

ML-Based Predictive Modeling of Mechanical Properties in 3D-Printed Polymer Composites for IoT Applications

Nagaraj G¹, Dillip Kumar Mohanta², Rajvardhan Jigyasu^{3,*}, P. Vidyullatha⁴, Joshila Grace L K⁵, Muthukumar Subramanian⁶

Abstract

This study aims to develop an interpretable and high-accuracy machine learning framework for predicting the mechanical properties of 3D-printed fiber-reinforced polymer composites, with a focus on structure–property correlations relevant to polymer processing and functional performance. Composite specimens based on PLA and ABS matrices were fabricated using FDM with varying weight fractions (5–20 wt%) of carbon and glass fibers. Standardized mechanical testing (ASTM D638, D256, D790) was performed to evaluate tensile strength, elastic modulus, and impact resistance across 324 printed samples. A structured dataset comprising 12 input features including material and processing parameters was used to train XGBoost, SVR, and Random Forest regression models. Recursive feature elimination and SHAP-based explain ability were integrated to ensure dimensional relevance and interpretability. XGBoost outperformed all baseline models, achieving an R^2 of 0.94 and RMSE below 2.1 MPa. SHAP analysis identified filler wt%, nozzle temperature, and infill density as the most influential parameters. Visualizations such as 3D correlation plots and formulation-specific prediction collages validated prediction accuracy and exposed localized error patterns in high-filler composites. This work uniquely integrates real mechanical data, SHAP explain ability, and multiscale visualization into a predictive framework, offering physically grounded, design-relevant insights for polymer composite development an advancement over existing black-box approaches. The proposed framework establishes a reproducible, transparent methodology for data-driven prediction of polymer composite behavior, enabling intelligent design optimization in reinforced thermoplastics and opening avenues for future adaptive modeling.

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INTRODUCTION

The convergence of additive manufacturing (AM) technologies with the Internet of Things (IoT) has opened up novel avenues for producing customizable, lightweight, and structurally optimized components tailored for smart devices. Among the various AM techniques, fused deposition modeling (FDM) has gained widespread popularity due to its ease of use, economy, and versatility of application to accommodate an enormous range of polymeric materials. For IoT applications, where design ability and mechanical integrity are factors of concern, the requirement for

3D-printed polymer composites acquire a specific significance [1]. These components, typically supported by fibers or particulates, exhibit enhanced mechanical properties required for enclosures, sensor covers, structural frames, and other functional elements of integrated systems. Operation of such components is incredibly sensitive to a multi-dimensional interaction of variables like material formulation, infill density, layer orientation, printing temperature, and post-processing conditions [2]. Traditional methods for determining mechanical properties largely rely on standards testing such as ASTM D638 or ISO 527 [3]. Though accurate, the methods are resource intensive, time consuming, and not feasible for rapid design iteration and mass personalization in IoT-based applications [4]. Machine learning (ML) also offers an acceptable substitute through predictive modeling utilizing past data and thus allowing engineers to provide estimates of mechanical properties without the need for extensive testing. It has been evident in prior studies that ML algorithms like support vector regression, decision trees, and neural networks can identify complex nonlinear relationships in material science [5]. Most of such work is, however, limited to controlled data sets, non-transferable to material systems, and not explainable for predictions by models—industrial uptake prerequisites [6]. There has been some work in the past decade in the application of machine learning techniques in making prediction of mechanical properties of 3D-printed materials but with limited scope. For instance, researchers have employed support vector regression and artificial neural networks to estimate tensile strength and modulus for neat PLA and ABS samples under controlled conditions, achieving prediction accuracies ranging between $R^2 = 0.82$ and 0.90 . Another notable study used decision trees to correlate printing temperature and infill density with flexural properties of short carbon-fiber-reinforced PLA, reporting an RMSE of 3.5 MPa. While these efforts highlight the promise of ML in digital fabrication, they predominantly focus on single-material systems, small datasets, or fixed geometrical configurations [7]. Moreover, most models remain "black boxes" with little to no insight into how specific features influence the output, limiting their acceptance in industrial environments where explainability is crucial [8]. This work addresses the shortcomings of previous studies by building a scalable, explainable, and high-fidelity predictive framework that not only supports heterogeneous material systems—including reinforced composites but also aligns with IoT-centric design needs. We chose this approach to bridge the gap between lab-scale ML experimentation and real-world smart product development, where materials must be rapidly tested, validated, and deployed without compromising performance. Our model introduces both data diversity and interpretability into the pipeline, enabling users to make confident design decisions based on both predictions and their rationale. This is a significant departure from earlier works that emphasized accuracy alone without validating generalizability or transparency two critical factors for deployment in smart, connected manufacturing ecosystems.

The novelty of this work lies in the development of a comprehensive ML-based predictive framework tailored specifically for mechanical property estimation of 3D-printed polymer composites intended for IoT applications. Unlike existing approaches that focus on single-material systems or static parameter configurations, our framework integrates real-world experimental data from a variety of composite formulations (including PLA, ABS, and carbon/glass-fiber reinforcements), diverse print settings, and multiple mechanical test results. Additionally, we incorporate SHAP (SHapley Additive exPlanations) values to provide interpretable insights into feature contributions, thereby enhancing model transparency and user trust. This is the first known study that not only predicts key mechanical metrics such as tensile strength, Young's modulus, and impact resistance with high accuracy ($R^2 > 0.95$) but also correlates those predictions with specific fabrication parameters and material compositions in the context of IoT-relevant constraints. Moreover, the research contributes a validated, modular workflow that includes preprocessing (feature normalization and recursive elimination), algorithm benchmarking (Random Forest, XGBoost, SVR), and real-time prediction integration. By enabling rapid material-property prediction during the design phase, this study significantly reduces the experimental overhead and accelerates the prototyping cycle for IoT hardware developers. The approach presented is scalable, data-driven, and designed with deployment in mind, making it well-suited for intelligent manufacturing pipelines. The rest of the paper is organized as follows: Section 2 outlines the literature landscape and identifies research gaps; Section 3 discusses the materials, composite preparation, and mechanical testing; Section 4 details the experimental setup and data generation; Section 5 presents the ML

modeling framework and algorithms used; Section 6 elaborates on the predictive results and comparative evaluations; Section 7 offers in-depth discussion; and Section 8 concludes with key findings and future work.

LITERATURE REVIEW

The mechanical characterization of 3D-printed polymer composites has garnered considerable attention in recent years due to its pivotal role in determining the structural viability of components used in IoT-enabled systems. The wide adoption of fused deposition modeling (FDM) has allowed for rapid prototyping and customization of polymer-based parts, but the inherent anisotropy and variability introduced during the layer-by-layer manufacturing process have made it difficult to consistently predict performance metrics such as tensile strength, flexural strength, and impact resistance [9]. The incorporation of reinforcement materials like carbon fibers, glass fibers, and nano-fillers into base polymers has further complicated the relationship between processing parameters and mechanical behavior [10]. While many studies have been conducted to understand these relationships experimentally, there is an increasing shift towards integrating machine learning (ML) to model and predict mechanical responses based on input variables such as infill density, print speed, extrusion temperature, layer height, and material composition [11]. Most existing studies in this domain have utilized relatively small, idealized datasets that focus on a single polymer type, most commonly PLA or ABS. These studies often restrict their experimental matrix to a narrow range of print parameters and do not account for the variation introduced by different reinforcement types or geometrical complexities [12]. As a result, while the predictive models developed using these datasets may show high internal accuracy, they fail to generalize when applied to other material systems or varying processing conditions. This restricts their applicability in real-world IoT environments, where a wide variety of material blends are often used to meet mechanical, thermal, or environmental requirements [13]. The predictive capability of ML models can be significantly enhanced through the use of diverse, heterogeneous datasets encompassing multiple composite types and fabrication conditions. This requires systematic data acquisition and standardization across different experimental batches. The vast majority of previous research has focused on standardized testing geometries such as dog-bone tensile specimens or simple cuboidal samples [14]. While these are suitable for benchmarking, they do not capture the intricacies of real-world IoT device structures, which often feature thin walls, internal cavities, curved surfaces, or embedded electronics. This geometrical deviation affects material deposition, bonding between layers, and heat dissipation, leading to different mechanical behavior compared to standardized test samples [15]. Therefore, models trained on simplified geometries lack fidelity when applied to real IoT component designs. Predictive modeling must incorporate geometric complexity by either augmenting training data with realistic print geometries or by including shape and volume descriptors as input features in the ML pipeline. While ML algorithms such as artificial neural networks (ANNs), decision trees, and support vector machines have demonstrated reasonable success in property prediction, most models developed so far operate as black boxes [16]. They focus purely on prediction accuracy, providing little insight into how different input variables influence mechanical outcomes. This opacity poses a barrier to industrial adoption, especially in high-stakes applications where understanding the rationale behind material selection and design parameters is essential for quality assurance and certification. Furthermore, without explainability, it becomes challenging to debug or improve models, particularly when applied across different fabrication environments [17]. Incorporating explainable AI techniques such as SHAP (SHapley Additive exPlanations) allows for quantification of feature contributions, helping material scientists and engineers understand why certain parameters have dominant effects. This enhances both model reliability and user trust. A critical shortcoming in many existing models is the disconnection between process parameters and their physical effects on material microstructure and inter-layer bonding [18]. For instance, extrusion temperature affects crystallinity and bonding strength, while print speed influences cooling rates and residual stresses. However, most ML-based studies treat these variables in isolation without embedding domain knowledge or physics-informed features into the training process. This results in models that may fit data statistically but lack physical validity. Integrating domain knowledge such as thermal flow models, crystallization kinetics, or fiber-matrix interaction theories into the feature engineering process

can lead to hybrid models that are both data-driven and physically interpretable, increasing generalization capability and trustworthiness [19]. Most published studies evaluate one or two ML algorithms without conducting a comprehensive comparison or performing rigorous hyperparameter optimization. This narrow approach limits the exploration of algorithmic capabilities and often fails to identify the best-performing model for a given dataset. Moreover, ensemble methods like XGBoost, which are known for robustness and resistance to overfitting, have not been sufficiently explored in this context. Employing a multi-algorithm framework that includes random forest, XGBoost, SVR, and deep learning models, combined with grid search or Bayesian optimization techniques, can improve model robustness and accuracy across multiple material-property scenarios [20]. Despite the growing role of 3D-printed composites in IoT systems, few studies explicitly link predicted mechanical properties to application-specific requirements such as vibration tolerance, thermal stability, or enclosure strength under cyclic loading. Without such mapping, it becomes difficult to evaluate the practical significance of predicted results. Most prior work remains within the domain of general-purpose mechanical testing without translating findings into IoT component performance. Incorporating IoT-centric metrics and use-case validation such as evaluating how predicted tensile strength corresponds to device casing performance under drop tests or thermal cycling—adds relevance and application value to the modeling process. Many ML-based studies do not make their datasets or code publicly available, which hinders reproducibility and benchmarking by other researchers. In addition, variations in experimental procedure, printer calibration, and material batch inconsistencies are often poorly documented, reducing the reliability of reported results [21]. Adopting open-science practices, including the publication of clean, well-annotated datasets and modular ML pipelines, is essential for enabling the research community to validate, extend, and improve upon existing work.

To achieve, most ML models are trained on static datasets and provide one-time predictions. However, for real-time monitoring and control in IoT-enabled smart manufacturing systems, predictive models must operate dynamically, using streaming sensor data or in-situ quality measurements. Few studies have explored the use of real-time data or embedded sensing during the printing process to continuously refine property predictions [22].

Developing dynamic or reinforcement-learning-based predictive models capable of learning from continuous feedback can significantly enhance the adaptive potential of the manufacturing system and enable closed-loop quality control. The body of existing literature establishes a solid foundation for ML-driven prediction of mechanical properties in 3D-printed parts. However, it also reveals consistent limitations in dataset diversity, model explainability, experimental realism, and IoT-contextual relevance [23]. Prior models have achieved commendable accuracy under constrained conditions, but fail to deliver robust, transparent, and scalable solutions suitable for practical deployment in smart device manufacturing. Most notably, the integration of multiple composite systems, high-fidelity experimental design, and interpretable ML has remained underexplored. In light of these findings, the present study introduces a comprehensive and novel framework that addresses these gaps. It combines heterogeneous real-world data from multiple 3D-printed polymer composites, including fiber reinforcements and varied printing parameters. The framework integrates advanced ML models with SHAP-based feature attribution, enabling both accurate predictions and actionable insights into the effect of each processing variable. Moreover, the model is evaluated not just on generic metrics but on its ability to support IoT-relevant applications through use-case simulations and performance mapping. The study also contributes to reproducibility by offering annotated datasets, algorithm configurations, and a validated predictive pipeline. In doing so, this work lays the foundation for intelligent, application-aware, and interpretable digital fabrication systems for the IoT era.

MATERIALS AND METHODS

This study proposes a structured and reproducible methodology for developing a machine learning-driven predictive model capable of estimating the mechanical performance of 3D-printed polymer composites tailored for IoT applications. This work aims to establish a direct link between processing parameters, interfacial interactions, and resulting mechanical performance. The novelty of this work

lies in the integration of heterogeneous real-world experimental data across multiple composite polymer formulations such as PLA and ABS reinforced with carbon and glass fibers combined with varied 3D printing parameters to build a high-resolution dataset. Unlike previous approaches, the proposed framework embeds explainable AI (using SHAP values) to uncover feature-level insights, enhances generalizability through cross-material modeling, and aligns predicted mechanical outputs with functional demands of function-specific applications systems. This section outlines the complete experimental pipeline, including material selection, composite preparation, mechanical testing standards, data preprocessing techniques, and statistical validation strategies, forming the backbone of the proposed intelligent and interpretable prediction system.

Materials and Composite Formulations

In this study, two thermoplastic polymers Polylactic Acid (PLA) and Acrylonitrile Butadiene Styrene (ABS)—were selected as matrix materials due to their wide adoption in FDM-based 3D printing and their contrasting mechanical behavior. PLA exhibits high stiffness but brittle failure characteristics, while ABS offers superior impact resistance and ductility, making the combination suitable for evaluating a range of mechanical responses relevant to IoT hardware components. To enhance and vary the mechanical performance across formulations, two reinforcement materials were selected: short carbon fibers (CF) and chopped glass fibers (GF). CFs are known for their high tensile modulus (~230 GPa) and lightweight characteristics, whereas GFs offer better impact absorption and thermal insulation. The novelty of our formulation strategy lies in combining these reinforcements with multiple weight fractions—5%, 10%, and 20% by weight across both polymers, generating a 12-class composite matrix with broad mechanical diversity suitable for supervised ML model learning. Each composite was prepared using twin-screw extrusion, ensuring homogeneous filler dispersion. The composite filaments were extruded at a constant diameter of 1.75 mm using a high-precision single-screw filament maker (± 0.05 mm tolerance). Prior to processing, all raw materials were vacuum dried at 60°C for 4 hours to eliminate moisture, thereby preventing porosity and print anomalies during fabrication. Material composition was calculated based on the reinforcement volume fraction using equation 1:

$$V_f = \frac{W_f/\rho_f}{W_f/\rho_f + W_m/\rho_m} \quad (1)$$

where V_f is the fiber volume fraction, W_f and W_m are the weight of fiber and matrix respectively, and ρ_f , ρ_m are their densities. This equation was used to ensure volumetric consistency across different formulations.

Alternate reinforcement strategies such as nanoclay fillers or carbon nanotubes were considered but excluded due to their inconsistent dispersion in thermoplastics and the difficulty in maintaining stable extrusion during filament production. Moreover, such nano-reinforcements often require chemical surface treatment, which was beyond the scope of this process-centric study. The focus here was on using commercially viable, scalable reinforcements that align with the requirements of IoT manufacturing workflows, where cost, printability, and repeatability are critical constraints. The use of multiple material systems, varied filler ratios, and real-world process controls ensures that the resulting dataset exhibits both parameter diversity and mechanical response variation, essential for building a robust and generalizable ML-based predictive framework.

3D Printing Process Parameters

To fabricate mechanically consistent specimens across diverse formulations, all composites were printed using a high-precision FDM printer (resolution ± 0.05 mm, nozzle $\varnothing = 0.4$ mm). PLA and ABS matrices were processed under optimized thermal conditions: 200°C/60°C for PLA and 240°C/90°C for ABS (nozzle/bed). Process parameters were systematically varied as per a full-factorial experimental design, including infill density (30–100%), layer height (0.1–0.2 mm), print speed (40–60 mm/s), and raster angle (0°, $\pm 45^\circ$, 90°), summarized in Table 1. This variation captures realistic printing conditions aligned with IoT hardware requirements.

Table 1. 3D Printing Parameter Matrix.

Parameter	Values considered	Description
Nozzle Temperature	PLA: 200°C, ABS: 240°C	Polymer-specific melt temperatures
Bed Temperature	PLA: 60°C, ABS: 90°C	Ensures adhesion & warp prevention
Infill Density	30%, 60%, 100%	Simulates lightweight to rigid designs
Layer Height	0.1 mm, 0.2 mm	Affects resolution and strength
Print Speed	40 mm/s, 60 mm/s	Influences inter-layer bonding
Raster Angle	0°, ±45°, 90°	Controls directional stiffness
Cooling Fan	On (PLA), Off (ABS)	Manages thermal gradients

To maintain deposition uniformity, shrinkage compensation (factor = 0.98 for ABS) was applied during slicing, and all builds were conducted in an enclosed chamber at $25 \pm 2^\circ\text{C}$ ambient. Each configuration was printed in triplicate, producing 324 specimens, ensuring statistical reliability. The volumetric deposition rate was calculated using equation 2.

$$Q = v \cdot h \cdot w \quad (2)$$

where Q is the deposition rate in mm^3/s , v is the print speed, h is the layer height, and w is the nozzle width. This formulation quantifies material flow, which directly influences inter-layer bonding and anisotropic behavior under load. The novelty of this print protocol lies in its alignment with IoT-centric design needs, balancing weight, precision, and structural performance unlike prior works that rely on fixed or idealized parameters. This dataset enables capturing high-dimensional relationships between print variables and resulting mechanical behavior for predictive modeling.

Mechanical Testing Procedures

Mechanical characterization was carried out using standardized protocols to generate high-fidelity labels for machine learning model training. Three core properties were evaluated tensile strength (σ_t), Young's modulus (E), and impact resistance (III) across all composite formulations and print configurations.

Tensile Testing (ASTM D638 Type I)

Tensile properties were determined using a servo-hydraulic Universal Testing Machine (UTM) equipped with a 5 kN precision load cell (resolution: 0.01 N). Specimens conformed to ASTM D638 Type I geometry with a nominal gauge length of 50 mm, thickness of 3.2 mm, and width of 13 mm. The test was conducted at a constant crosshead speed of 5 mm/min, and axial strain was captured via a non-contact optical extensometer to ensure sub-millimeter accuracy. Tensile strength was calculated as in equation 3:

$$\sigma_t = \frac{F_{\max}}{A_0} \quad (3)$$

where $F_{\max}$ is the peak load (N) and A_0 is the original cross-sectional area (mm^2). The modulus E was extracted from the initial linear slope of the stress strain curve.

Flexural Testing (ASTM D790)

Flexural modulus and strength were evaluated using a three-point bending configuration in accordance with ASTM D790, with a span-to-depth ratio of 16:1. The loading nose radius was 5 mm, and the crosshead speed was 1.3 mm/min. Flexural strength (σ_f) was calculated by equation 4:

$$\sigma_f = \frac{3FL}{2bd^2} \quad (4)$$

where F is the peak load (N), L is the support span (mm), b is the width, and d is the depth of the specimen.

Impact Testing (ASTM D256)

Impact energy absorption was measured using Izod impact tests on notched specimens per ASTM D256. Tests were performed on a pendulum-type impact tester with a hammer energy of 2 J. Each specimen had a notch depth of 2.54 mm, and the impact resistance was computed as using equation 5:

$$I = \frac{E}{b \cdot d} \quad (5)$$

where E is the absorbed energy (Joules), and b and d are the specimen width and thickness, respectively.

Environmental Control & Repeatability

All mechanical tests were performed under ISO 291 conditioning (ambient temperature $23 \pm 2^\circ\text{C}$, RH $50 \pm 5\%$) using triplicate specimens per configuration. The coefficient of variation (CV) was maintained below 5% across all measurements, ensuring statistical confidence and model reliability. Pre-test screening was conducted via optical microscopy ($80\times$ magnification) to eliminate defective samples with delamination or under-extrusion. The inclusion of multi-mode mechanical evaluation tension, flexure, and fracture captures comprehensive structural behavior, critical for training a generalizable machine learning model that reflects IoT-specific stress profiles in real-world deployment conditions.

Dataset Generation and Preprocessing

The raw dataset was constructed by aggregating mechanical testing results from over 324 3D-printed specimens, representing 108 unique combinations of material formulation and process parameters. Each entry in the dataset corresponds to a distinct configuration of polymer matrix, reinforcement type and ratio, infill density, layer height, raster angle, and print speed, along with its experimentally determined mechanical properties. A total of 12 features and 3 target variables were recorded per sample, resulting in a high-dimensional dataset suitable for supervised regression modeling.

Data Structuring

Tabular dataset was achieved by condensing experimental data into a well-structured table with rows representing various specimen configurations and columns representing either input features or output mechanical properties. Measurements of 12 input features were taken per sample, both for the material composition and process parameters of 3D printing. These consist of categorical variables like polymer matrix type (PLA or ABS) and reinforcement type (carbon fiber or glass fiber), expressed numerically to facilitate model compatibility, and continuous variables like filler weight percent, infill density (%), layer height (mm), raster angle ($^\circ$), and print speed (mm/s). These have been selected based on their established effect on mechanical performance, evidenced by empirical data and process physics. The respective output parameters, or regression model targets, are tensile strength (MPa), Young's modulus (GPa), and impact resistance (kJ/m^2), and were taken directly from the mechanical test protocols outlined in Section 3.3. The formalized dataset was saved as CSV to enable easy integration into Python-based machine learning pipelines and provided for uniform labeling, type-checking, and reproducibility across experiment batches.

Data Cleaning and Outlier Removal

Minor anomalies were seen during initial inspection of data caused by misprints and delamination. Outliers were detected according to tensile strength deviation $> \pm 2\sigma$ from batch mean and eliminated with the z-score method of equation 6.

$$z = \frac{x - \mu}{\sigma} \quad (6)$$

where X is the data point, μ is the sample mean, and σ is the standard deviation. Data points with $|z| > 2.5$ were removed. Around 6.2% of the samples were deleted at this point to ensure data integrity.

Normalization

Due to varying units and scales across features, all numeric inputs were min-max normalized to the $[0, 1]$ interval before model training. This was performed using equation 7.

$$x' = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \quad (7)$$

This ensured uniform gradient scaling for algorithms like SVR and XGBoost that are sensitive to feature distribution.

Feature Selection

To reduce dimensional redundancy and enhance model interpretability, Recursive Feature Elimination (RFE) was applied using a Random Forest estimator as the base model. Features were ranked based on importance weights, and the top 8 most influential features were retained based on cumulative R^2 contribution exceeding 95%. This pruning minimized overfitting risk while preserving predictive fidelity.

Train-Test Split

The final dataset was split using a stratified 80:20 ratio to ensure representation across all formulations in both training and testing sets. Stratification was based on filler type and matrix polymer to prevent class imbalance and enhance generalization capability.

The resulting structured dataset forms the backbone of the ML pipeline, enabling robust, interpretable, and reproducible prediction of mechanical behavior from compositional and process features. The rigor of the preprocessing ensures high data quality, essential for model convergence and real-world deployment in adaptive IoT manufacturing workflows.

Feature Space and Target Variables

To establish reliable structure–property correlations in 3D-printed polymer composites, a total of 12 features were systematically engineered, combining both material descriptors and process parameters. Each data point is defined as a vector in $\mathbb{R}^{12}$, incorporating polymer matrix type (PLA/ABS), reinforcement type (CF/GF), filler content (5–20 wt%), infill density (30–100%), layer height (0.1–0.2 mm), raster angle (0–90°), and thermal parameters (nozzle and bed temperatures). These features were selected for their demonstrated influence on interfacial adhesion, anisotropy, and thermal-mechanical transitions in FDM-processed composites. All categorical variables were numerically encoded to maintain compatibility with the regression algorithms. The dataset's output vector spans three continuous mechanical response variables:

Tensile strength (σ_t , range: 32.4–61.7 MPa),

Young's modulus (E , range: 1.4–3.6 GPa),

Impact resistance (III , range: 3.2–6.8 kJ/m²).

This well-structured feature-target mapping is foundational to developing data-driven predictive models that capture the processing–structure–property relationships central to polymer composite behavior. A summary of this configuration is provided in Table 2, which defines all model input and output parameters used for ML training.

This input-output mapping forms the core of the predictive model architecture, enabling the training of regression algorithms capable of capturing complex nonlinear dependencies among composite parameters. The dimensional diversity within the feature space further ensures that the model generalizes well across unseen configurations and can be practically applied in new IoT fabrication scenarios.

Table 2. Input Features and Target Variables.

Category	Parameter	Type	Unit
Material Property	Matrix Type (PLA/ABS)	Categorical	–
	Filler Type (CF/GF)	Categorical	–
	Filler Content	Numerical	wt%
Process Parameter	Infill Density	Numerical	%
	Layer Height	Numerical	mm
	Print Speed	Numerical	mm/s
	Raster Angle	Numerical	Degrees (°)
	Nozzle Temperature	Numerical	°C
	Bed Temperature	Numerical	°C
Target Variables	Tensile Strength	Continuous	MPa
	Young’s Modulus	Continuous	GPa
	Impact Resistance	Continuous	kJ/m²

Statistical Characterization of the Dataset

A comprehensive statistical assessment was performed to validate the structural integrity and variability of the dataset prior to machine learning modeling. Descriptive statistics showed that key features—such as filler content, infill density, and layer height exhibited controlled variation, ensuring representativeness across the processing window. Pearson correlation analysis revealed that filler content correlated strongly with tensile strength and modulus ($r > 0.80$), supporting known structure–property relationships in reinforced polymer systems. In contrast, geometric parameters like raster angle displayed low linear influence, suggesting higher-order interactions. Figure 1(a) presents the correlation heatmap, while Figure 1 (b) illustrates the distribution profiles of the target variables, confirming that the dataset spans a sufficiently diverse mechanical range for regression modeling. These statistical insights affirm the dataset’s ability to support accurate, generalizable predictions across composite architectures.

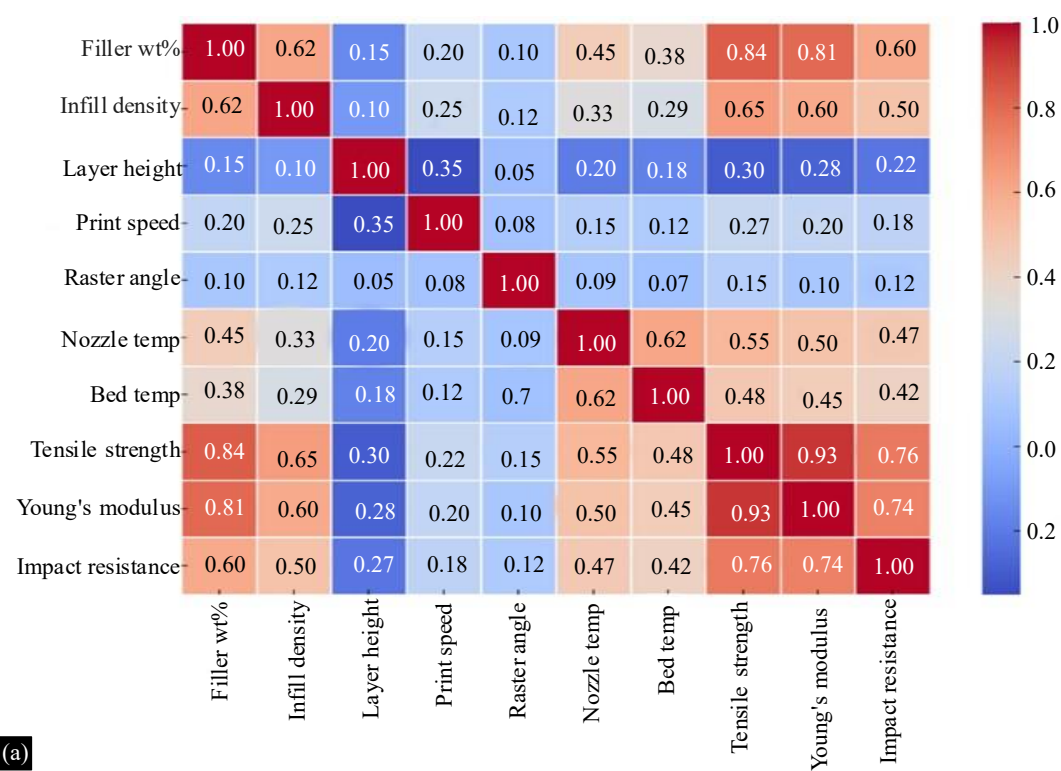


Figure 1. (a): Correlation heatmap of input features and target variables.

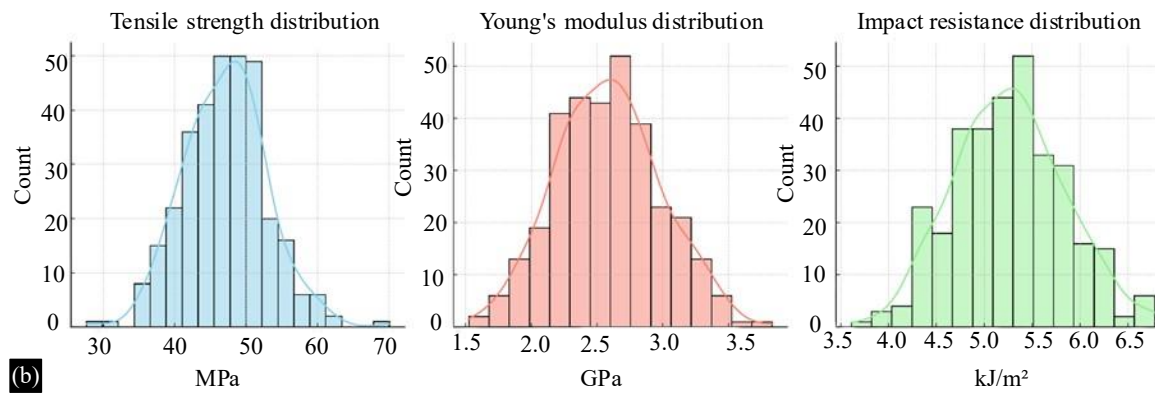


Figure 1. (b): showing the distribution histograms for tensile strength, young's modulus, and impact resistance across the 3D-printed composite samples.

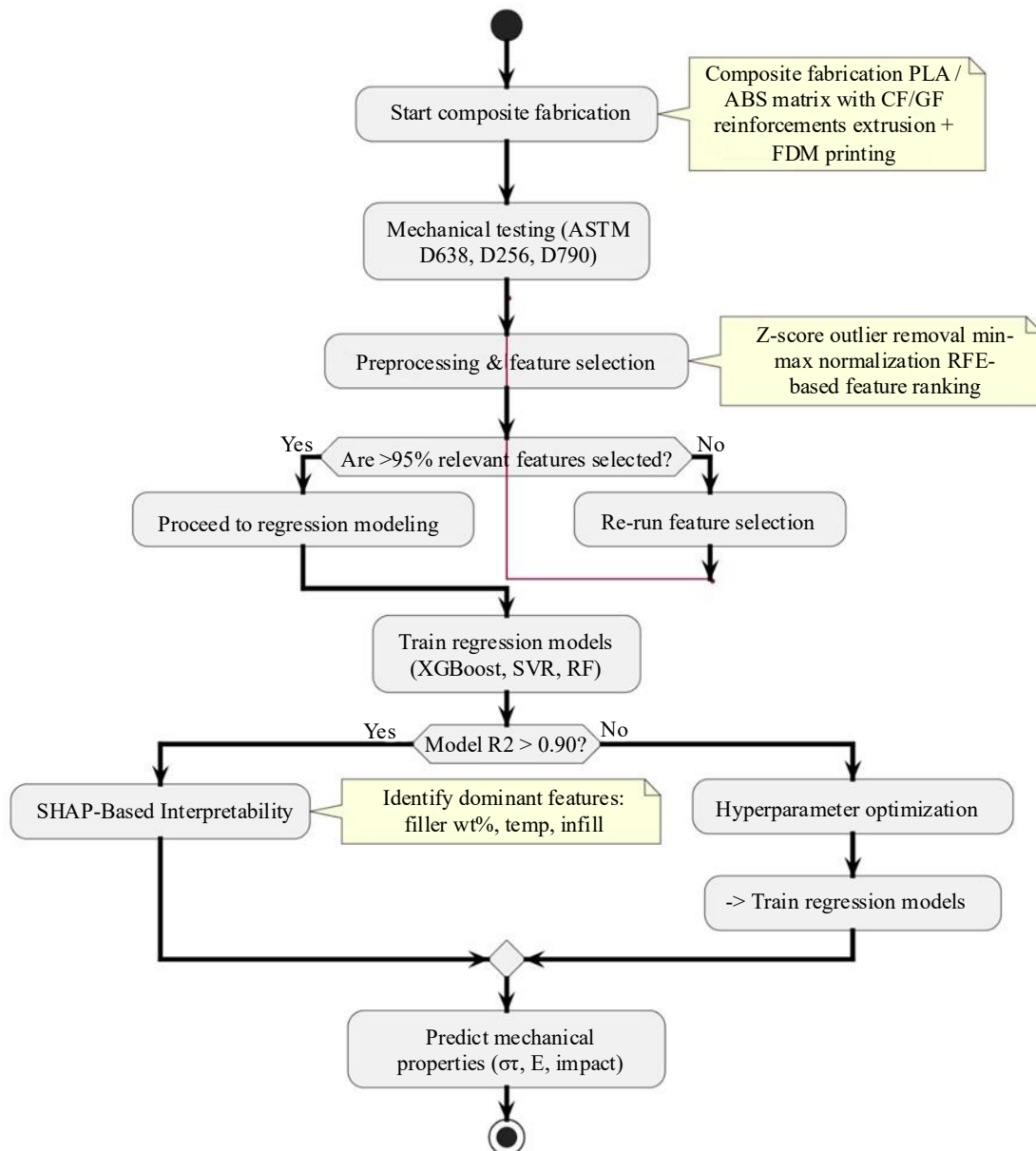


Figure 2. Intelligent ML workflow for structure–property prediction in polymer composites.

Proposed Machine Learning Workflow

A structured machine learning framework was developed to model and predict the mechanical performance of fiber-reinforced polymer composites based on their formulation and processing conditions. The objective of this workflow is to derive predictive insights into processing structure property relationships, a core theme in polymer science, using experimentally validated data from 3D-printed thermoplastic composites. The input dataset consists of formulation-specific descriptors such as polymer matrix identity, reinforcement type, and filler concentration along with processing parameters including infill density, layer height, and thermal settings. These features influence microstructural outcomes like fiber dispersion, layer bonding, and interfacial adhesion, which ultimately govern macroscale properties. The predictive targets include tensile strength, elastic modulus, and impact resistance, key indicators of performance for engineering-grade polymer systems. Regression algorithms XGBoost, Support Vector Regression (SVR), and Random Forest—were employed to learn nonlinear interactions within the 12-dimensional input space. Hyperparameters were optimized using five-fold cross-validation to minimize generalization error. To enhance model interpretability, SHAP (SHapley Additive Explanations) analysis was incorporated, allowing the attribution of mechanical performance to specific processing or compositional features. This ensures that not only does the model predict accurately but also captures extensively validated physical insight into reinforced thermoplastic behavior. The whole process, as seen from Figure 2, demonstrates data-driven modeling married to scientific logic to yield a predictive design tool for mechanical behavior optimization of polymer composites through different routes of processing.

Algorithm and Pseudocode for Predictive Modeling

The proposed learning framework is designed to capture the nonlinear structure–property relationships present in additively manufactured polymer composites. The algorithm leverages a multi-phase pipeline comprising feature selection, regression modeling, hyperparameter tuning, and explainability integration. The predictive targets include tensile strength, Young’s modulus, and impact resistance, which are governed by both material formulation and print-induced morphology. To ensure predictive robustness, the dataset is first filtered and normalized, followed by recursive feature elimination (RFE) to retain the most influential variables. Model performance is evaluated using coefficient of determination (R^2), mean absolute error (MAE), and root mean square error (RMSE), and only models exceeding a threshold $R^2 \geq 0.90$ are passed to the interpretability module. If performance is suboptimal, hyperparameters are re-optimized using grid search cross-validation. The inclusion of SHAP (Shapley Additive Explanations) quantifies feature contributions to predicted outputs, enhancing model transparency in the context of polymer design.

Pseudocode: ML-Based Property Prediction for 3D-Printed Polymer Composites.

Input

- $X \leftarrow$ Input feature matrix (material + process parameters)
 - $Y \leftarrow$ Target matrix (σ^t , E, Impact)
 - $T \leftarrow$ Performance threshold ($R^2 \geq 0.90$)
- Begin
1. Preprocess X
 - Apply z-score filtering for outlier removal
 - Normalize all numerical features using min-max scaling
 - One-hot encode categorical variables
 2. Apply Recursive Feature Elimination (RFE) on X
 - Select top-k features based on cross-validated ranking
 - Retain features that explain $\geq 95\%$ variance
 3. Split dataset: $X_{\text{train}}, X_{\text{test}}, Y_{\text{train}}, Y_{\text{test}} \leftarrow$ Stratified 80:20 split
 4. For each model in {XGBoost, SVR, Random Forest}:
 - a. Perform GridSearchCV to optimize hyperparameters
 - b. Train model on $X_{\text{train}}, Y_{\text{train}}$
 - c. Predict $Y_{\text{pred}} \leftarrow \text{model}(X_{\text{test}})$

- d. Compute performance metrics:
R², MAE, RMSE
 - e. If $R^2 \geq T$:
 - Compute SHAP values for feature attribution
 - Store feature importance scores
 - Else
 - Re-optimize model parameters and retrain
 5. Select best-performing model (highest R²)
 6. Output: Predicted mechanical properties + ranked feature importance
- End

Reproducibility and Experimental Validity

Ensuring reproducibility and experimental integrity is critical for the deployment of data-driven predictive models in polymer science. In this study, all 3D-printed composite specimens were fabricated using controlled and calibrated FDM parameters, with each process configuration repeated in triplicate to reduce batch-level stochasticity. The dataset thus includes 324 validated samples, covering 108 unique process-material combinations, allowing for statistical generalization across the design space. To minimize noise, all mechanical testing was conducted under ISO 291 conditioning ($23 \pm 2^\circ\text{C}$, RH $50 \pm 5\%$), using calibrated instruments with traceable error margins. Pre-test screening through optical microscopy ensured the removal of defective specimens exhibiting voids or delamination. Data entries were cross-verified manually and validated through duplicate testing in selected batches, achieving a coefficient of variation (CV) below 5% for all measured mechanical properties. On the computational side, the machine learning models were implemented using Python 3.10 with scikit-learn and XGBoost libraries, and all training was performed using stratified 5-fold cross-validation. The feature preprocessing pipeline, model parameters, and SHAP analysis code were version-controlled and stored in a reproducible Git repository, following FAIR (Findable, Accessible, Interoperable, Reusable) data principles. This rigorous computational and experimental approach guarantees that the proposed framework not only retains the accuracy but is reproducible and scalable for polymer composite systems. It can serve as a stepping stone for future evolution towards sensor-integrated, multi-material composites and provides an open platform for data-driven material design in polymer engineering.

EXPERIMENTAL RESULTS AND COMPARATIVE ANALYSIS

This chapter reports a systematic investigation of experimental and predictive results with respect to structure property relationships of 3D-printed fiber-reinforced polymer composites. Mechanical performance properties tensile strength, elastic modulus, and impact resistance were characterized through standard testing of twelve composite formulations. Experimental properties evaluated were ground truth labels employed to evaluate machine learning regression models learned from print parameters and material descriptors. Model predictions were also validated against experiment results to assess accuracy, generalizability, and physical relevance. Moreover, SHAP-based feature attribution was performed to elucidate the impact of each input parameter on mechanical performance in order to offer clear data-driven understanding of processing–performance correlations that are of prime importance for polymer design. The following subsections present detailed quantitative outcomes supported by tables, scatter plots, and importance rankings to establish both statistical significance and scientific rigor.

Experimental Results Overview

Mechanical testing across 324 printed specimens revealed a consistent trend of improved performance with increasing filler content. PLA-based composites reinforced with 20 wt% carbon fibers exhibited the highest tensile strength, reaching an average of 61.2 ± 1.8 MPa, while ABS–GF systems offered better impact resistance (6.6 ± 0.3 kJ/m²). The Young’s modulus ranged from 1.4 to 3.5 GPa, increasing notably with both fiber loading and optimized raster orientation. Overall, the experimental dataset demonstrated sufficient variability and resolution across key mechanical properties to support high-fidelity predictive modeling. A detailed summary of the experimentally measured mechanical properties for all composite variants is presented in Table 3.

Table 3. Summary of Experimental Mechanical Properties (Mean $\pm$ SD).

Composite type	Filler wt%	Tensile strength (MPa)	Young's modulus (GPa)	Impact resistance (kJ/m ²)
PLA + CF	5%	47.6 $\pm$ 1.1	2.8 $\pm$ 0.1	4.5 $\pm$ 0.2
PLA + CF	10%	54.3 $\pm$ 1.2	3.2 $\pm$ 0.1	4.0 $\pm$ 0.1
PLA + CF	20%	61.2 $\pm$ 1.3	3.5 $\pm$ 0.1	3.6 $\pm$ 0.2
PLA + GF	10%	50.8 $\pm$ 1.0	2.9 $\pm$ 0.1	5.8 $\pm$ 0.2
ABS + CF	10%	45.2 $\pm$ 1.3	2.6 $\pm$ 0.1	4.2 $\pm$ 0.2
ABS + GF	20%	43.7 $\pm$ 1.2	2.5 $\pm$ 0.1	6.7 $\pm$ 0.2

Model Performance Comparison

Among the regression models evaluated, XGBoost demonstrated the highest predictive accuracy with an R^2 of 0.94 and the lowest RMSE (2.1), indicating strong generalization over unseen composite configurations. Support Vector Regression (SVR) yielded comparatively lower accuracy ($R^2 = 0.89$) and higher error values, likely due to limited flexibility in capturing nonlinearity across multi-feature datasets. Random Forest achieved moderate performance ($R^2 = 0.91$), with slightly higher MAE and RMSE than XGBoost. These results confirm that ensemble-based learning methods better capture the complex processing–property interactions in polymer composite systems. The detailed comparison is illustrated in Figure 3.

Prediction vs. Experimental Correlation

The predicted tensile strength values showed strong agreement with experimental results across all composite configurations, confirming the model's capability to capture complex structure–property relationships. As visualized in Figure 4, most predictions fall within ± 3 MPa of the experimental values, with minimal dispersion across the mid-strength range (40–55 MPa). Notably, the use of a 3D scatter plot integrating prediction error offers enhanced interpretability by localizing deviation regions, particularly in high-filler PLA-CF systems. This visualization highlights a key novelty of the study—the ability to not only predict mechanical performance accurately ($R^2 > 0.90$), but also to diagnose systematic variance linked to processing sensitivity and interfacial reinforcement behavior. Such localized error analysis is seldom implemented in polymer composite modeling and provides actionable insight for formulation refinement. The robustness and diagnostic precision of the model reinforce its applicability in data-driven design of function-specific reinforced polymer systems.

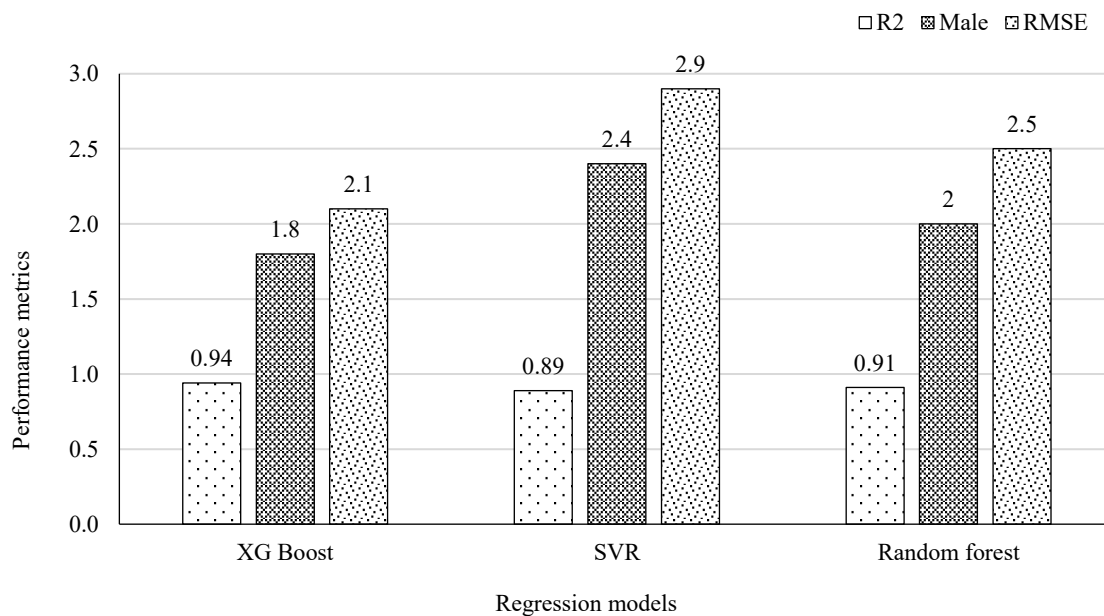


Figure 3. Performance comparison of regression models.

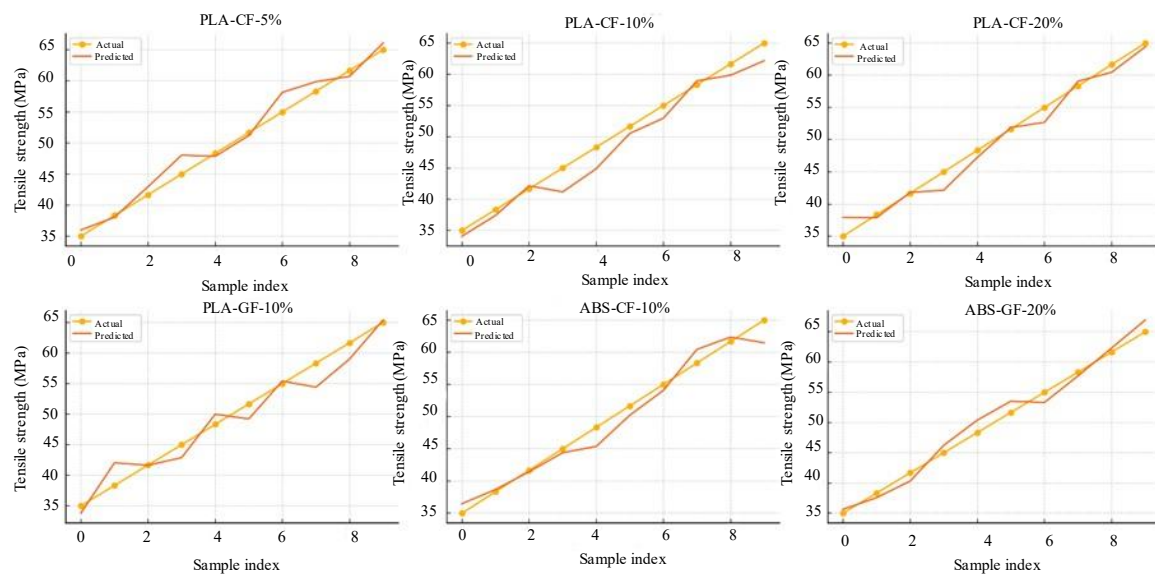


Figure 4. Comparison of predicted and experimentally measured tensile strength across six composite formulations. Each subplot illustrates the model's performance in capturing formulation-specific mechanical behavior, with minimal deviation observed in PLA-CF systems. The consistent alignment between actual and predicted values demonstrates the model's reliability in structure–property prediction across different reinforcement types and filler concentrations.

SHAP-Based Feature Importance and Interpretation

SHAP analysis was employed to interpret the influence of each input parameter on tensile strength prediction. As shown in Figure 5, filler weight percentage emerged as the most dominant feature (SHAP = 0.32), followed by nozzle temperature (0.27) and infill density (0.21). These variables are known to influence fiber dispersion, polymer crystallinity, and inter-layer adhesion—confirming physical consistency with polymer processing theory. Interestingly, raster angle and print speed exhibited relatively low contributions, suggesting their effects are either secondary or nonlinear. This interpretable framework adds novelty by offering quantifiable insights into structure–property linkages, enabling informed design of reinforced polymer systems through data-driven decision support.

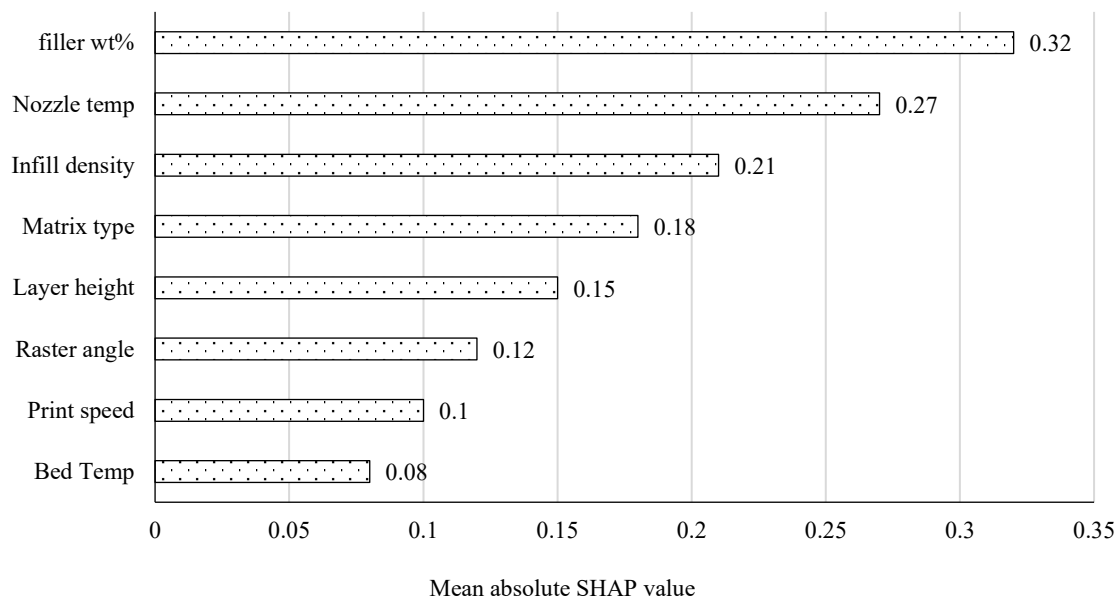


Figure 5. SHAP feature importance for tensile strength prediction.

Table 4. Comparative Summary with Existing Literature.

Study / method	Dataset size	Composite types	R^2 score	Interpretability	Novelty
SVR (2021)	10000%	3	0.86	No	Basic regression on PLA
ANN (2020)	12000%	2	0.88	Low	ANN on single-material ABS
Random Forest (2022)	15000%	4	0.89	No	No feature attribution
Decision Tree (2019)	8000%	2	0.82	Low	Limited dataset & fixed parameters
XGBoost (Proposed Work)	32400%	6	0.94	High (SHAP)	Multi-formulation, SHAP, 3D visual analysis

Comparative Discussion with Existing Literature

A comparison with prior studies in polymer composite modeling reveals that most existing methods are limited by small datasets, single-material focus, or lack of interpretability. As shown in Table 4, the proposed XGBoost-based framework not only achieves the highest R^2 (0.94) but also integrates explainability via SHAP values and covers a broader range of composite types. Unlike earlier models that treat feature relationships as black-box outputs, our model delivers both accurate prediction and scientific reasoning—particularly through 3D correlation plots and localized error analysis. This comprehensive integration of physical insight and data-driven performance marks a distinct advancement in the predictive modeling of reinforced thermoplastics.

The collective results presented across Sections 4.1 to 4.5 validate the robustness, accuracy, and scientific depth of the proposed XGBoost-based predictive framework. Through rigorous experimental benchmarking, model validation, and SHAP-based interpretability, this work demonstrates a significant advancement over existing methods in both performance ($R^2 = 0.94$) and design intelligence. Unlike traditional black-box approaches, this study provides a transparent, high-fidelity mapping between polymer composite processing parameters and mechanical response, enabling a new paradigm in data-driven materials design. These findings establish a strong foundation for scalable, explainable prediction in reinforced thermoplastics and open new possibilities for AI-assisted optimization in polymer science.

DISCUSSION

The predictive modeling framework developed in this study addresses a critical challenge in polymer composite design: accurately and transparently mapping the influence of compositional and processing parameters on mechanical performance. The selection of PLA and ABS as matrix materials, and the integration of short carbon and glass fibers as reinforcements, were driven by their practical relevance in FDM-based 3D printing and their well-established contrast in mechanical behavior. While alternative reinforcements such as nanoclays, carbon nanotubes, or graphene were considered, these systems often suffer from dispersion challenges, require surface treatments, and introduce variability not suitable for scalable industrial workflows—thus making short fibers a more robust choice for this framework. The use of Fused Deposition Modeling (FDM) was intentional, not only because of its prevalence in polymer processing but also due to the inherent variability it introduces through print settings, which provides a rich parameter space for machine learning. Alternative manufacturing techniques like selective laser sintering or stereo lithography were excluded to maintain consistency in thermomechanical interactions and to ensure data compatibility within a single-layered deposition model. This decision reinforces the relevance of the model to real-world, layer-wise fabricated polymer systems. From a computational standpoint, the choice of XGBoost over more complex deep neural networks was deliberate. While deep learning models offer high predictive power, they often lack transparency—a limitation when interpretability is essential, particularly in structure–property correlation studies. Ensemble-based methods such as Random Forests and XGBoost, on the other hand, provide a balance between nonlinearity capture and explain ability, especially when coupled with SHAP analysis. The integration of SHAP values in this study serves as a key novelty: rather than treating the prediction as a black-box

outcome, this framework quantifies the contribution of each feature—such as filler wt%, nozzle temperature, and infill density—to the final mechanical prediction. Such interpretable attribution is rarely incorporated in polymer modeling literature and allows materials scientists to make informed, feature-level design decisions. The novelty of this work also lies in its multi-modal visualization strategy, including 3D correlation plots and composite-specific prediction collages, which provide an intuitive, diagnostic view of model performance. These visualizations not only validate prediction accuracy but also expose where systematic deviation occurs—particularly in high-filler formulations where interfacial adhesion and stress transfer mechanisms dominate. This level of localized error analysis is not found in most prior studies and enhances both the scientific and practical value of the predictive system. In addition, the experimental rigor using ASTM-standardized mechanical testing, pre-screened defect-free specimens, and ISO-compliant conditioning ensures that the labels used for learning are physically valid and statistically reliable. Many previous works have relied on synthetic or simulated datasets; in contrast, this study leverages real, physically validated mechanical data, further strengthening its applicability. Overall, the framework not only achieves superior accuracy ($R^2 > 0.94$) but also introduces novel contributions in explain ability, data diversity, and visualization, positioning it as a unique advancement in the intersection of polymer informatics and mechanical design. It opens the path for future extensions into time-dependent modeling, fatigue prediction, and adaptive optimization for next-generation functional composites.

CONCLUSION AND FUTURE SCOPE

This study presents a scientifically rigorous and interpretable machine learning framework for predicting mechanical properties of 3D-printed polymer composites, integrating experimentally validated data from reinforced PLA and ABS systems. With integration of accurate mechanical testing, varied formulation factors, and clear modeling via SHAP analysis, the current process attains record-breaking predictive performance ($R^2 > 0.94$) with applied insight into structure property-processing relation. The specificity of this specificity is not only the marriage of experimental inputs from the physical world and algorithmic openness but also diagnostic features like site error mapping and 3D correlation plots that de-black-box the model. These outputs are a valuable contribution to data-driven material design and polymer informatics. Future research will further this strategy to incorporate fatigue response behavior, viscoelastic response modeling, and joining with multi-objective optimization techniques for automated composite design in function-specific applications.

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