

Tree-Based Machine Learning Approach for Predicting the Impact Behavior of Carbon/Flax Bio-Hybrid Fiber-Reinforced Polymer Composite Laminates [†]

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Abstract: In this research, the effect of change in stacking sequences on the impact performance of bio-hybrid fiber-reinforced polymer (bio-HFRP) composite materials was analyzed and evaluated. The methodology was developed, based on the mechanical testing and utilization of tree-based machine learning regression models. Low-velocity impact (LVI) testing was performed on five distinct stacking sequences of carbon/flax bio-HFRP at energies ranging from 15 J to 90 J. For all tests, peak impact force was recorded and compared. Symmetric configurations with a uniform distribution of flax layers across the composite laminate exhibited better impact performance. Additionally, two tree-based machine learning (ML) algorithms were used: random forest (RF) and decision tree (DT). The performance metrics used to assess and compare the efficiency were the coefficient of determination (R^2), mean square error (MSE), and mean absolute error (MAE). The most accurate model for the prediction of peak impact force was DT with the R^2 training and test dataset values of 0.9920 and 0.9045, respectively. Furthermore, lower MSE and MAE values were attained using the DT model as compared to the RF model. The developed methodology and the model serve as powerful tools to predict the damage-induced properties of bio-HFRP composite laminates utilizing minimal resources and saving time as well.

Keywords: bio-hybrid composites; impact behavior; machine learning; decision tree; random forest



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1. Introduction

Hybrid fiber-reinforced polymer (HFRP) composite materials have gathered significance in recent times for use in the defense and automotive aerospace sectors as a result of their increased strength/weight ratio and enhanced resistance to impact [1]. Research studies conducted over the last years have confirmed that HFRP composites offer superior structural performance than other traditional materials. In these multi-layered composites, fiber hybridization and changes in stacking sequences offer adaptability in terms of superior stiffness, strength, and impact damage resistance [2]. The optimization of fiber hybridization and stacking sequence in HFRP composites results in the development of composites with enhanced impact damage resistance. Furthermore, the traditional HFRP relies on synthetic reinforcements, such as carbon, glass, and Kevlar, due to ease in availability [3]. Nevertheless, the widespread use of these synthetic fibers prompts concerns

about the rapid depletion of the earth's natural resources, the potential for pollution of the environment, and the problems with recycling [4]. In light of this, demand for green composites made of environmentally benign sustainable natural fibers like flax, hemp, and jute has increased dramatically. Therefore, the hybridization of synthetic fibers with natural fibers contributes to developing eco-friendly composite materials, referred to as bio-hybrid composite materials [5].

The effect of fiber hybridization and change in stacking sequences have been widely investigated in bio-hybrid composite materials for use in different applications. However, the development of such bio-hybrid composite materials and their experimental testing includes extensive experimentation and significant time investment along with substantial economic resources. As a result, in recent decades, the usage of alternative techniques like finite element analysis (FEA) to model various mechanical and impact tests has increased [6]. However, despite their benefits, FEA techniques may fall short of physical testing in terms of accuracy and dependability because of model simplifications and assumptions. Therefore, techniques based on ML offer alternate methods for the estimation of the performance of composite materials subjected to various types of static and dynamic loadings [7]. Depending on the nature and intricacy of the dataset, ML-based algorithms can use various types of strategies, which include regression and classification. These ML-based algorithms can be applied to forecast the electrical, mechanical, tribological, thermal, and acoustic properties of different types of HFRP composites. Recently, tree-based machine learning models have gained considerable attention for the design and optimization of composite laminates [8]. For example, Wang et al. [9] compared the efficiency of the artificial neural network (ANN) based algorithm and DT ML algorithm to predict the projectile penetration in aramid/carbon HFRP laminates. It was concluded that the DT model exhibited better accuracy for the prediction of the training dataset; however, ANN showed better generalization capabilities for the test dataset. Similarly, Machello et al. [10] used tree-based ML approaches, i.e., DT and RF for forecasting the tensile strength of FRP composites. The findings concluded that the most accurate model is the DT model with a test R^2 value of 0.88. In another study [11], damage characteristics of FRP composite impact loading were predicted using different machine learning models, and the highest R^2 value of 0.8693 was attained for the test dataset. The above-mentioned research demonstrates the effectiveness of different ML-based algorithms to forecast the performance of the bio-HFRP composite laminates under impact loading.

In this study, a novel method combining experimental work and prediction using a machine learning model was used to investigate the effect of change in stacking configuration and change in impact energies on the mechanical behavior of carbon/flax bio-HFRP composite laminates. The design variables were the stacking sequence and the impact energy, whereas the output variable was the peak impact force. Following the detailed experimentation, the gathered dataset was used as an input for the DT- and RF-based machine learning models. The outcome of the fiber hybridization and the change in stacking sequence on the LVI behavior of carbon/flax composite Bio-HFRP composite laminates as a function of peak impact force was investigated.

2. Materials and Methods

2.1. Experimental Methods

2.1.1. Materials

In this research, the bio-HFRP composite laminates were fabricated using carbon and flax fabrics. Both fabrics have an areal weight of 200 g/m² and are woven in a 2 × 2 twill arrangement. Carbon fabric was obtained from TEi Composites Ltd., Chang Hua, Taiwan, with a tensile modulus of 230 GPa, tensile strength of 3750 MPa, and failure strain of 1.8% in the warp and weft direction. The flax fabric was obtained from Easy Composites Ltd., Stoke-on-Trent, United Kingdom, with a tensile modulus of 6 GPa and 7 GPa in the weft and warp direction, respectively, a tensile strength of 58 MPa and 61 MPa in the warp and weft direction, respectively, and a failure strain of 1.8% and 1.5% in the warp and weft

direction, respectively. Furthermore, laminating epoxy supplied by RIAERO Ltd. and formulated amine hardener was used as a resin system with a weight ratio of 2:1 to fabricate the bio-HFRP composite laminates. The laminating epoxy has a tensile modulus of 3.5 GPa, tensile strength of 75 MPa, and a failure strain of 6% [12]. To ascertain the impact of varying stacking configurations on the mechanical behavior of bio-HFRP composite laminates, a series of five distinct sequences, each including fifteen layers, were carefully designed and manufactured by the vacuum bagging process to guarantee optimal quality [2,12]. The details of the bio-HFRP composite laminate stacking configurations are listed in Table 1.

Table 1. Investigated stacking configurations of bio-HFRP composite laminates.

Specimen Type	Laminate Code	Resulting Layup
Sandwich	S	[C/C/C/C/C/C/F/F/F/C/C/C/C/C/C]
Asymmetric	A-CFa	[C/F/F/F/C/C/C/C/C/C/C/C/C/C/C]
	A-CFb	[C/C/C/C/C/C/C/C/C/C/C/F/F/F/C]
Symmetric	SUa	[C/F/C/C/C/C/C/F/C/C/C/C/C/F/C]
	SUb	[C/C/F/F/C/C/F/F/F/C/C/F/F/CC]

C: Carbon fiber; F: Flax fiber.

2.1.2. Drop Weight Impact Test

As per the ASTM standard D7136 [13], the impact damage resistance of the five different bio-HFRP composite stacking configurations was examined and assessed with the help of a drop-weight impact tower (BESMAK materials testing equipment, Kazan, Turkey). The impactor used for the LVI was the cylindrical impactor, with a 16 mm diameter and hemispherical nose. In order to record the impact force produced at the surface of the Bio-HFRP composite laminate, the impactor was fitted with a load sensor [12]. The impactor weighed 9.67 kg in total along with the carriage. From the manufactured panels, a flat specimen measuring 100 mm by 150 mm was cut. The impactor's release height was adjusted to alter the impact energy in each test. In this research, the LVI tests were executed at six energy levels ranging from 15 J to 90 J. To ensure the consistency of the performed tests, three repeats were performed for each stacking configuration at each energy level. After the LVI, the peak impact force was recorded using the inbuilt data acquisition system.

2.2. Tree-Based ML Models

2.2.1. Decision Tree (DT)

Popular machine-learning models called decision trees are widely employed in problems involving regression and classification. By dividing data into values, DTs anticipate continuous targets for regression problems. A regression-based DT has the same architecture as a regular DT with each internal node representing a feature, and each branch represents a possible value for that particular feature [7]. Furthermore, hyperparameters also aid in controlling the model's complexity and preventing overfitting. The maximum depth of the tree, minimum samples for node splitting, minimum samples per terminal node, maximum leaf nodes, and splitter are a few of the important hyperparameters that were employed in this investigation [7].

2.2.2. Random Forest (RF)

The RF is a popular ensemble regression approach that blends the flexibility and interpretability of DT with the capacity to integrate numerous models. Employing "parallel ensembling" creates many unique DTs with different training datasets and random features. Every tree undergoes independent training, generating a set of rules that enable it to segment the data based on particular attributes and generate predictions. Depending on whether the problem is one of regression or classification, the final solution is determined by either majority voting or averaging the predictions made by each tree. Random forests increase accuracy and generalizability while decreasing bias and volatility by mixing numerous decision trees. The number of estimators, minimum samples for node splitting,

maximum tree depth, bootstrap technique, and maximum features are the algorithm's primary hyperparameters.

Furthermore, accurately calibrating the model's hyperparameters is essential for achieving optimal performance in DT and RF models. Methods like GridSearchCV and RandomizedSearchCV are utilized for this. These techniques essentially search the hyperparameter space for the optimal set of parameters to maximize the model's efficacy. Moreover, these techniques establish a range of potential values for each hyperparameter that has ever been studied, forming a structure akin to a grid. GridSearchCV carries out comprehensive cross-validation to identify the configuration that performs the best. Conversely, RandomizedSearchCV uses a random sample to evaluate the performance of a subset of options.

In this study, the input dataset fed to train the machine learning models comprises the stacking configuration of composite laminates consisting of fifteen layers and the impact energy. For machine learning models, the stacking sequence is converted from the categorical form of data to the numerical form of data. For this purpose, the carbon layer was assigned 1 as a binary code, and the flax layer was assigned 0 as a binary code. Therefore, due to fifteen layers in a stacking sequence, fifteen input variables were created. Moreover, the impact energy was assigned as the sixteenth input variable. On the other hand, the investigated output variable was the peak impact force. Furthermore, the Python 3.11.7 programming language and the Scikit-learn 1.2.2 module were used to implement both DT and RF.

Furthermore, three performance criteria, namely R^2 , MSE, and MAE, were employed in this work to assess how effectively various machine learning models predicted the peak impact force of bio-HFRP composite laminates. These metrics were employed to evaluate the ML-based regression algorithms' generalization, accuracy, and precision capabilities.

3. Results and Discussion

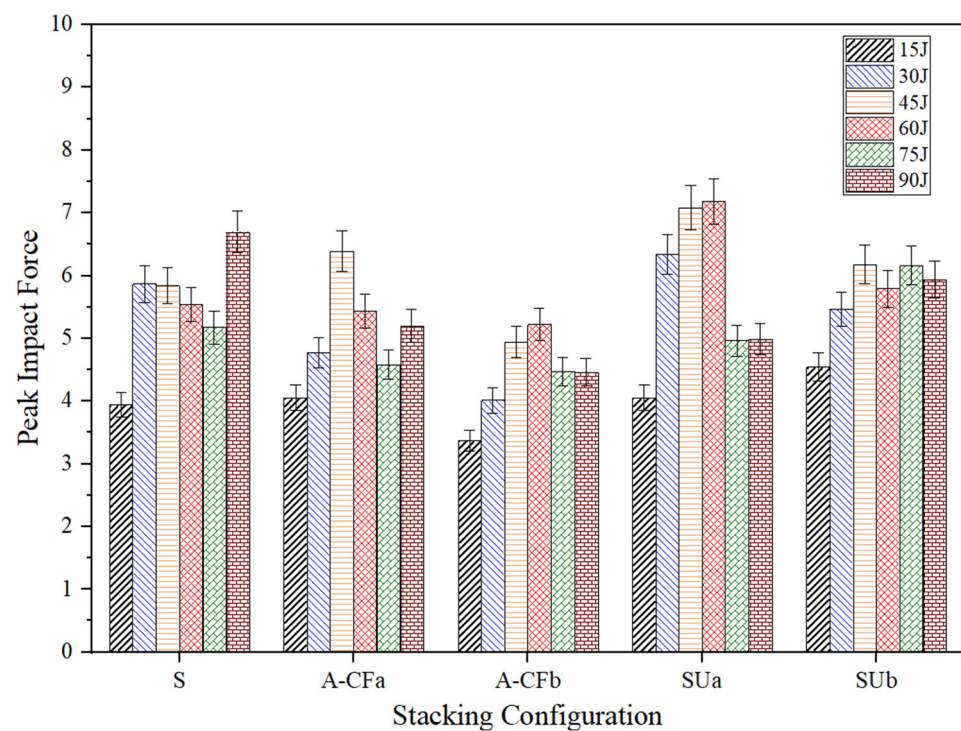
3.1. LVI Experimental Results

During the LVI process, there are three primary stages, i.e., contact, deformation, and rebound/perforation. When the impactor is released from the height, its kinetic energy is transformed into the elastic energy of the specimen. The contact force increases until it hits the maximum value, known as the peak impact force, as a result of this energy conservation from kinetic energy to elastic energy. The composite laminate with the highest peak impact force has a superior ability to withstand damage since it can absorb more energy before failing. Table 2 presents the experimentation results on the peak impact force of five different bio-HFRP composite laminates that were subjected to impact at energies of 15 J, 30 J, 45 J, 60 J, 75 J, and 90 J.

Additionally, for all impact energies, Figure 1 compares the peak impact force of five different bio-HFRP composite laminates. The comparison shows that, at the impact energy of 15 J, the symmetric configuration SUB with a carbon-to-flax ratio of 1.14 showed the highest peak impact force as compared to other stacking sequences. However, the other symmetric configuration SUa with a carbon-to-flax ratio of four performed better than the other stacking configurations in terms of peak impact force for impact energies of 30 J, 45 J, and 60 J. For the impact energies of 75 J, SUB exhibited better impact resistance as compared to the other stacking sequences. Furthermore, for the impact energy of 90 J, the sandwich stacking sequence S showed a better impact performance. This indicates that the homogeneous distribution of natural flax layers raises the material's ability to endure deformation resulting from impact events by increasing the peak force. However, for all impact energies, the asymmetric stacking sequence A-CFb displayed the lowest peak force. This suggests that the LVI performance in terms of the composite laminates in terms of impact strength is greatly reduced when three consecutive natural flax layers are present in the tensile region of the laminates.

Table 2. Experimental results for the LVI of bio-HFRP composite laminates.

Impact Energy (J)	Laminate Code	Peak Impact Force (kN)	Impact Energy (J)	Laminate Code	Peak Impact Force (kN)
15 J	S	3.94	30 J	S	5.87
	A-CFa	4.05		A-CFa	4.77
	A-CFb	3.37		A-CFb	4.01
	SUa	4.05		SUa	6.34
	SUb	4.54		SUb	5.46
45 J	S	5.84	60 J	S	5.54
	A-CFa	6.39		A-CFa	5.43
	A-CFb	4.94		A-CFb	5.22
	SUa	7.08		SUa	7.18
	SUb	6.18		SUb	5.79
75 J	S	5.17	90 J	S	6.7
	A-CFa	4.58		A-CFa	5.2
	A-CFb	4.47		A-CFb	4.46
	SUa	4.96		SUa	4.99
	SUb	6.16		SUb	5.94

**Figure 1.** Comparison of the peak impact force of carbon/flax bio-HFRP composite laminates.

3.2. Prediction of Peak Impact Force Using Tree-Based ML Models

In this study, two tree-based ML algorithms, namely DT and RF, were applied to the available dataset in order to forecast the mechanical properties of carbon/flax bio-HFRP composite laminates. For the ML models, 80% of the dataset was allocated for training and 20% was allocated for testing. Furthermore, tuning and optimizing the hyperparameters for all the ML models is a crucial step during the training stage. The key hyperparameters have been tuned and optimized for both regression models utilized in this investigation. Performance data from the prediction models were used to determine the best combination of hyperparameters. This section will present the coefficient of determination R^2 , for each of the machine learning models, to determine which combination of hyperparameters will yield the highest accuracy for each model.

3.2.1. DT

In this study, the efficiency of a DT regression model was evaluated using utilizing both GridSearchCV and RandomizedSearchCV. However, before implementing DT, it is imperative to define the ranges for different key hyperparameters. The ranges of common hyperparameters used for the GridSearchCV and RandomizedSearchCV techniques [7] in the DT regression model are given in Table 3.

Table 3. Hyperparameter ranges for tuning of the DT regression model.

Hyperparameters	Ranges
Maximum depth of tree	0–81
Minimum samples for node splitting	1–5
Maximum leaf nodes	1–61
Minimum samples per terminal node	1–50
Maximum features	1–60

Additionally, Table 4 displays the outcomes of the DT regression model with both search strategies applied. The accuracy of both techniques was assessed in terms of the training dataset and test dataset R^2 values. To find the optimal combination of hyperparameters given in Table 3, optimization was performed by exploring the different combinations of hyperparameters. For the GridSearchCV, it was found that the maximum depth of the tree and the maximum number of leaf nodes are the critical factors and have the strongest effect on the performance of the model. For optimization, the minimum samples for node splitting, the minimum samples per terminal node, and the maximum features were fixed at 2, 1, and 11, respectively. The results in Table 4 show that the increase in the maximum depth of the tree improved the DT regression model's performance in terms of R^2 values for the training and test datasets. With R^2 values of 0.9920 and 0.9045, respectively, for both training and test data, the GridSearchCV approach performed best at a maximum depth of 8 and a maximum number of leaf nodes of 28 when using a random splitter. Comparably, using the RandomizedSearchCV method, the model's performance was enhanced for both the training and test datasets when the maximum depth of the tree was increased. At a maximum lead node count of 34 and a maximum tree depth of 8, the optimal performance was attained. These findings imply that the optimal hyperparameter combinations employ GridSearchCV and RandomizedSearchCV, along with a maximum tree depth of 8, emphasizing the benefit of the model's use of a deep tree structure to detect the underlying patterns in the data and prevent overfitting.

Table 4. Training and test dataset R^2 scores for various hyperparameters and search approaches in regression DT for predicting peak impact force.

Search Approaches	Splitter	Maximum Depth of Tree	Maximum Leaf Nodes	R^2 Train	R^2 Test
GridSearchCV	Random	5	18	0.8999	0.7721
	Random	6	26	0.9835	0.8967
	Random	7	28	0.9894	0.9020
	Random	8	28	0.9920	0.9045
RandomizedSearchCV	Best	5	19	0.9387	0.6897
	Random	6	47	0.9835	0.8967
	Random	7	45	0.9894	0.9020
	Random	8	34	0.9920	0.9045

3.2.2. RF

In order to forecast peak impact force, the effectiveness of an RF-based regression model that made use of both the GridSearchCV and RandomizedSearchCV search approaches was evaluated in this section. Prior to employing these search methods, it was

important to establish the ranges for the key hyperparameters of the RF regression model. The ranges of key hyperparameters used for the tuning of the RF regression model [7] are given in Table 5.

Table 5. Hyperparameter ranges for tuning of DT regression model.

Hyperparameters	Ranges
Number of estimators	1–200
Maximum depth of tree	1–200
Minimum samples for node splitting	2
Maximum features	1–16

The results of the RF model showing the training and test dataset R^2 values utilizing the GridSearchCV and RandomizedSearchCV are given in Table 6. For both search strategies, the outcome of changing the maximum depth of the tree and the number of estimators on the R^2 train and test dataset values was observed. For the GridSearchCV search method, it was noted that, as the number of estimators varied from 200 to 25, the maximum depth of the tree decreased from 9 to 8 and then remained constant. This decrease in the number of estimators from 200 to 25 resulted in an improvement in R^2 test values from 0.6859 to 0.7309, while the R^2 training dataset values remained constant at 0.9920, showing a strong fit on the training test data. Furthermore, the results showed that the reduction in the number of estimators may help in mitigating the overfitting, therefore, improving the performance and generalization. Furthermore, the consistent maximum depth of the tree value of eight suggested that this depth was sufficient for capturing the data complexity without affecting the accuracy of the model. However, for RandomizedSearchCV, the tree's maximum depth increased progressively from 22 to 68 when the number of estimators varied from 200 to 25. However, the trend for the change in training and test dataset R^2 values remained the same as in GridSearchCV with a peak R^2 test dataset value of 0.7309 attained at 25 estimators. Overall, the comparison of GridSearchCV and RandomizedSearchCV search techniques in the RF regression model exhibited the same trend. The results also concluded that the reduction in the number of estimators improved the model's performance for the test dataset.

Table 6. Training and test dataset R^2 scores for various hyperparameters and search approaches in regression RF for predicting peak impact force.

Search Approaches	Number of Estimators	Maximum Depth of Tree	R^2 Train	R^2 Test
GridSearchCV	200	9	0.9920	0.6859
	100	8	0.9920	0.6879
	50	8	0.9920	0.7003
	25	8	0.9920	0.7309
RandomizedSearchCV	200	22	0.9920	0.6859
	100	39	0.9920	0.6879
	50	50	0.9920	0.7003
	25	68	0.9920	0.7309

3.3. Error Assessment of the Tree-Based ML Models

In this section, the comparison of performance metrics in terms of R^2 , MSE, and MAE for both training and test datasets was carried out to choose the effective prediction model from the DT and RF models (Table 7). The comparison of R^2 values showed that the most effective model was the DT model with R^2 training and test dataset values of 0.9920 and 0.9045, respectively. Similarly, for the MSE and MAE comparison, a model with lower values was considered to perform better due to small average prediction errors. Table 7 concluded that the DT model showed lower values for the MAE test (0.1977) and MSE test (0.11031), respectively.

Table 7. Comparison of performance metrics.

Performance Metrics	DT	RF
R ² training	0.9920	0.9920
R ² test	0.9045	0.7309
MSE training	0.0069	0.0069
MSE Test	0.1031	0.2906
MAE training	0.0155	0.0155
MAE test	0.1977	0.3319

4. Conclusions

The LVI performance of the carbon/flax bio-HFRP composite laminates is strongly influenced by the change in stacking configurations. However, the process of design, development, and optimization of such bio-HFRP composite laminates requires a significant number of financial resources as well as substantial experimentation. Therefore, in this study, a methodology incorporating experimental testing and prediction using tree-based machine learning models was utilized. Five distinct bio-HFRP composite laminates were subjected to LVI with energies ranging from 15 J to 90 J. The comparison of peak impact force for all stacking configurations revealed that symmetric configuration SUa has a carbon-to-flax ratio of 4 and an even dispersion of flax layers across the laminate thickness, exhibiting better impact performance at 30 J, 45 J, and 60 J. However, at 15 J and 75 J, the other symmetric configuration SUB with eight flax layers exhibited the highest impact resistance, and at the impact energy of 90 J, the sandwich configuration S outperformed other composite laminates. Furthermore, the effectiveness of the tree-based machine learning regression models, namely DT and RF, to forecast the peak impact force, was evaluated. The tuning of key hyperparameters was also performed for both DT and RF. Regarding the peak impact force, it was concluded that the best-performing algorithm is DT with training and test dataset R² values of 0.9920 and 0.9045, respectively. Moreover, the relatively lower values of MSE and MAE for the DT model as compared to the RF model also confirm the better performance ability of the DT model. In conclusion, the tree-based ML models' outcomes confirmed that the algorithm could accurately forecast the peak impact force. Numerous significant benefits of this approach include a significant reduction in the quantity of laboratory testing as well as an improvement in the time and cost of procuring materials and conducting recurrent physical testing.

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