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Data-driven machine learning regression methods to predict the residual strength in FRP composites subjected to fatigue

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Abstract

Fiber-reinforced polymers (FRPs) are widely recognized as ideal materials for transport structures due to their customizable properties, high strength, and stiffness combined with low density. These materials exhibit significant resistance to atmospheric conditions but are susceptible to fatigue loading. Unlike conventional metals, which possess an endurance limit, FRPs are prone to failure under any external load when subjected to a substantial number of fatigue cycles. This makes the estimation of residual strength a critical aspect of composite engineering. This study evaluates the efficacy of various machine learning (ML) regression models, integrated with materials informatics, in predicting the post-fatigue residual strength of carbon- and glass-based FRPs (CFRPs and GFRPs). A total of 10 features that closely affects the fatigue behavior in FRPs were used to train the ML models; five from materials and manufacturing aspects, four from testing parameters, and one representing composite properties. The study tested regression models from linear, non-linear, decision tree, ensemble, support vector, and artificial neural network (ANN) approaches to identify the best fit for the dataset. R-squared (R^2), Mean Absolute Error (MAE), Median Absolute Error (MedAE) and Root Mean Square Error (RMSE) were used as evaluation metrics to assess model performance. The findings indicate that the available numerical data is sufficient to initiate training and develop robust ML models for residual strength prediction, though the scope for improvement remains with the expansion of the

Abbreviations: ADAB, Adaptive Boosting; Adadelta, Adaptive Delta; Adagrad, Adaptive Gradient Algorithm; ANN, Artificial Neural Network; BPNN, Back propagation neural network; BR/R, Bayesian ridge regressor; CFRP, Carbon fibre reinforced polymer; CG, Conjugate gradient; CV, Cross-validation; DAN, Deep autoencoder networks; DNN, Deep neural network; DT, Decision tree; ELM, Extreme learning machine; EN/R, ElasticNet/regressor; *f*, frequency; FRCs, Fibre reinforced concrete; FRPs, Fibre reinforced polymer/plastics; GBR, Gradient boost regressor; GFRP, Glass fibre reinforced polymer; GRNN, Generalized regression neural network; GWO, Grey wolf optimizer; IFSS, Interfacial shear strength; KNN, K-nearest neighbour; L-BFGS, Limited-memory Broyden–Fletcher–Goldfarb–Shanno; LR, Linear regressor; LSQR, Least square QR; MAE, Mean absolute error; MARS, Multivariate adaptive regression spline; MedAE, Median absolute error; ML, Machine learning; MLP, Multilayer perceptron; N/N_f, Normalized fatigue life, ratio of actual fatigue cycles and cycles at failure; N_f, Number of cycles to failure; NSGA, Non-dominated Sorting Genetic Algorithm; PCA, Principal Component Analysis; Poly, Polynomial function; QDA, Quadratic Discriminant Analysis; QSI, Quasi-static indentation; R, Stress ratio; R^2, Coefficient of determination; RBF, Radial basis function; RELU, Rectified Linear Unit; RF/R, Random forest/regressor; RMSprop, Root Mean Square Propagation; RR, Ridge regression; SAG, Stochastic average gradient; SAGA, Stochastic Average Gradient Augmented; SELU, Scaled Exponential Linear Unit; SQRT, Square root; SVD, Single value decomposition; SVM, Support vector machine; SVR, Support vector regressor; XGBoost, Extreme gradient boosting; ρ_{ampl}, Stress amplitude.

dataset. Among the tested models, the Multi-Layer Perceptron (MLP), an ANN-based regressor with two hidden layers comprising 30 and 20 neurons, achieved the best performance, with R^2 values of 0.88 on the validation set and 0.95 on the test set and the best RMSE of 72.42. Additionally, the decision tree (DT) and AdaBoost regressors recorded a MedAE of zero on the validation data, suggesting that at least half of their predictions were accurate. The boosted DT model also demonstrated the lowest MedAE on the test dataset, with a value of 2.13.

Highlights

- Data compiled from various literatures contains outliers that degrades ML model.
- Feature importance set the accuracy of ML models.
- ANN model takes the highest training time and presents the best fit.
- GridSearchCV improves the model prediction.
- Models presenting negative fit on the data can be improved by varying parameters.

KEYWORDS

artificial neural network, fatigue, Fiber reinforced polymers, machine learning, residual strength

1 | INTRODUCTION

Fiber-reinforced polymer (FRP) composites being heterogenous and anisotropic requires a great deal of analysis to make them worthy of application in sectors, such as transportation, defense, sports, and so forth.[1] Fiber-reinforced polymers are known for their tailoring properties[2] and must undergo numerous test, such as bending and tensile to safeguard against the external loads.[3] But structural components made out of such materials are susceptible to failure when subjected to fatigue loadings; owing to the accumulation of damages in form of crack propagation[4] during the service life, which can initiate from stress concentration in form of internal defects or machined stress raisers.[5,6] Effective estimation of residual strength by experimentations ensures that the components satisfy the safety criteria; which is a time consuming and labor-intensive process but is paramount to safer components. Analytical methods are quicker than the experimental one, but the results are always an estimation. Estimative methods could be probabilistic[7] or empirical[8] in nature and can provide us with reasonable results using means such as reliability level and coefficient of variation respectively. Another predictive method, which is gaining popularity, is based on Machine Learning models.[9] The method relies on a large set of data for training and based on it could come up with solutions ranging from continuous prediction, optimization, feature identification, uncertainty quantification, reliability, and sensitivity analysis.[10] The learning models are classified as supervised and unsupervised ones, where the earlier one uses structured data such as data sheet to train the model; while the later one uses unstructured data, such as images or acoustic signals to gain the pattern on the test data. Supervised, semi-supervised, unsupervised, and reinforcement learning are the further classifications of ML models.[11] Supervised learning suits best for polymer composites and could handle a vast range of targets that could be either predictive or descriptive or both in nature.[12,13] A predictive model is used to predict outcomes, while a descriptive model is designed to learn from the data and provide detailed answers to the queries. In this context, Loh et al.[14] investigated the fire structural survivability of load-bearing FRP laminates using both experimental methods and artificial neural network (ANN) modeling. Experimental tests under fire and tension load conditions reveal significant scatter in structural performance due to variations in material properties and testing conditions. Artificial neural network-based deep neural networks (DNN) were developed to predict critical parameters, such as failure time, surface temperatures, and axial displacement under fire conditions, achieving high predictive accuracy ($R^2 \geq 0.972$). The study highlights the potential of DNN models to complement experimental methods by reducing testing requirements while addressing inherent variability in material behavior. The findings provide valuable insights for improving the fire-safe design and performance assessment of composite structures.

Ensemble machine learning models that includes extreme gradient boosting (XGBoost), multivariate adaptive regression spline (MARS) and random forest (RF) were used by Milad and his associates.[9,15] The models were trained on a total of 729 data points comprising a total of 5 features in combinations; where, MARS model was found to be fairly accurate, while RF presented better accuracy only when strains were used as training features among the tested models. Yin and Liew[16] used 5 ML models and ANN to predict the interfacial shear strength of FRP composites using data from literatures on micro-bond tests using 11 features. Fiber diameter was found to be the most influential feature for IFSS and use of smaller fiber diameter was recommended. They concluded that GBR and ANN could produce reasonable results on small data. Das and his co-workers[17] used machine learning techniques and broadband dielectric spectroscopy (BbDS) to predict moisture content in fiber-reinforced polymer composites under hygrothermal aging. Multilayer Perceptron (MLP) achieved the highest classification accuracy (97.83%) but was computationally expensive, while SVM and QDA with PCA provided competitive accuracy at lower costs. Regression models, including MLR, DTR, and MLP, demonstrated excellent predictive performance with R^2 >0.95, identifying dielectric properties at specific frequencies as key features. Principal Component Analysis (PCA) effectively reduced dimensionality and multicollinearity, improving model efficiency and performance for classification and regression tasks. Kumar et al.[18] trained and tested ANN, RF, and Gradient Boosting Machine (GBM) models on five features to predict the specific wear rate (SWR) of GFRP samples filled with graphene. Sliding distance was the most influential parameter across models, emphasizing the system-dependent nature of tribological properties. ILSS and tensile strength × elongation (Se) ranked second in importance for RF and GBM models, respectively.

Osa-uwagboe et al.[19] employed machine learning (ML) techniques to predict damage properties in fiber-reinforced polymer composites under quasi-static indentation (QSI) with different indenter geometries. Models based on total energy absorption delivered exceptional performance, achieving R^2 values between 0.9932 and 0.9999, while force-based models were less accurate for specific geometries, such as conical indenters. Among the evaluated ML regressors, k-Nearest Neighbors (k-NN) excelled in handling nonlinear relationships and complex data variability, especially with larger indenter surface areas. The findings highlighted the ability of ML models to reduce time and cost in material design optimization. Moreover, the ensemble regressors were boosted using gridsearch and cross-validation (CV); which adjust the weights to improve predictability.[20–22] He and his associates[23] investigated machine learning techniques for detecting delamination in FRP composite beams using vibration-based structural health monitoring. Three machine learning algorithms—back propagation neural networks (BPNN), extreme learning machines (ELM), and support vector machines (SVM)—are evaluated for predicting delamination interface, location, and size based on natural frequency shifts. The research includes theoretical modeling, numerical simulations, and experimental validation with FRP beam specimens. Among the algorithms, SVM demonstrated superior accuracy, particularly in predicting discrete interfaces, and required fewer samples. The findings highlight the effectiveness of SVM for improving delamination damage prediction and advancing structural health monitoring methodologies. Ding et al.[24] predicted macroscopic mechanical properties and microscopic crack patterns in unidirectional fiber-reinforced polymer (UD FRP) composites. Using data from Discrete Element Method (DEM) simulations, two deep neural networks (DNN) were developed for regression and classification tasks. The regression model predicts tensile strength and Young's modulus, while the classification model identifies crack patterns. Both models exhibited high prediction accuracy, highlighting DNNs as effective tools for modeling complex anisotropic composite behavior with considerations of random fiber distributions.

Machine learning regression models are used in predicting the fatigue life of FRP composites as well. Li et al.[25] focused on predicting the fatigue life of fiberglass-reinforced polyester composites using a novel data-intelligence model, the Extreme Learning Machine (ELM). This modern approach was compared against the traditional Generalized Regression Neural Network (GRNN) and was found to outperform it in accuracy and efficiency. Experimental data involving geometry, stress, and fiber orientation variables were used to train and validate the models, with the ELM achieving a 39% improvement in root-mean-square error and a 38% reduction in mean absolute percentage error over the GRNN. The results demonstrated ELM's advantages in non-iterative tuning and reliability, making it a favorable tool for engineering applications. Mirzaei and co-workers[26] presented a novel model combining ANN with the Non-dominated Sorting Genetic Algorithm II (NSGA-II) to predict the fatigue life of laminated composites. The model is trained using experimental data and finite element simulation results, incorporating features like stress, strain, and geometrical parameters. By employing optimization and data augmentation techniques, the model achieved high predictive accuracy, with R^2 scores of up to 97% for both test and validation datasets. Comparative analysis revealed its superiority over conventional machine learning approaches, especially in handling complex behaviors of composite materials. Min et al.[27] introduced a novel stacking ensemble model, termed Stacking-SXDG, for predicting the flexural fatigue life of fiber-reinforced concrete (FRC). This model integrates Deep Autoencoder Networks (DAN), XGBoost, Random Forest, and a Gray Wolf Optimizer (GWO)-optimized Deep Neural Network (DNN). It demonstrated superior predictive accuracy compared to conventional methods, achieving an R^2 value of 0.938. Key findings emphasize the defining influence of stress level, fiber properties (type, length, and content), and specimen size on fatigue life. The research established the potential of ensemble machine learning models in advancing material performance prediction and highlighted opportunities for further dataset expansion. Table 1 presents the state-of-the-art summary of literature survey.

The learning models provide reasonable results and thus, has the capability of shifting material research toward computation based from existing experimentation-based approach. While several studies have estimated fatigue life using machine learning (ML), most have been limited to 5–7 features for training on small datasets and a narrow range of ML models. This study introduces a novel approach by utilizing 10 features significantly influencing the fatigue performance of FRPs, applying them across 12 ML regression models for training, validation, and testing. Notably, this work pioneers the use of hyperparameter tuning via grid search in this domain. Thus, this work evaluates various ML regression models for their fitting on the data to estimate the residual fatigue life in FRP composites by linear and non-linear mapping of 10 features. The 4-steps process includes data collection, selection of features and training and testing of models (Figure 1). Out of the 10 features, 5 are from materials and manufacturing aspects, 4 selected aspects are from testing conditions and 1 from the mechanical property comprising a total of 968 data points (details in Table 1). Tensile and compressive moduli, fiber volume fraction (v_f) and void fraction could not be included as training feature due to inconsistent reporting; since missing values from the training feature degrade the ML models.

2 | MACHINE LEARNING FRAMEWORK, DATA AND METHODS

Machine learning has expedited the materials exploratory process and can come up with quick solutions, which is not possible in conventional methods. The objective of machine learning process is to train the models using data to make predictions based on regression and/or classification. Scikit Learn[28] on Jupyter notebook was used for programming and to train the ML models on the data. The article tests a total of 12 machine learning regression models for their fit which includes Linear Regressor (LR), Ridge Regressor (RR), ElasticNet (ER), LASSO, Support Vector Regressor (SVR), Bayesian Ridge Regression (BR), K-Nearest Neighbor (KNN), Multilayer Perceptron (MLP(ANN)), Decision Tree (DT), Gradient Boosting Regressor (GBR), Random Forest Regressor (RFR) and ADA Boost Regressor (ADAB) respectively. More details on the regression function and loss functions of the models could be found out in the work by Yin and Liew[16] or on the scikit learn website.[29] The models are further tuned using GridSearchCV.

The evaluation metrics for this study are, 1. coefficient of determination (R^2) for which the best score is 1.0. It can be negative as well referring to worse fitting, or zero presenting a disregard to input data. 2. Mean absolute error (MAE) which is a non-negative entity that has the best value is 0.0. 3. Median absolute error (MedAE), a non-negative float with the best value of 0.0 that presents the regression loss. 4. Root mean square error (RMSE), a non-negative float with the values ranging from 0 (perfect predictions) to ∞, where smaller values indicate better model performance. More about the metrics could be found out at the reference [29]. Moreover, standard deviation, average, minimum and maximum values predicted by various models are also presented in results section.

2.1 | Data

Fatigue behavior of FRP composites depends upon a number of parameters expanding to materials, mechanical properties and test parameters. A comprehensive data frame containing 968 inputs was prepared from the literature,[30–34] and can be assessed from the URL (https://github.com/Dewa1989/Residual-Fatigue-Strength/tree/main). Table 2 shows the feature representation of the training-validation-test (65:20:15) data with 10 independent features containing information on reinforcing materials and weave pattern, stacking sequence and number of plies, ultimate strength of the composites and test parameters that include stress ratio and stress amplitudes, test frequency, fatigue life and normalized fatigue life. Fiber material and weave patterns has a defining effect on the fatigue performance where CF are found to outperform GF, while woven fabric possess poor fatigue life owing to the stress concentrations arising from the tow cross-over points.[1,35] Number of plies that closely controls the stacking sequence of laminates,[35,36] and static strengths are important parameters to establish

TABLE 1 Summary of the state of the art.

Training features	Target	Data points	Split ratio	Models used	Metrices	Ref.
Thickness, width, v_f, v_m, stress, time-to-failure, heat flux exposure time, failure temperature, temporal temperature evolution on heated surface and temporal temperature evolution on unheated surface	Front failure temperature, Back failure temperature, Axial displacement at failure, Failure time, Temporal temperature evolution on unheated surface, Temporal temperature evolution on the unheated surface	48 to 111,967	~80/20	DNNs with 4 hidden layers and 2048 neurons per layer 149 to 479 Epochs	R^2 = 0.97 to 0.99 RMSE = 0.27 to 74.04 MAE =0.18 to 47.99	Loh et al.[14]
Strain, density, fiber strength, diameter and thickness in combinations	Strain enhancement ratio	729	-	XGBoost, MARS, RF	R^2 = 0.99874, RMSE = 0.39, MAE = 0.20, Nash = 0.99	Milad et al.[15]
Fiber type, diameter and length, fiber and matrix stiffness, fiber and matrix poison's ratio, matrix type, loading rate, preparation and test temperature	Fmax and IFSS	818	80/20	LR, BR, EN, SVR and GBR	R^2 = 0.999 & 0.987 on Fmax and IFSS, MSE = 0.0002 & 11.737, MAE = 0.008 & 2.29, EVS = 0.999 & 0.987	Yin and Liew[16]
Permittivity, Dielectric relaxation strength and thickness	Moisture content	1024	80/20	MLR, DT and MLP	Accuracy for classification and R^2. R^2 = 0.962 accuracy = 97.83%	Das et al.[17]
GNP content, applied load, sliding distance, product (se), Vicker hardness, and ILSS	Specific wear rate	72	70/30	ANN, RFR, and GBR	R^2 = 0.9884 MAE = 0.221 MSE = 0.066, RMSE = 0.257	Kumar et al.[18]
Quasi-static indentation, Acoustic emission, X-ray micro-CT, SEM images	Damage	700	80/20	ADAB, ANN DT, ET, GBR, K-NN, LGBM, NuSVR, RFR and XGBoost	R^2 = 0.9879, MAE = 0.0165, MSE = 0.0042	Osa-uwagboe et al.[19]
Manufacturing, interface damage, location, size and the modal frequencies	Delamination damage	60 to 2387	90/10 to 50/50	Back propagation neural network, Extreme learning machine, and Support vector machine	MAE = 1.22	He et al.[23]
Discrete Element Method (DEM) simulations of 2000 Representative Volume Element (RVE) with 200 different sets of fiber volume fractions and fiber radii	Transverse tensile strength and Young's modulus	2000 for regression 1600 for classification	-	DNN Regression	R^2 = very close to 1	Ding et al.[24]
Material, Density, Modulus of elasticity, Strength, Poisson's ratio,	Fatigue cycles	–	–	ELM, GRNN	RMSE = 11.7846, MAPE = 10.9232, WI = 0.9908,	Li et al.[25]

(Continues)

TABLE 1 (Continued)

Training features	Target	Data points	Split ratio	Models used	Metrices	Ref.
geometry dimension, stress, and fiber orientations					NS = 0.9767, R = 0.9927	
Stress, strain, mapped layup, mapped notch geometry, maximum of the applied fatigue load, and ultimate tensile strength	Fatigue life	5–128	55/30/15 for train-test-validate	ANN-NSGA-II with one to 5 layers	$R^2 = 0.95$	Mirzaei et al.[26]
Water-to-cement ratio, sand-to-cement ratio, coarse aggregate-to-cement ratio, fiber properties, key concrete mixture parameters, specimen dimensions, stress levels, stress ratios, and reliability	Fatigue life	–	80/20	DNN, CatBoost, DT, SVR	$R^2 = 0.896$, RMSE = 66,831, MAE = 26,207	Min et al.[27]

FIGURE 1 Workflow of the machine learning process.

TABLE 2 Features of the training, validation and test data.

Features	Min value	Max value	Mean value	Class
Input features				
Material	0	1	–	Discontinuous (0–1)
Nature of Reinforcement	0	2	–	Discontinuous (0–2)
Stacking type	0	3	–	Discontinuous (0–3)
Number of plies	4	20	–	Discontinuous
Ultimate tensile strength (MPa)	89.54	769	451.58	Continuous value
Stress amplitude (MPa)	54.8	600	318.60	Continuous value
Stress ratio (R)	−0.47	0.5	0.10	Continuous value
Test frequency (Hz)	2	10	–	Discontinuous
Endured fatigue cycles	10	10,000,000	634411.11	Continuous value
Normalized fatigue life (N/N_f)	0.1	1.0	0.735	Continuous value
Target feature				
Residual strength (MPa)	0	734	195.66	Continuous value

Note: Materials: 0- CF & 1-GF; Nature of Reinforcement: 0- UD, 1-Woven & 2- Satin weave; Stacking type: 0- In-plane, 1-Angle-ply, 2- Cross-ply & 3- Symmetric laminates.

the fatigue loads. Moreover, test features such as R, σ_{amp}, f, N_f and N/N_f possess great influence over the fatigue performance of FRP composites.[35,37,38] It is worth mentioning that stress amplitude is usually set at a fraction of the ultimate strength and R is based on the application cycles. Moreover, there is no standard that establishes the test frequency, but it mostly remains in the range of 1–10 Hz; since higher frequencies tend to reduce fatigue life due to hysteretic heating.[39] More information on material's attribute could be found in the literature.[40] For the models, post fatigue residual strength was the target and the matrix material was epoxy. Figure 2 presents the distribution of the target with respect to the training features. Pearson correlation coefficient, that traces the linear dependence among the training features is shown in Figure 3, and shows great nonlinearity, which is suitable for effective model training.

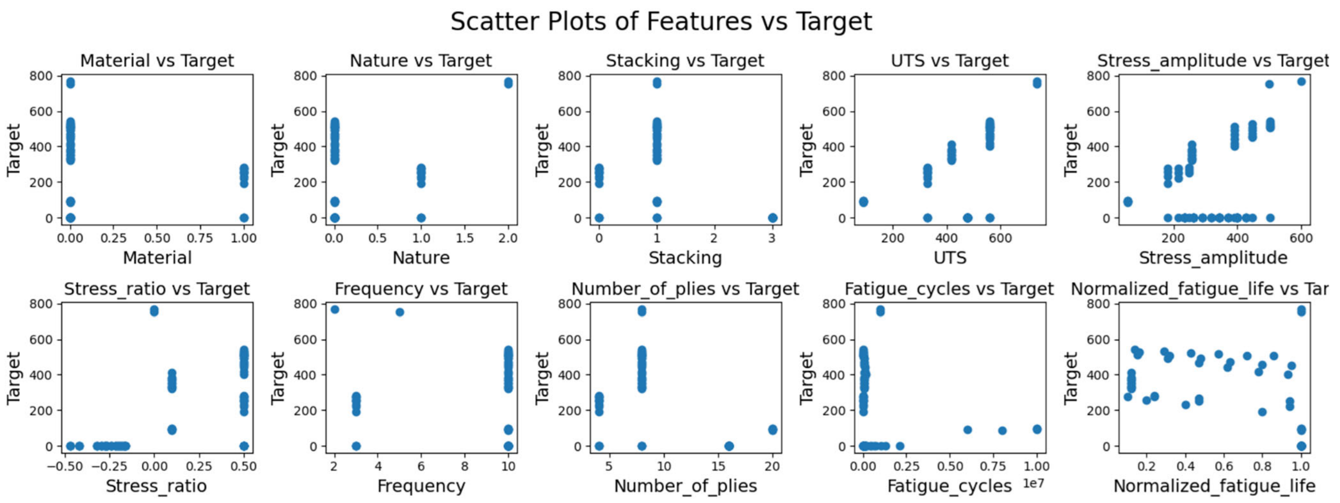

FIGURE 2 Target distribution versus training features. (Material, nature of reinforcement, kind of stacking, number of plies and test frequency presents a discontinuous distribution).

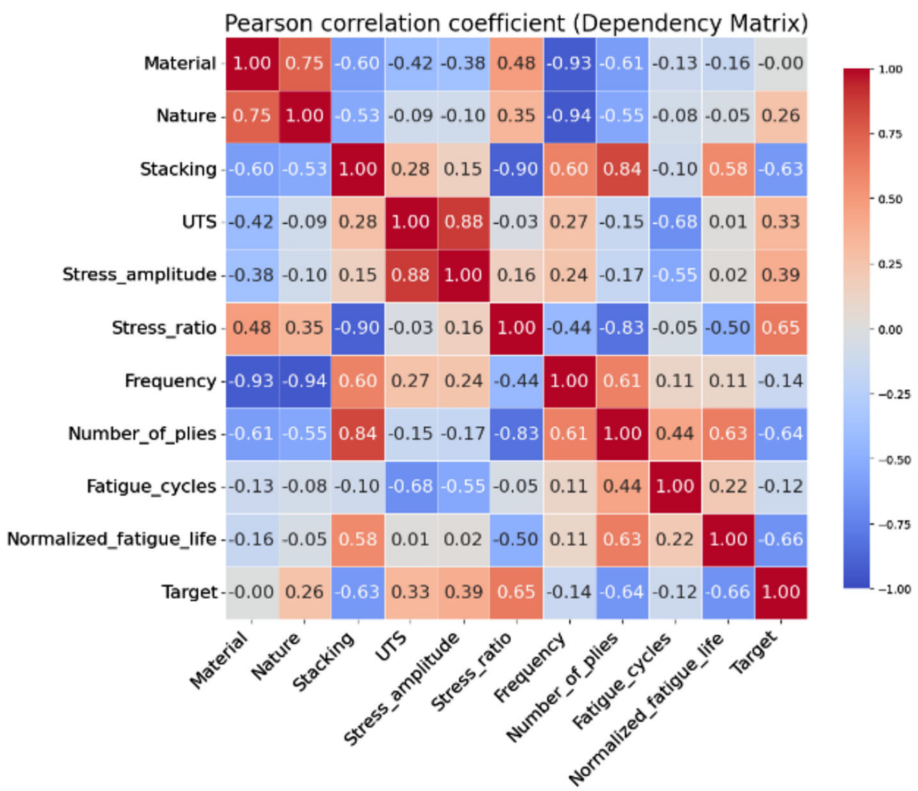

FIGURE 3 Pearson correlation coefficient of the training the target features (Highest positive correlation is between stacking sequence and number of plies; highest negative correlation between test frequency and nature of reinforcement and reinforcement materials).

2.2 | Cross-validation and gridsearch parameters

The work explores a total of 12 ML regression models out of which 11 models were boosted using grid search and cross validation (CV) to be collectively called as GridSearchCV that could improve the evaluation metrices of ML models. Five-fold cross validation that includes 5 independent shuffling of data was done to improves their generalization (schematic in Figure 4). Out of the 12 tested models, BRR and KNN presented a negative fit on the data and SVR initially presented a zero fit on the data that improved after the boosting; and hence BRR and KNN will not be the part of further discussions. However, the results could be accessed from the provided URL.

Hyperparameter selection and optimization is critical to ML models and dictates the learning and behavioral aspects of ML models.[41–44] Table 3 presents the details of hyperparameters of different ML models used in this work. The optimum combination of params could improve the model's performance; but comes at great time and computational costs.[43] While most of the ML regression models have limited parameters to control, ANN, an extremely powerful model requires intervention on many params, such as number of hidden layers, activation function of the layers, learning rate, and so forth, to inhibit the overfitting on the data. In this work, the number of hidden layers and neurons in DNN were optimized using Keras Tuner, while MinMaxScaler was used for normalization of the input data. More details on the optimization steps could be found in the works;[41–44] and specifics on params for models could be assessed from the reference.[29]

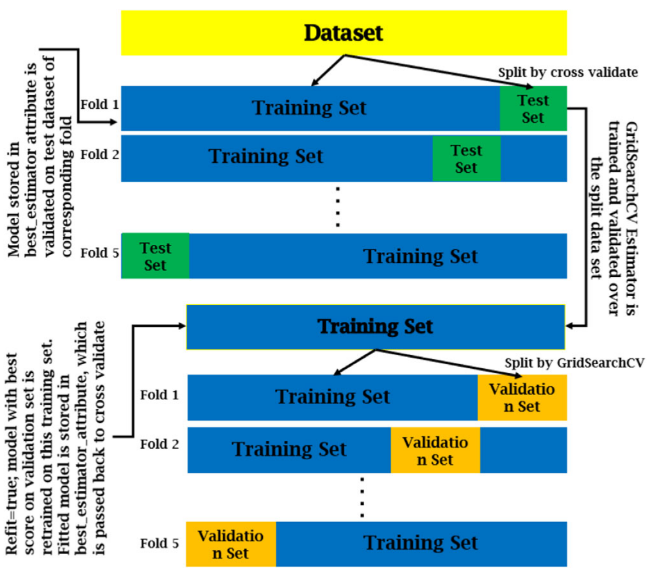

FIGURE 4 Flow of grid search and 5-fold cross-validation on the tested models.

Figure 4 presents the schematic of applied cross-validation and grid search method across models.

3 | RESULTS AND DISCUSSIONS

3.1 | Fit and metrices

3.1.1 | Linear and non-linear regression models

The performance of the models, both tuned and unturned, is summarized in Tables 4 and 5 for the validation and test datasets, respectively. Linear and non-linear models, with the exception of Elastic Net Regression (ER), showed comparable fits, achieving R^2 values in the range of 0.75–0.79 on the validation set. The ER model, however, had a lower R^2 value of 0.59 on validation data but improved significantly to 0.79 after fine-tuning using GridSearchCV, matching the performance of the tuned Ridge Regression (RR) and Lasso models. Interestingly, parameter tuning did not affect the fit of RR and Lasso models on the validation dataset. On the test data, the models generally exhibited better fit compared to the validation dataset. For instance, the ER model's R^2 improved from 0.62 to 0.8 after fine-tuning, aligning with the RR and Lasso models. A slight improvement of 0.01 in test data fit was observed, likely due to the smaller size of the test dataset (15% of the entire data). Despite improved R^2 on the test set, the models exhibited higher Mean Absolute Error (MAE), potentially attributable to random variability, a challenging test set, or the ubiquitous presence of outliers in fatigue data. Additionally, the models demonstrated an improvement in Median Absolute Error (MedAE) on the test data compared to the validation set, suggesting either better generalization or possible underfitting on the validation dataset, as indicated by the lower fit values.[45] Interestingly, Linear Regression (LR) achieved the highest fit and the lowest RMSE on the test dataset, despite the features being non-linearly associated. This highlights the model's ability to adapt and learn patterns in the data beyond the constraints of its linear regression function. Moreover, it was observed that models predicted negative minimum residual strengths, which is physically unrealistic as the minimum residual strength cannot be less than 0 MPa and hence considered as model's limitations.

3.1.2 | Tree and ensemble based regressors

Tables 6 and 7 present the model parameters for the validation and test datasets, respectively. Ensemble regressors are broadly classified into parallel and sequential ensembles, both of which combine predictions from simpler base

TABLE 3 Details of the grid search parameters of the implied models.

Model	Grid search parameter(s)
Ridge Regression	'alpha': [0.0001, 0.001, 0.01, 0.1, 1.0], 'solver': ['auto', 'svd', 'cholesky', 'lsqr', 'sparse_cg', 'sag', 'saga', 'lbfgs']
ElasticNet	alpha: 50 values between 0.001 to 1.0 l1_ratio#: 0.1, 0.2, 0.4, 0.5, 0.6, 0.8, 0.9 #Mix of L1 (Lasso) and L2 (Ridge) regularization
LASSO	alpha: 50 values between 0.0001 to 1.0
Support Vector Regression (SVR)	kernel: 'linear', 'poly', 'rbf', 'sigmoid' Regularization parameter C#: 0.001–0.1 #small to eliminate overfitting Tube width ε: 50 values between 0.01–1.0 Polynomial degree##: 2, 3, 4, 5 ##Only relevant for 'poly' kernel Gamma###: 'scale', 'auto' ###Kernel coefficient for 'rbf', 'poly', and 'sigmoid'
MLP (ANN) Hyperparameters	Number of neurons in the input layer: 10 Number of neurons in the output layer: 1 Number of hidden layers: 2 Number of neurons in the Hidden layer: 20 to 50 (in combinations) Normalization scaler on input data: MinMaxScaler Activation functions for hidden layers: ReLU, Sigmoid, SELU, Tanh Activation function in output layer: Linear Optimizer: Adam, Adagrad, Adadelta, RMSprop (learning rate of 0.0001)
Decision Tree	Max depth: 3–10 Minimum sample split: 2–10 Minimum sample leaf: 1–4 Max features: None, 'sqrt', 'log2'
Gradient Boosting Regression (GBR)	n_estimators: 100(min) –10,000, learning_rate: [0.001–1.0], max_depth: 3–10, subsample: [0.001–1.0], criterion: 'friedman_mse', 'squared_error', loss: squared_error', 'absolute_error', 'huber', 'quantile'
Random Forest Regressor (RFR)	n_estimators: 50, 100, 200, max_depth: None – 30, min_samples_split: 2–10, min_samples_leaf: 1–4
ADA Boost Regressor (ADAB)	Number of estimators: 50–200 Learning rate: 50 values between 0.001 to 1.0 Loss function: 'linear', 'square', 'exponential'

TABLE 4 Results of linear and non-linear models on validation set.

Model	R^2	MAE	MedAE	RMSE	SD	Average	Min	Max
LR	0.79	50.94	27.46	97.49	211.13	190.31	−27.46	597.02
RR	0.79	48.36	28.11	96.64	203.13	189.65	−34.94	565.27
RR_GS	0.79	50.93	27.45	97.49	211.13	190.31	−27.45	596.99
ER	0.59	79.34	35.72	135.43	182.4	188.12	−5.05	492.77
ER_GS	0.79	50.09	26.28	97.13	210.7	190.05	−26.28	594.78
LASSO	0.78	49.75	23.29	97.89	208.63	190.21	−11.92	588.72
LASSO_GS	**0.79**	47.45	22.17	**96.03**	209.35	189.09	−22.17	586.74

Note: The bold value indicates results of the best model from each class.

TABLE 5 Results of linear and non-linear models on test set.

Model	R^2	MAE	MedAE	RMSE	SD	Average	Min	Max
LR	**0.80**	81.98	25.42	**99.07**	198.66	224.27	−27.89	538.05
RR	0.79	52.55	25.37	100.47	198.97	220.25	−50.56	518.37
RR_GS	0.80	51.98	25.40	97.49	198.66	224.27	−27.87	538.04
ER	0.62	76.47	33.07	134.72	193.80	226.78	−24.40	479.55
ER_GS	0.80	51.53	24.36	99.05	198.93	223.92	−26.77	537.90
LASSO	0.79	52.11	22.91	101.81	201.74	223.05	−23.31	548.23
LASSO_GS	0.80	51.25	21.51	99.22	200.01	222.86	−22.89	537.59

Note: The bold value indicates results of the best model from each class.

TABLE 6 Results of tree and ensemble models on validation set.

Model	R^2	MAE	MedAE	RMSE	SD	Average	Min	Max
DT	0.65	38.18	0	123.76	213.59	179.09	0	525.00
DT_GS	0.65	38.05	0	124.79	214.48	179.76	0	510.67
GBR	0.67	37.45	2.47	120.13	215.35	181.46	−0.43	547.07
GBR_DT	**0.77**	30.95	0.20	**100.90**	208.19	175.24	−0.20	527.73
RFR	0.76	33.40	2.98	103.98	206.72	175.81	0	524.84
RFR_GS	0.73	35.83	3.28	109.63	207.33	176.25	0	522.79
ADAB	0.65	39.74	0	123.66	210.73	177.37	0	506.00
ADAB_GS	0.66	42.68	0	121.94	205.70	173.06	0	507.29

Note: The bold value indicates results of the best model from each class.

TABLE 7 Results of tree and ensemble models on test set.

Model	R^2	MAE	MedAE	RMSE	SD	Average	Min	Max
DT	0.69	44.63	10.50	122.30	216.57	239.51	0	517.00
DT_GS	0.67	49.41	2.13	126.45	215.62	238.001	0	510.67
GBR	0.67	56.38	7.30	126.05	205.42	220.27	−0.25	511.75
GBR_DT	**0.87**	32.28	6.92	**80.18**	208.19	175.24	−0.20	506.01
RFR	0.79	38.66	5.93	100.48	206.09	227.62	0	503.91
RFR_GS	0.76	40.49	5.04	107.21	208.64	229.90	0	514.27
ADAB	0.69	46.24	9.61	122.74	212.54	234.26	0	504.50
ADAB_GS	0.66	50.87	7.92	128.31	207.66	228.66	0	506.42

Note: The bold value indicates results of the best model from each class.

models to enhance overall accuracy. Random Forest is an example of a parallel ensemble method, where base learners (decision trees) are generated and trained independently in parallel, a technique also known as bagging. The final prediction is derived by averaging the outputs of these trees, each trained on different features and bootstrapped samples. In contrast, Gradient Boosting is a sequential ensemble method, where base learners are trained sequentially, and each learner is dependent on the performance of the previous ones. This approach improves predictions by adjusting the weights of previously misclassified samples, thereby reducing bias in the final estimator. The final predictions are made using a weighted sum or weighted majority vote of the base learners. Figure 5A,B illustrates the schematics of the Random Forest and Gradient Boosting regressors.

The results of the tree and ensemble models on the validation set (Table 6) highlight the superior performance of Gradient Boosting Regressor (GBR) models, particularly the GBR_DT variant, which achieved the highest R^2 value of 0.77 and the lowest RMSE of 100.90. This establishes the model's ability to accurately capture patterns in the data. Random Forest Regressor (RFR) also performed well, with an R^2 of 0.76 and an RMSE of 103.90, which slightly improved when hyperparameter tuning was applied (RFR_GS: RMSE 109.63, R^2 0.73). Decision Tree (DT) and Adaptive Boosting (ADAB) regressors, even after tuning (DT_GS and ADAB_GS), exhibited relatively lower performance metrics, with RMSE values exceeding 120 and R^2 values around 0.65–0.66, indicating weaker generalization on the validation

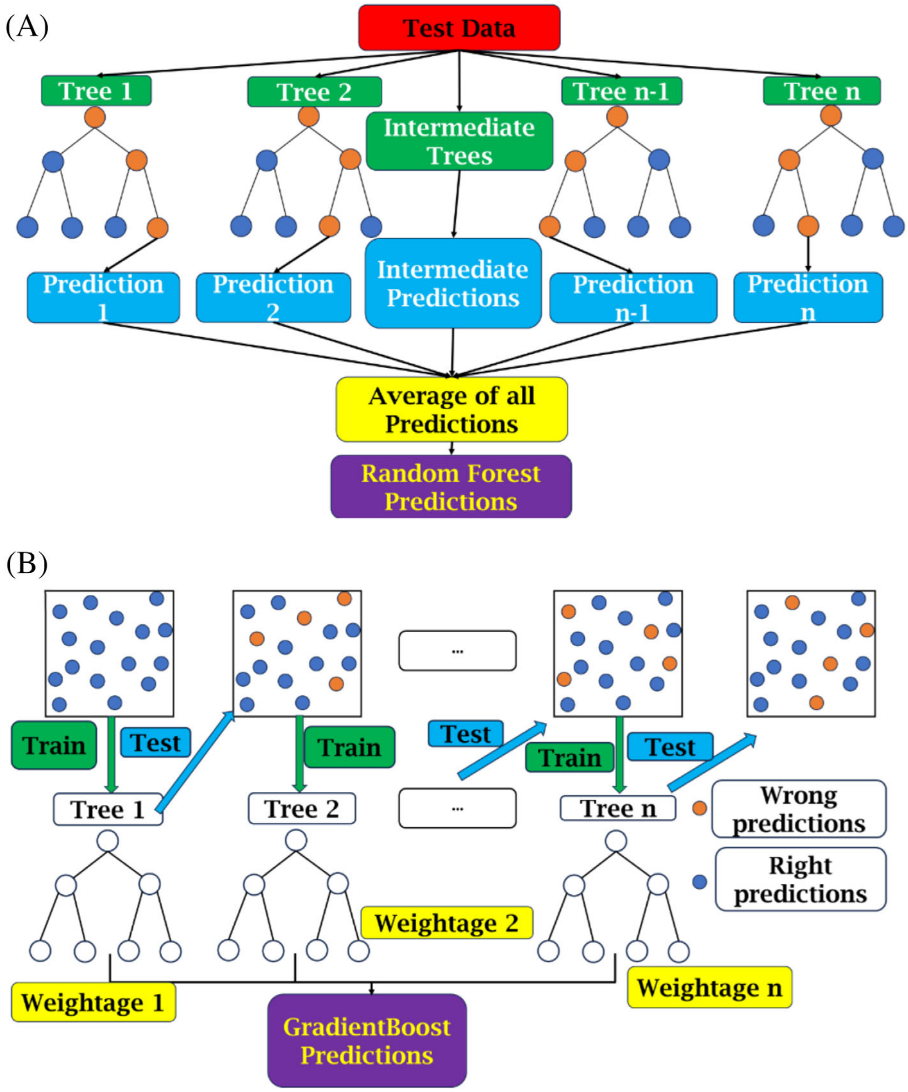

FIGURE 5 Representation of (A) Random Forest and (B) Gradient Boosting ML models.

TABLE 8 Results of SVR and ANN models on validation set.

Model	R^2	MAE	MedAE	RMSE	SD	Average	Min	Max
SVR	0	166.25	85.9	210.5	11.3	96.76	84.47	110.2
SVR_GS	0.70	45.88	3.39	115.12	205.97	189.01	−0.12	530.14
MLP	**0.88**	27.71	1.51	**72.42**	210.48	169.08	−47.82	563.54
MLP_GS	**0.88**	27.71	1.51	**72.42**	210.48	169.08	−47.82	563.54

Note: The bold value indicates results of the best model from each class.

TABLE 9 Results of SVR and ANN models on test set.

Model	R^2	MAE	MedAE	RMSE	SD	Average	Min	Max
SVR	−0.18	201.43	132.56	238.45	11.51	98.13	84.32	110.90
SVR_GS	0.71	47.05	9.15	118.22	213.05	233.99	−0.14	528.89
MLP	**0.95**	21.56	3.66	**47.81**	205.94	214.70	−7.53	504.64
MLP_GS	**0.95**	21.56	3.66	**47.81**	205.94	214.70	−7.53	504.64

Note: The bold value indicates results of the best model from each class.

set. On the test set (Table 7), the GBR_DT model continued to exhibit acceptable performance, achieving the highest R^2 of 0.87 and the lowest RMSE of 80.18, reinforcing its robustness and generalization capabilities. The RFR model also performed reasonably well, with an R^2 of 0.79 and an RMSE of 100.48, maintaining its

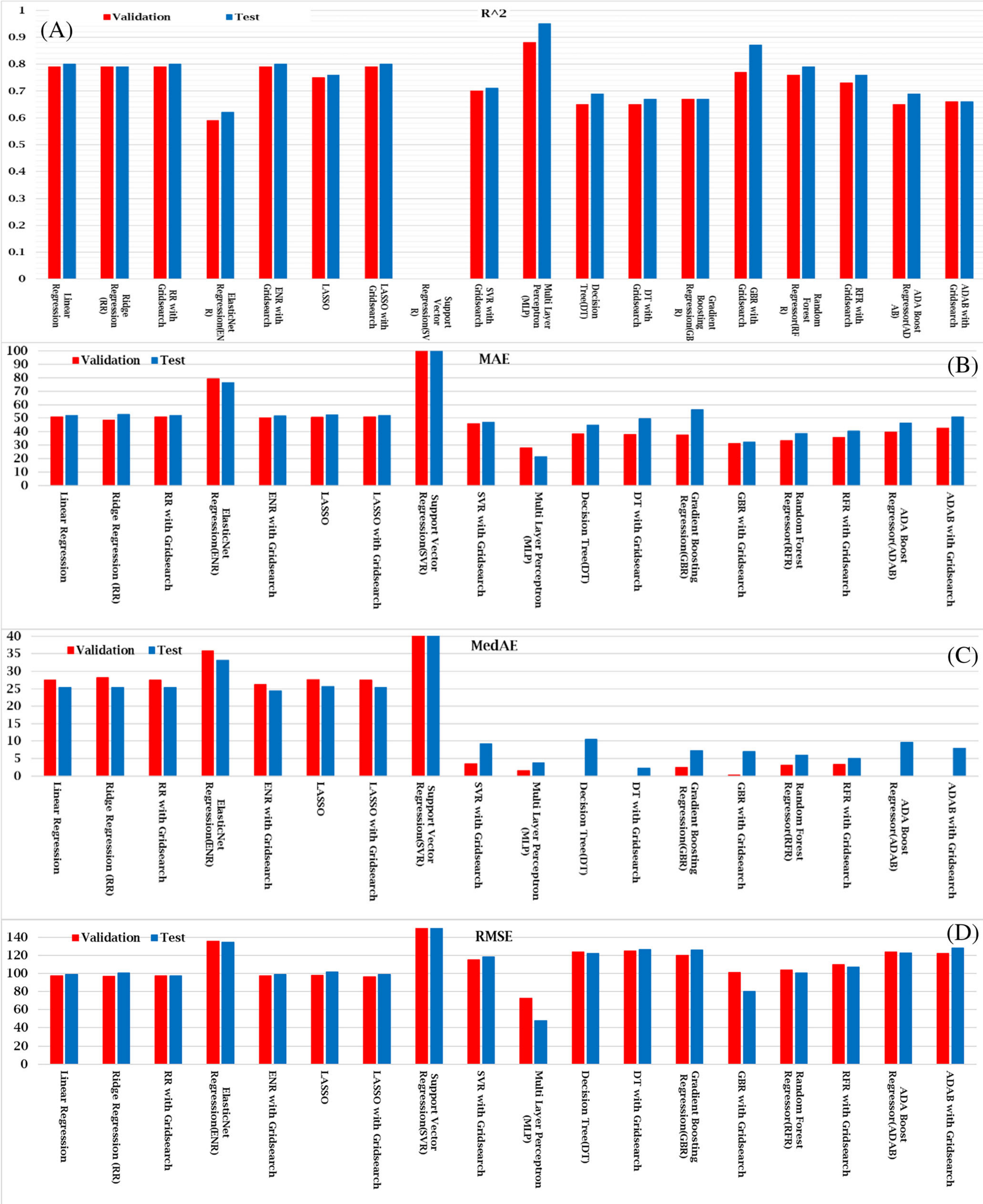

FIGURE 6 Comparison of evaluation metrices (A) R^2; (B) MAE; (C) MedAE; and (D) RMSE [SVR regression had a 0-fit and −0.18 fit on validation and test data respectively, thus the highest MAE and MedAE].

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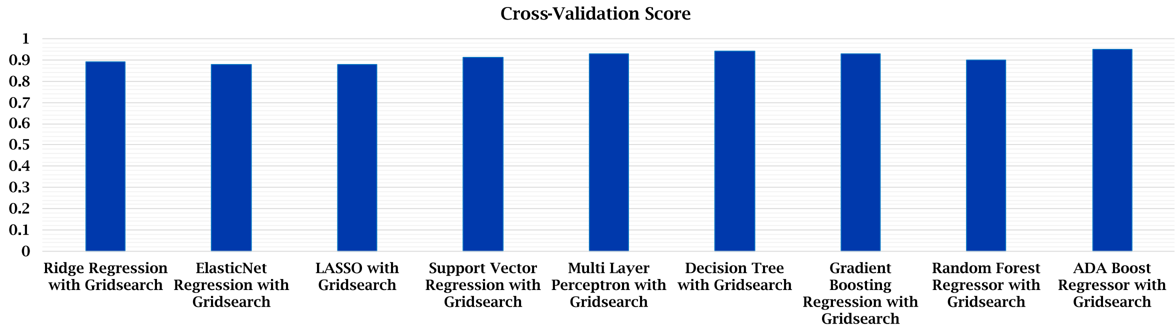

FIGURE 7 Cross validation score of the tested models.

TABLE 10 Best grid parameters for the tested models.

Model	Best parameters
RR	'alpha': 0.0001, 'solver': 'sparse_cg '
ER	'alpha': 0.001, 'l1_ratio': 0.9, 'max_iter': 5000
LASSO	'alpha': 0.0001, 'solver': 'auto'
SVR	'C': 1000.0, 'degree': 2, 'epsilon': 0.1, 'gamma': 'scale', 'kernel': 'linear'
MLP	'activation': 'relu', 'alpha': 0.0001, 'hidden_layer_sizes': (30, 20), 'learning_rate': 'constant', 'solver': 'adam'
DT	'max_depth': 5, 'max_features': None, 'min_samples_leaf': 1, 'min_samples_split': 5
GBR	'learning_rate': 0.1, 'max_depth': 7, 'n_estimators': 200, 'subsample': 0.8
RFR	'max_depth': None, 'min_samples_leaf': 1, 'min_samples_split': 5, 'n_estimators': 100
ADA Boost	'learning_rate': 0.01, 'loss': 'exponential', 'n_estimators': 50

consistency over the data. DT and ADAB regressors, along with their tuned versions, showed modest improvements in R^2 (ranging from 0.66 to 0.69 for DT variants and 0.65 to 0.66 for ADAB variants) but continued to deliver higher RMSE values above 120, indicating larger prediction errors. These results suggest that ensemble models, particularly sequential ensembles like GBR, provide superior predictive accuracy compared to standalone regressors or less optimized ensemble approaches. Moreover, models from these class except GBR predicted the minimum residual strength of 0; indicating their ability of interpreting a physically possible minimum strength.

3.1.3 | SVR and MLP (ANN)

The performance of Support Vector Regression (SVR) and ANN models, as presented in Tables 8 and 9, highlights the significant differences between these approaches. On the validation set, the MLP model outperformed all others, achieving the highest R^2 of 0.88 and the lowest RMSE of 72.42, both before and after hyperparameter tuning (MLP_GS). This indicates the MLP model's strong capability to generalize the patterns in the dataset. In contrast, the baseline SVR model showed no predictive power on the validation set ($R^2 = 0$), with a high RMSE of 210.5 and MAE of 166.25. However, hyperparameter tuning significantly improved the SVR's performance, resulting in an R^2 of 0.70 and a reduced RMSE of 115.12. Despite this improvement, SVR remained inferior to the MLP model in all performance metrics. On the test set (Table 9), the MLP model again demonstrated the best performance, achieving an R^2 of 0.95 and the lowest RMSE of 47.81, reflecting its robustness and ability to generalize well on unseen data. Conversely, the baseline SVR model exhibited poor performance, with a negative R^2 of -0.18, indicating its inability to capture the underlying data distribution. Tuning significantly enhanced the SVR model's performance ($R^2 = 0.71$, RMSE $= 118.22$), but it still fell short of the results delivered by MLP models. The overall results highlight the superiority of ANN models, particularly MLP, in capturing complex, non-linear relationships in the dataset, making them the most effective regressors among the tested models. Despite achieving the best metrics among all the models, the MLP also exhibited a notable limitation by inaccurately predicting the physically minimum residual stress of zero, and produced negative residual stress values, which are not feasible in real engineering applications. Moreover, Table 10 presents the best hyperparameters of the GridSearch modified models.

Figure 6A–D presents comparative bar chart of the performance indicators for various regression models based on multiple evaluation metrics of R-squared (R^2), Mean Absolute Error (MAE), Median Absolute Error (MedAE), and Root Mean Square Error (RMSE) for validation and test datasets. Linear Regression (LR), Ridge Regression (RR), and Bayesian Ridge Regression (RR_GS) consistently perform well, with R^2 values of

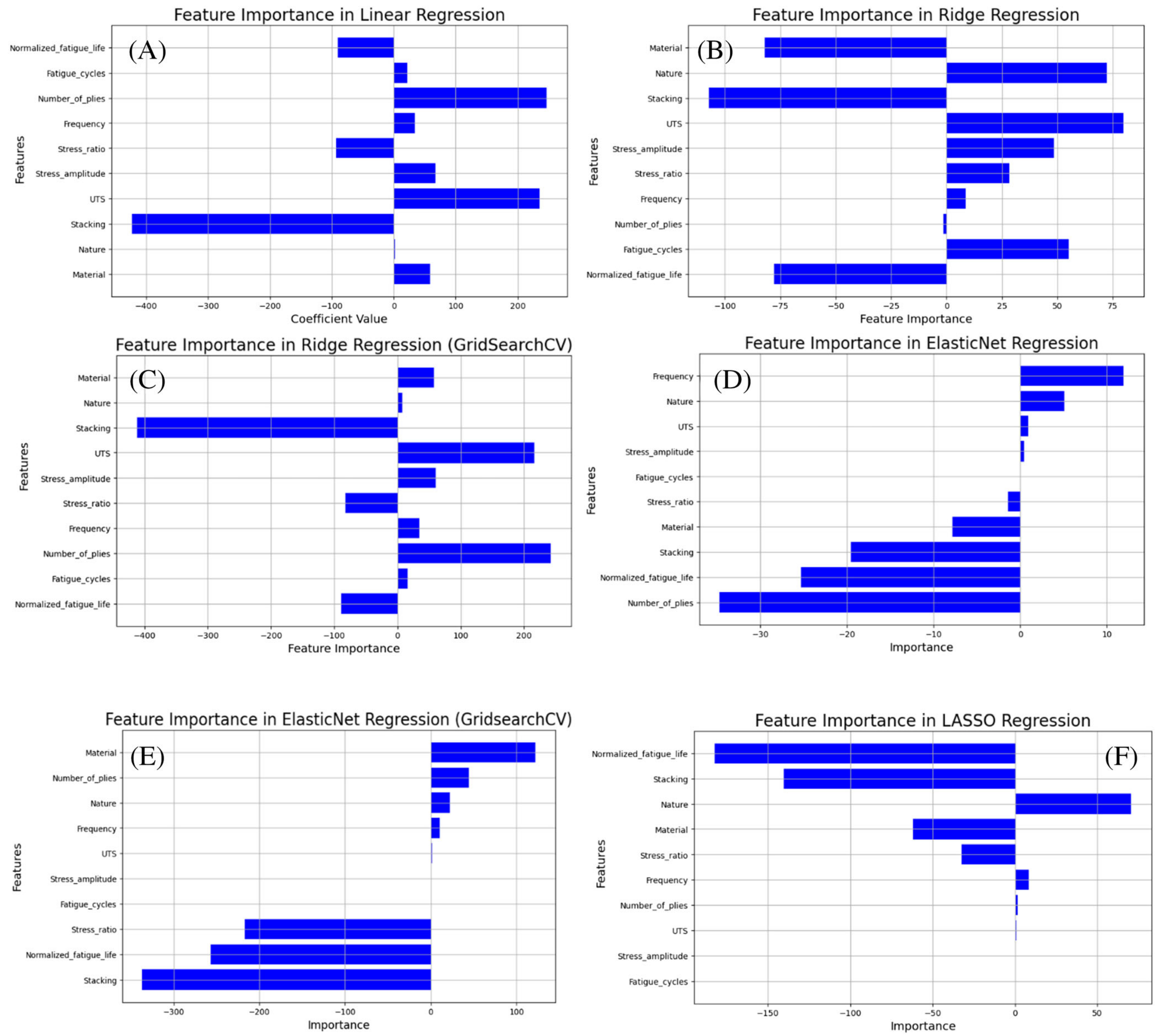

FIGURE 8 Feature importance for different models (A) LR, (B) RR, (C) RR with gridsearch, (D) ER, (E) ER with Gridsearch, (F) LASSO, (G) LASSO with gridsearch, (H) SVR, (I) SVR with gridsearch, (J) MLP, (K) DT, (L) DT with gridsearch, (M) GBR, (N) GBR with gridsearch, (O) RFR, (P) RFR with gridsearch, (Q) ADA Boost, and (R) ADA Boost with gridsearch.

0.79–0.80, and relatively low MAE, MedAE, and RMSE values. ElasticNet Regression (ER) exhibits lower R^2 (0.59–0.62) and higher error metrics, but when boosted with GridSearch (ER_GS), it improves to R^2 values comparable to LR and RR. LASSO Regression and its GridSearch variant perform similarly to the best models, achieving R^2 around 0.75–0.80 with moderate error metrics. Support Vector Regression (SVR) underperforms significantly with negative R^2 (−0.18 on the test set) and high error values, but optimization (SVR_GS) boosts R^2 to 0.71 and reduces errors. The Multi-Layer Perceptron (MLP) is the standout model, achieving the highest R^2 (0.88–0.98) and the lowest MAE, MedAE, and RMSE, showcasing its strong predictive ability. Decision Tree (DT) and Gradient Boosting Regression (GBR) models have moderate performance, with R^2 values of 0.65–0.67 and slightly higher errors, which GridSearch does not significantly improve. Summarily, MLP outperforms all models, while SVR shows the weakest baseline performance. Linear and Ridge methods maintain consistent reliability across all metrics. Figure 7 plots the cross-validation (CV) scores of regression models after optimization. Ridge Regression, ElasticNet Regression, and LASSO with GridSearch achieve consistent CV scores of 0.88–0.89, indicating reliable performance on generalizability. Support Vector Regression (SVR) shows

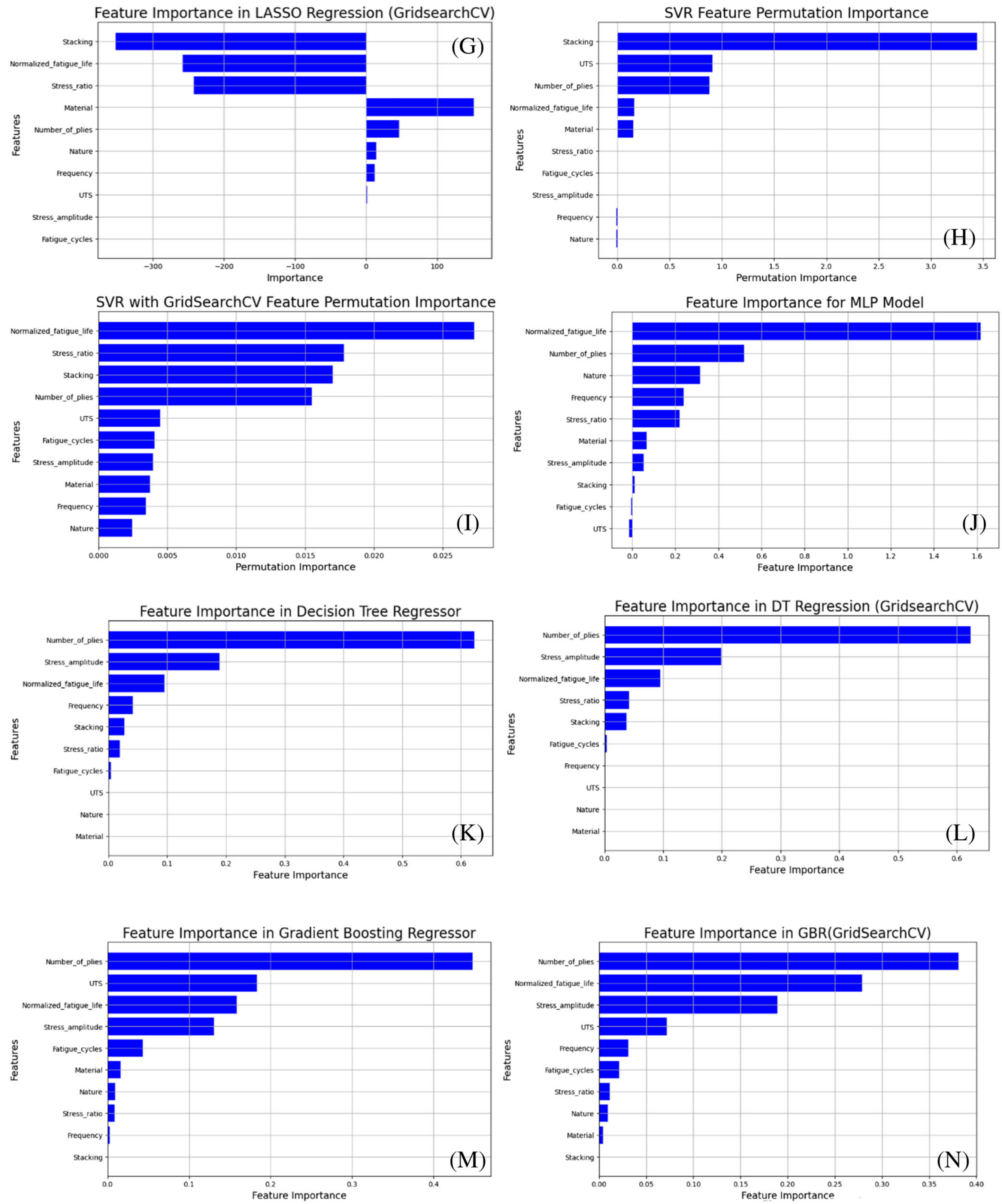

FIGURE 8 (Continued)

improvement with a CV score of 0.91. Multi-Layer Perceptron (MLP) and Gradient Boosting Regression (GBR) both exhibit strong performance with scores of 0.93. The Decision Tree with GridSearch achieves a slightly higher score of 0.94, while the Random Forest Regressor (RFR) follows closely at 0.90. Notably, the AdaBoost Regressor

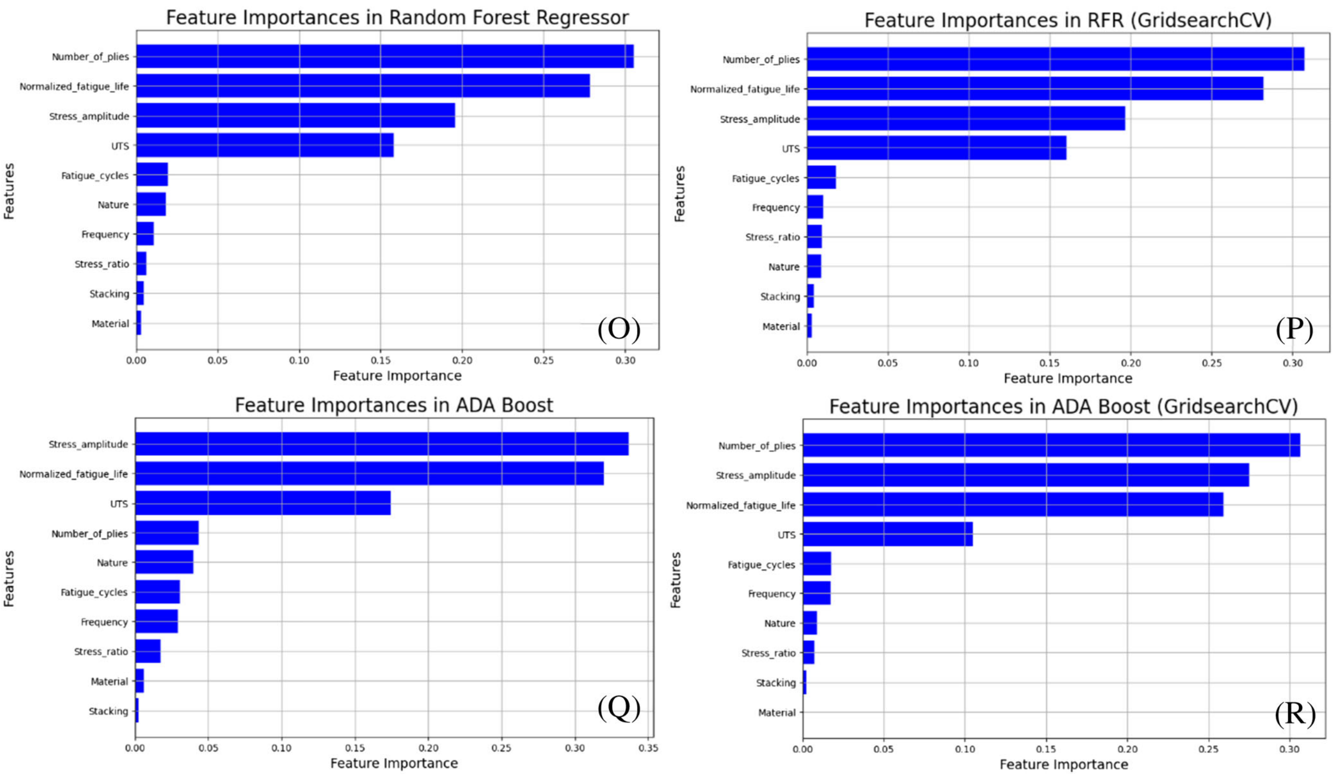

FIGURE 8 (Continued)

with GridSearch delivers the best CV score of 0.95, highlighting its superior generalization ability.

3.2 | Feature importance and predictions

Predictions are influenced by the feature importance determined by each algorithm, where the selection of features is guided by the model's handling of outliers. Linear Regression, Ridge Regression, and Boosted Ridge Regression models utilized all available features to generate predictions, ensuring comprehensive coverage of the dataset. In contrast, ElasticNet (EN), LASSO, and SVR models largely disregarded the fatigue-cycles feature, likely due to the presence of outliers in this parameter. Additionally, these models exhibited low or no sensitivity to stress amplitudes and the ultimate tensile strength (UTS) of the composites. Interestingly, the Linear Regression model excluded the nature of reinforcement as a training feature. The SVR model also deemed the stress ratio a trivial feature, while the tuned SVR model incorporated all parameters as training features. For tree-based models, ensemble methods, and ANN, feature importance was assessed using the permutation method, wherein feature weights were varied to evaluate their impact on predictions, eliminating negative magnitudes. The Decision Tree (DT) regressor did not utilize UTS, reinforcement nature, and reinforcing materials for training, while the boosted DT regressor added test frequency as a feature. Gradient Boosting Regressor (GBR) and boosted AdaBoost Regressor excluded stacking sequence and reinforcement materials from their training features. Feature importance plots are provided in Figure 8A–R.

Figure 9A–J illustrates a comparison of predictions made by various machine learning models. An effective ML model should capture the underlying patterns in the training data rather than memorizing them, ensuring valid predictions on unseen test data. A smaller Median Absolute Error (MedAE) is indicative of this ability. In this study, the ANN model and the boosted Gradient Boosting Regressor (GBR) demonstrated the most accurate predictions, achieving R^2 values of 0.87 and 0.95, respectively, on the test data. These results are consistent with the findings of Yin and Liew.[16] Both models showed strong generalization capabilities, as indicated by cross-validation R^2 scores exceeding 0.9. In comparison, linear and non-linear models exhibited cross-validation R^2 scores below 90%, suggesting a relatively lower capacity for generalization. However, this does not imply poor performance, as their R^2 values were still higher than those of tree-based and ensemble-based regressors. The figure also highlights that predicting residual strength

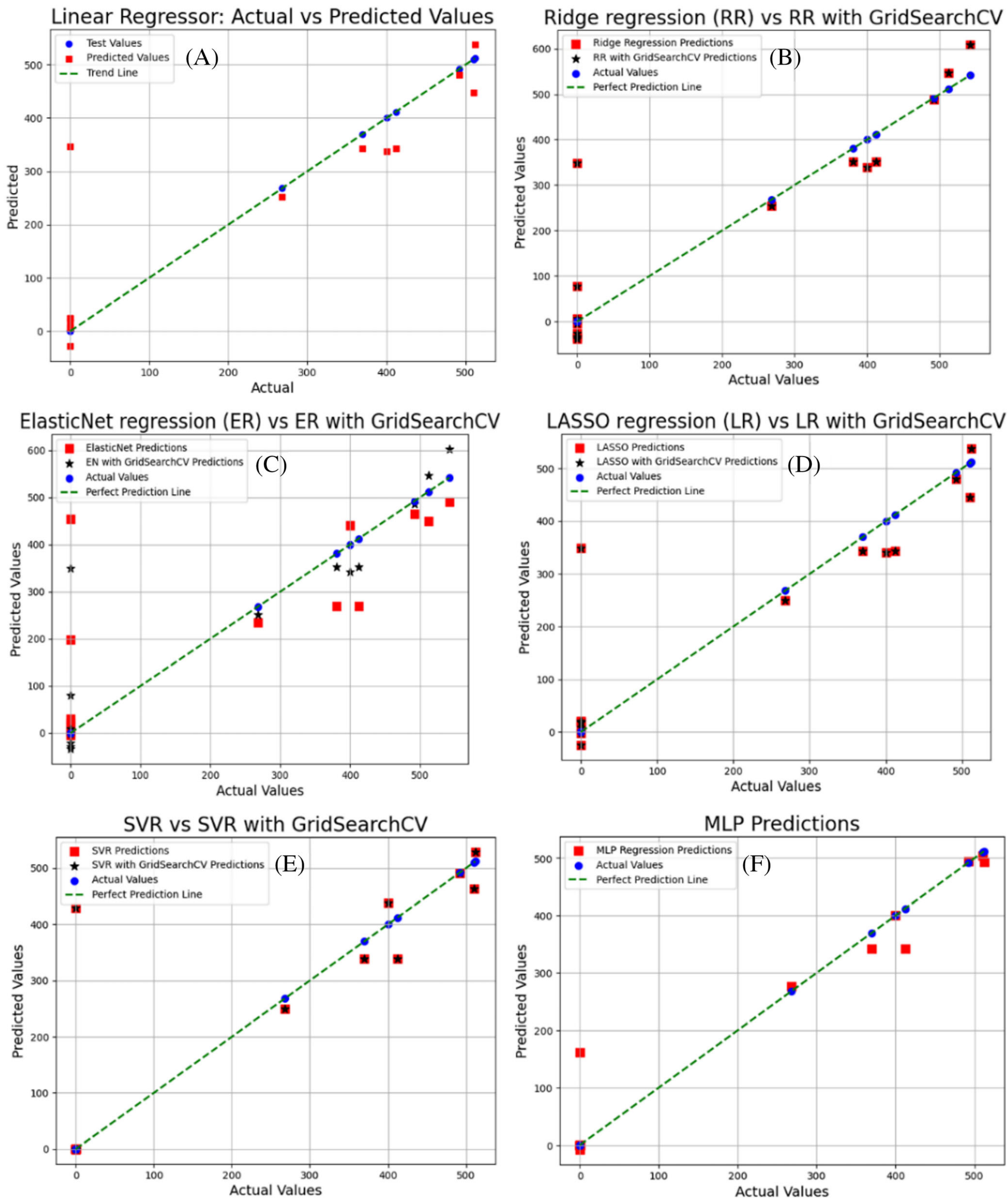

FIGURE 9 Actual versus prediction of the models (A) LR, (B) RR versus RR with gridsearch, (C) ER versus ER with Gridsearch, (D) LASSO versus LASSO with gridsearch, (E) SVR versus SVR with gridsearch, (F) MLP, (G) DT versus DT with gridsearch, (H) GBR versus GBR with gridsearch, (I) RFR versus RFR with gridsearch, (J) ADA Boost versus ADA Boost with gridsearch.

was particularly challenging for most models, especially at low magnitudes, which correspond to conditions involving a very high number of fatigue cycles. Notably, only the boosted ElasticNet Regression (ER) and the ANN-based Multi-Layer Perceptron (MLP) models successfully achieved high accuracy in these scenarios.

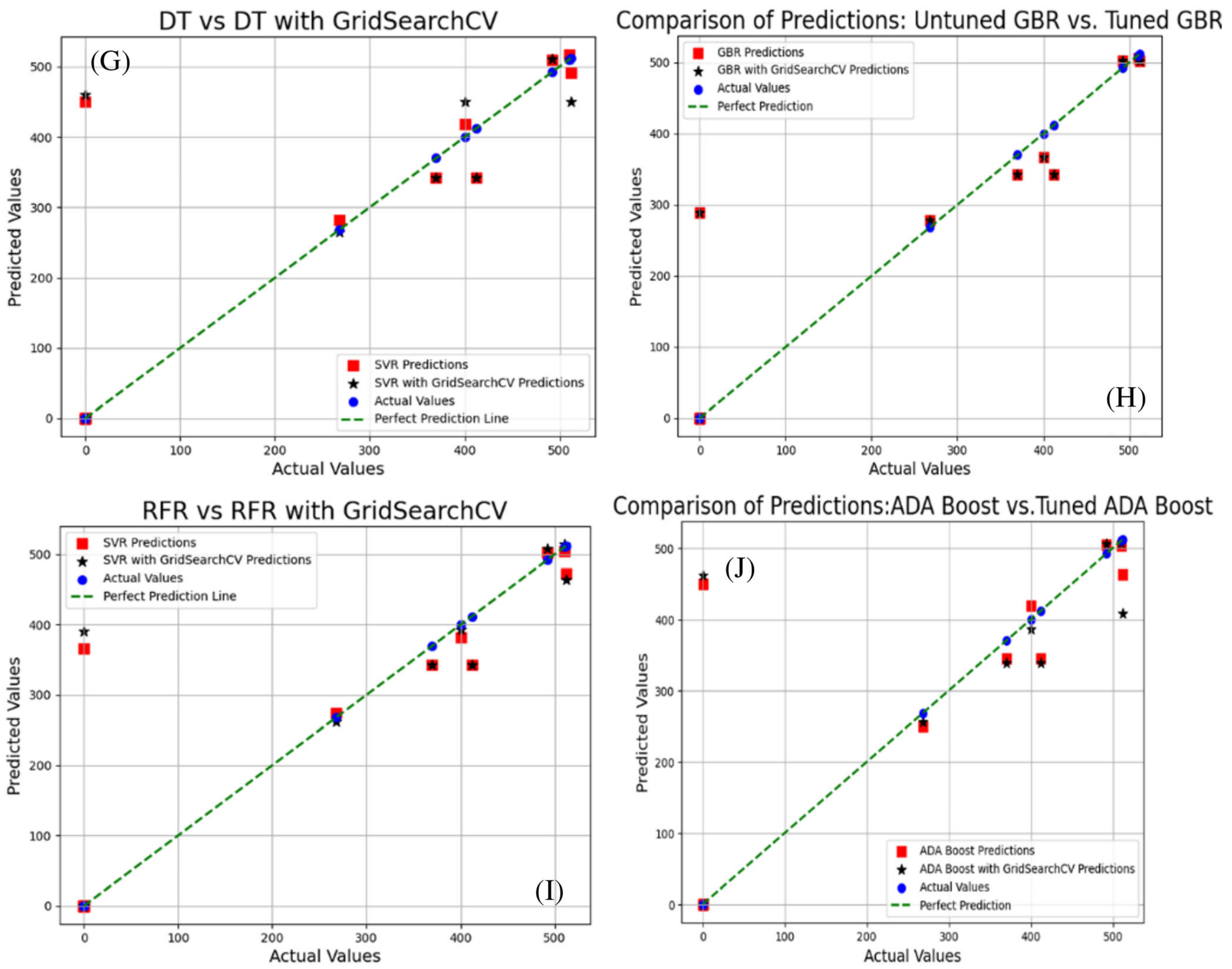

FIGURE 9 (Continued)

4 | CONCLUSIONS

This work uses the concept of materials informatics combined with the machine learning method to predict the residual strength of FRPs subjected to fatigue. A total of 18 ML models that included pristine and GridSearchCV modified LR, RR, ER, LASSO, SVR, MLP, DT, GBR, RFR and ADA Boost models were trained using 10 features on 968 data points, which is unique and never been reported. The training-validation and testing data were compiled from the literatures that performed manufacturing and experimentation under variable conditions and hence, the presence of outliers was ubiquitous. Such data also required normalization for effective training.

Fatigue behavior of FRP composites is controlled by a number of variables arising from materials and manufacturing, testing and/or mechanical properties aspects and hence effective training features must contain data from these attributes. This work included reinforcement material, nature of reinforcement, stacking type, number of plies from materials attribute, ultimate tensile strength (MPa), stress amplitude (MPa), stress ratio (R), test frequency (Hz), endured fatigue cycles (N), normalized fatigue life (N/N_f) from properties and testing aspects to predict the residual strength (MPa) as target feature. Fiber volume fractions and void fractions as training features could be used for training, but data unavailability eliminated these attributes as training features. The dependency matrix established strong positive relationship between the stress amplitudes & the UTS and number of plies and stacking sequence, which is always the case; while a negative dependency was found between the material and nature of reinforcement & test frequency, indicating the parameters do not affect the selection of the test frequency.

Linear Regression (LR), Ridge Regression (RR), and LASSO demonstrated consistent performance, achieving

R^2 values in the range of 0.79–0.80 on both validation and test datasets. The models showed relatively low error metrics, with MAE and RMSE values reflecting their ability to generalize well across datasets. For example, the tuned Ridge Regression (RR_GS) achieved an R^2 of 0.80 and RMSE of 97.49 on the test set. ElasticNet Regression (ER), however, initially exhibited weaker performance with an R^2 of 0.59 on the validation set. Fine-tuning using GridSearchCV significantly enhanced its performance, resulting in an R^2 of 0.80 on the test set, comparable to other regression models. A notable limitation across these models was their tendency to predict negative residual strengths, which is physically unrealistic. Tree-based models, such as Decision Tree (DT) and its tuned variant (DT_GS), exhibited moderate performance, with R^2 values ranging from 0.65–0.69 and relatively high RMSE values exceeding 120 on both validation and test datasets. Ensemble methods provided a marked improvement in predictive accuracy. For instance, Gradient Boosting Regressor with tuned Decision Trees (GBR_DT) achieved the highest R^2 of 0.87 and the lowest RMSE of 80.18 on the test dataset, showcasing its robustness and ability to capture complex patterns. Random Forest Regressor (RFR) and its tuned variant (RFR_GS) also performed well, achieving R^2 values of 0.79 and 0.76, respectively, on the test dataset, with RMSE values slightly exceeding 100. AdaBoost (ADAB), however, demonstrated lower predictive accuracy, with R^2 values ranging from 0.65–0.69 and higher error metrics, indicating its limitations in generalizing across the dataset.

Support Vector Regression (SVR) displayed the weakest baseline performance, with an R^2 of 0.0 on the validation set and $-$ 0.18 on the test set, along with the highest MAE and RMSE values (e.g., 210.5 and 238.45, respectively). Hyperparameter tuning significantly improved the model's performance, boosting the R^2 to 0.71 and reducing RMSE to 118.22 on the test set. Despite these improvements, SVR remained inferior to most other models in all performance metrics. The Multi-Layer Perceptron (MLP) model consistently outperformed all other models. On the validation set, MLP achieved the highest R^2 of 0.88 and the lowest RMSE of 72.42. After tuning, its performance on the test set further improved, with an R^2 of 0.95 and an RMSE of 47.81. These results highlight the MLP model's superior capability to capture non-linear and complex relationships in the dataset. However, a significant limitation was its occasional prediction of negative residual strengths, which, like other models, contradicts physical feasibility.

The results underscore the strength of ensemble methods, particularly GBR_DT, and neural network-based approaches like MLP in handling complex datasets with non-linear relationships. While regression models, such as LR, RR, and LASSO offer reliable performance with low computational complexity, their limitations in capturing complex patterns and predicting physically feasible values highlight the importance of model selection based on problem specifics. Tree-based methods and SVR exhibited moderate to weak performance, with the latter showing substantial improvement post-optimization. Among all models, MLP stands out as the most robust, achieving the best metrics. MLP model with two hidden layers containing 30 and 20 neurons (10-30-20-1), regularization of 0.0001, relu as activation function, constant learning rate, Adam optimizer and admin solver presented the best fit of 0.95 on the test data; while boosted GBR with the params of 'learning_rate': 0.1, 'max_depth': 7, 'n_estimators': 200, 'subsample': 0.8 offered the second-best fit of 0.87 on the test data; but on the expense of greater computational time. Overall, this study highlights the potential of machine learning in advancing materials informatics, providing valuable insights for predicting the properties of FRPs under fatigue.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are openly available in GitHub at https://github.com/Dewa1989/Residual-Fatigue-Strength/tree/main.

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