17, 18].

Standardization and preparation of data

Before ML models can be constructed, the data must be cleaned, missing and anomalous values dealt with, shuffled, normalized, and separated into training and test sets. To perform the data preparation operations, python, and its libraries in combination with manual methods were relied on. Datasets with missing or unusual values were manually corrected. The data were shuffled to eliminate any potential for bias in the ML models.

The created models' responsiveness is enhanced when the inputs are brought within the same numerical range. This was accomplished with the help of Robust Scaler, a program that standardizes data and scales its characteristics to accommodate for outliers [19]. The dataset must be divided into a training set and an evaluation set before ML regression models can be created.

ML models

Predictions may be produced using a supervised ML regression model and a set of input variables. For this purpose, it is crucial to train the models using actual input-output data. Al-Gr MMCs WR and friction were predicted using 15 material and tribological input characteristics and 5 ML regression models. Among the models used were an ANN, GBM, RF, SVM, and a K-Nearest Neighbor algorithm (KNN). Python and the scikit-learn package have been our go-to for ML modelling and analysis. Our prior works [20] provide extensive coverage of the ML models.

The output of non-parametric KNN regression models is predicted by using a threshold of the training data nearest neighbors. In KNN, a new datapoint is predicted based on its nearest neighbors (datapoints) in the training set, as the name suggests. Common locations where the KNN regression model may be adjusted are the number of neighbours examined (neighbours). Underfitting can make the KNN model less sensitive to incoming datapoints, whereas overfitting happens when the number of neighbours is too small.

SVM regression techniques allow for predictions to be produced by projecting data on higher-dimensional hyperplanes. Data with complicated nonlinear connections can be used with SVM. Some examples of kernel functions that may be used to organize hyperplane data are the linear kernel, the polynomial kernel, the radial basis function (RBF), the sigmoid kernel, etc. According to the literature [21], the RBF function is superior for processing tribological data. Optimal operation of the SVM model depends on settings for both the kernel coefficient gamma and the regularization parameter C. SVM models function well even when there are few observations but many input variables.

Nonlinear interactions may be taken into consideration in prediction using contemporary models based on artificial neural networks (ANN). This model's approach to learning is commonly compared to that of the human brain. Several subfields of material science and tribology have found success using ANN models [22]. To accomplish the complicated task of linking the ANN model's input and output layers, many hidden layers of neurons or intermodal units are employed. A hierarchical, inter-unit network processes raw data to produce useful insights. When creating our ANN models, we considered the feed-forward processing strategy of the multilayer perceptron (MLP).

The ANN architecture used in this study is illustrated in figure 2 and consists of a feed-forward MLP regressor. The study employed a three-stage ANN regression model, where each of the 10 layers incorporated multimodal units, also known as neurons, to process information. To improve the accuracy of the ANN models for predicting the COF and WR, activation functions such as tanh and relu were employed. Adjusting parameters like the activation function type, the number of neurons in each hidden layer, and the regularization parameter (alpha) all play crucial roles in optimizing the efficiency and performance of the ANN model.

Both the GBM and RF models construct their prediction models with the use of ensemble techniques that are based on decision trees. Effectiveness of decision tree-based regression models in dealing with tribological data has been documented [23, 24]. These models' decision trees are created in radically different ways. When creating decision trees, RF will always use a random subset of the available data, whereas GBM will choose data progressively. This is why RF and GBM employ bagging and boosting. When the bagging approach is used on RF data, overfitting is decreased, efficiency is improved, and model resilience is boosted. The accuracy of a model may be improved by expanding its decision trees to include additional features and levels of branching. By optimizing loss functions (which are arbitrarily differentiable), the boosting method fixes the errors introduced by the previous tree. As a result, GBM is an effective strategy for investigating multifaceted causal networks.

ML optimization

The developed ML models are fine-tuned for best possible prediction accuracy. Optimizable model parameters

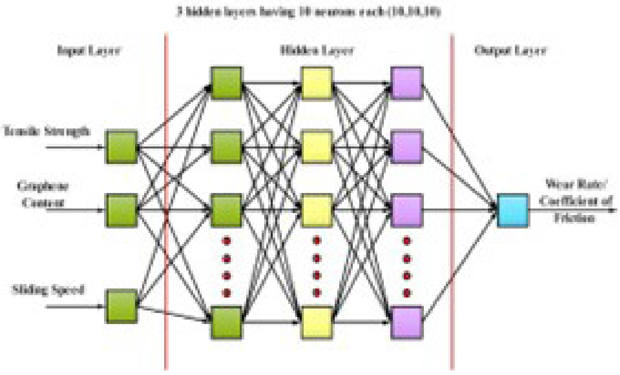

Figure 2: ANN design using a MLP.

were introduced in the previous paragraph. The best parameter settings for the prediction models were determined using a grid search and cross-validation. The optimization strategies were used to test several iterations of our prediction models, each with a unique set of values for the parameters. The optimized parameters for predicting wear rates and COFs are provided in table 1. The number of neurons and the depth of the hidden layers both contribute to the complexity of an ANN model. An ANN model's activation function calculates the output by giving weights to each of the inputs. The best predictions were made by a three-layer, ten-neuron ANN model for COF using alpha = 0.012 regularization and tanh as the activation function (Table 1).

Similar efforts were made to optimize the parameters of other models to improve their forecasting abilities with respect to COF and WR.

Results and Discussion

Standard performance assessment criteria have been used to evaluate the effectiveness of the created findings, and the results of the ML analysis have been reported. We have also discussed the findings of the data-driven investigation, which reveals the sensitive dependence of wear and friction on the input parameters for Al-Gr MMCs.

Prediction of COF results

The R^2, MAE, MSE, and RMSE are common statistical performance measures used to assess the efficacy of a ML regression model. R^2 values between 0.7 and 0.9 suggest a satisfactory regression model, whereas R^2 values more than 0.9 indicate a highly successful prediction model. All five models for predicting COF did quite well, with R^2 values between 0.8693 and 0.9646 and relatively tiny error values (Table 2). The best prediction results, however, were achieved by the RF (R^2 = 0.9638) and GBM (R^2 = 0.9646) models, both of which are based on a decision tree (RMSE, MAE and MSE = 0.0375, 0.0256, and 0.0015, respectively). The best parameter settings for the prediction models were determined using a grid search and cross-validation.

The optimal number of boosting steps (n estimators) for predicting COF with the GBM model was 150, and the maximum depth for each regression unit was set at 2. The COF data was used to evaluate the efficacy of a maximum learning rate of 0.8 and other tweaked parameters. Figure 3 shows how well the best-performing GBM model predicts the COF vs the COF observed in experiments. There was a strong relationship between the predicted and observed COF values.

The RF model's optimal split R^2 value of 0.9638 was discovered for a collection of 80 decision trees in which 4 characteristics were considered (max features). When compared to other models, those based on GBM and RF decision trees fared the best. The KNN model, which depended on distances between instances, was the simplest to build but also the least successful of the models developed. When creating a forecast for a new datapoint, the KNN model performed best when

Table 1: COF Optimizing models.

Model name	Selected factors	COF	WR
K-Nearest neighbors (KNN)	Weights, n_neighbors	Uniform, 5	Uniform, 3
GBM	n_estimator, learning rate, max_depth	160, 0.8, 3	160, 0.8, 0.01
RF	Max_features, n_estimators	4, 80	6, 30
ANN	Activation function, hidden layers, alpha	Tanh, (10,10,10), 0.012	Relu, (10,10,10), 0.04
SVM	Gamma, C, kernel	0.08,100, rbf	0.3,100, rbf

Table 2: Measures of COF prediction model performance.

ML model	MSE	MAE	RMSE	R2 value
KNN	0.0052	0.0409	0.0683	0.8693
GBM	0.0013	0.0221	0.0359	0.9646
RF	0.0015	0.0256	0.0375	0.9638
ANN	0.0039	0.0398	0.0614	0.8946
SVM	0.0035	0.0342	0.0584	0.9047

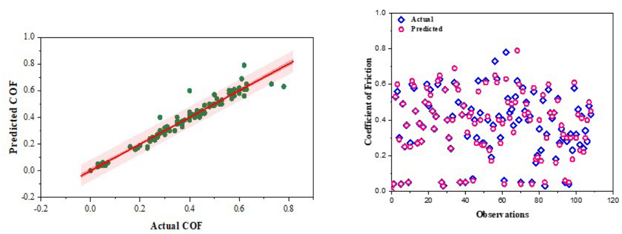

Figure 3: Evaluation of the experimental COF and the predicted COF by gradient boosting machine (GBM) model.

it gave equal weight to each of the five nearby datapoints. Comparing the model's performance on the challenging COF dataset to that of other ML models, it still fares poorly. The ANN model accurately predicted the COF 89.36% of the time (R^2 = 0.8946). Given how small the error terms are, the ANN model does a decent job at making predictions.

Impact of input factors in COF prediction

To predict the COF for Al-Gr MMCs, the RF model's feature significance is attributed to rank the importance of each input variable (Figure 4). In a feature significance analysis chart like this, the sum of the individual variable scores is 1. The relevance of each factor in determining the result is represented by a score between zero and one. The COF shifts if and only if the input scores are not all zero (Figure 4). COF was shown to be most reliably predicted by graphene content, hardness, and load.

Lubricating layer generation and maintenance need both asperity contact between the sliding surfaces and normal load. The graphene weight percentage is also crucial for promoting the self-lubrication effect and lowering friction. The material's hardness was also a crucial consideration in creating COF. Furthermore, it was shown that the COF predictions do not change with the graphene type in Al-Gr MMCs.

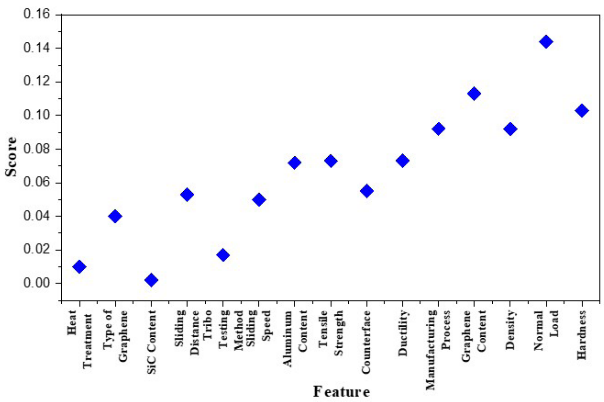

Figure 4: Significance of input factors for forecasting the COF.

WR prediction

Several ML models were used to forecast the WR of Al-Gr MMCs, and the results are shown in table 3. The R^2 values between 0.8899 and 0.9471 were obtained by the top-performing models. These methods comprised RF, GBM, ANN, and SVM. KNN's model, which was based on a distance function, exaggerated WR since it was unable to consider the complicated relationships included in wear data. Outstanding performance (R^2, RMSE, MAE and MSE = 0.9335, 0.0261, 0.0094, and 0.0008, respectively) was achieved by ANN on this difficult dataset of WR. The GBM model built atop the decision tree scored the best in terms of overall prediction accuracy (R^2, RMSE, MAE and MSE = 0.9471, 0.0232, 0.0098, and 0.0006, respectively). When calculating the WR, the model reached a best-case accuracy of 94.67 percent. Despite the existence of categorical variables in the WR data, the GBM regression model's boosting approach yielded trustworthy results.

Figure 5 displays a contrast between the observed (experimentally measured) WR and its projected GBM regression model equivalent. WR measured in experiments were found to correlate very well with those expected.

The wear may be accurately anticipated by the RF model, which is also based on a decision tree. Indicators of effective model implementation include a high R-squared value and small error term values. The ANN model accurately predicted wear far more often than the gold standard (as measured by Mean Absolute Error, Root Mean Squared Error, and Mean Absolute Deviation, respectively). The ANN model was able to effectively analyse the complex WR data by using a small regularization term (alpha = 0.04), three hidden layers of ten neurons, and the "relu" activation function. When applied to complicated wear data, alternatives once again outperformed the KNN model based on distance.

Effect of the input factors on prediction on WR

Predictions of WR for Al-Gr MMCs may be made with high precision using the RF model's feature importance characteristic (Figure 6). If an input variable's score is more than zero, it has a discernible impact on the WR. Wear may be predicted using a material's graphene content, hardness, and normal load, as determined by a feature significance analysis. Researchers have determined that graphene plays a pivotal role in enhancing the mechanical properties and self-lubricating effect of Al-Gr MMCs. Notably, the concept of hardness acting as a barrier against wear during tribological interactions has allowed engineers to make more accurate wear predictions. Unlike in bulk materials, where surface hardness is more effective at resisting material removal than the bulk material's strength, it was observed that hardness has a greater impact on friction and wear compared to tensile strength. The tribosurface, asperity contact, graphene layer formation and maintenance, and the onset of moderate to severe wear were all influenced by the applied normal stress. Graphene type was shown to be more influential than COF in determining WR in Al-Gr multi-material composites. The bonding between aluminum and graphene, as well as other surface and mechanical characteristics, might change depending on the kind and number of graphene layers used. It's worth noting that the WR of Al-Gr MMCs can be affected by graphene's structure, which makes it susceptible to microcracking and shattering during tribological interactions.

Table 3: Evaluation criteria for models predicting the WR.

ML model	MAE	MSE	RMSE	R^2 value
GBM	0.0098	0.0006	0.0232	0.9471
KNN	0.0138	0.0027	0.0520	0.7352
RF	0.0087	0.0009	0.0314	0.9041
ANN	0.0094	0.0008	0.0261	0.9335
SVM	0.0123	0.0012	0.0342	0.8899

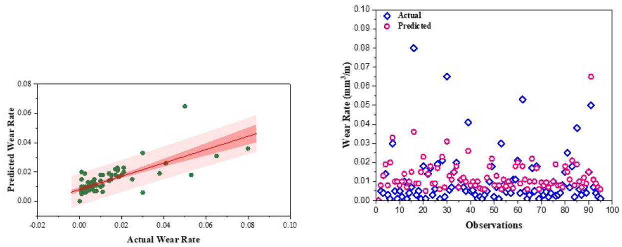

Figure 5: Evaluation of the experimented and the predicted WR by gradient boosting machine model.

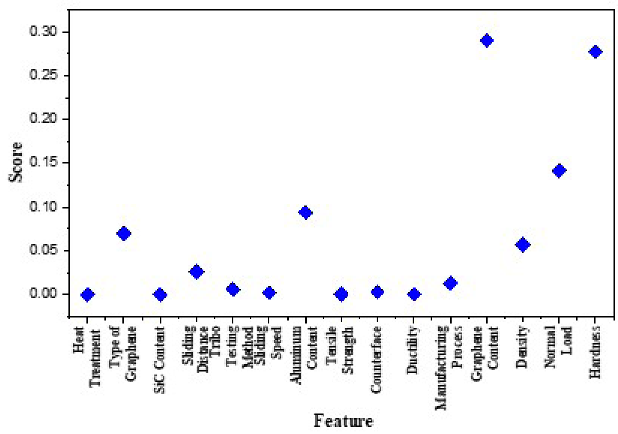

Figure 6: Significance of input factors for prediction of the WR.

Evaluation of performance of prediction

The purpose of this study was to evaluate and contrast the ML models used to estimate COF and WR in dry circumstances for aluminum alloys, Al-Gr composites, and Al-Gr composites [25]. Both the GBM and the RF, which are decision tree-based ML models, performed well when asked to predict future friction and WR using just categorical input data. Models trained on composites of Al-Gr outperform those trained on aluminum base alloys statistically. It was shown that for these two composites, changes in graphene and graphite concentrations had a greater impact on predicted friction and wear. Because of this, our models were able to make accurate predictions. Wear and the COF were found to be particularly sensitive to material hardness and other tribological factors when working with aluminum base alloys. The dataset highlighted the complex interaction between input and result components, as well as the role of chance. However, the ML models performed worse than their graphene and aluminum composite counterparts.

The COF and WR of Al-Gr MMCs may be predicted by our developed ML models with an accuracy of up to 96%. For many combinations of loading conditions and material qualities, it is possible to make educated guesses about the COF and wear with little to no requirement for experimental verification. These models may be used to analyse data from over 20 separate experiments to determine which variables have the most impact on COF and WR in Al-Gr MMCs. With this knowledge, Al-Gr MMC production might be optimized, leading to wider use.

Conclusion

Al-Gr MMCs were studied to learn more about their combined characteristics. Phenomenological studies were also conducted on the COF and WR behavior of these MMCs in dry conditions and with sliding contacts. Tribological applications of these MMCs are likely to be the focus of future research, with an emphasis on optimizing production process factors and tribological test conditions.

Graphene's inclusion in Al-Gr MMCs led to significant increases in both their hardness and tensile properties.

Al-Gr MMCs showed a dramatic decrease in COF and WR as graphene concentration increased. This was attributed to a graphene-rich layer on the tribosurface.

Under the same tribological circumstances, a linear comparative analysis showed that the COF could be lowered by the same amount of graphene was used as the reinforcement phase in the aluminum matrix. The WR of these MMCs were consistent with this pattern.

Al-Gr multi-material composites (MMCs) wear and friction models performed exceptionally well. However, the decision tree-based R 2, RMSE, MAE and MSE based RF (0.9638, 0.0375, 0.0256, and 0.0015) and GBM (0.9646, 0.0358, 0.0219, and 0.0012) COF prediction models showed higher performance, while the GBM (0.9471, 0.0232, 0.0098, and 0.0006) and ANN (0.9335, 0.0261, 0.0094, and 0.0008) models provided the optimum prediction for wear.

Load, graphene content, and hardness were found to be the most significant factors in predicting COF by the ML analysis. It was found that the graphene content, normal load, and hardness of Al-Gr MMCs had the most influence on their wear behaviour.

Acknowledgements

None.

Conflict of Interest

None.

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