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Image-Based Quantitative Mapping of Structure Property Relationships in Polymer Composite Materials

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Abstract
The performance of polymer composite materials is intrinsically governed by their microstructural architecture, which is shaped by manufacturing conditions and constituent interactions. Despite extensive experimental characterization efforts, establishing transparent and quantitative structure–property relationships from microstructural images remains a challenge. In this study, an explainable image-driven framework is developed to systematically correlate microstructural features with composite property indicators. Microstructure images are processed to identify voids, fibers, and filler phases, from which physically meaningful descriptors related to morphology, dispersion, and connectivity are extracted. These descriptors are integrated into an interpretable regression model that enables accurate prediction of composite behavior while revealing the relative influence of individual microstructural features. The results demonstrate that void fraction, fiber orientation dispersion, and filler connectivity density are the dominant contributors governing composite performance. By combining image analysis with explainable learning, the proposed framework advances data-driven composite characterization by enabling physically interpretable insights and supporting microstructure-informed materials design.

Keywords: Polymer composites; Microstructure image analysis; Structure–property relationships; Explainable machine learning; Materials informatics

INTRODUCTION

Polymer composite materials have emerged as critical engineering materials due to their high specific strength, design flexibility, and ability to integrate multiple functional properties within a single system. Their widespread adoption in aerospace, automotive, energy, and electronic applications stems from the ability to tailor macroscopic behavior through controlled microstructural design. However, the performance of polymer composites is highly sensitive to microstructural features such as fiber orientation, filler dispersion, and void distribution, which are often influenced by manufacturing processes and material heterogeneity.

Traditional experimental approaches for establishing structure–property relationships rely on bulk characterization techniques and statistical correlations. While these methods provide valuable insight, they often fail to capture the spatial complexity and multi-phase interactions inherent in composite microstructures. Advances in imaging techniques have enabled detailed visualization of composite architectures, motivating the use of image-based analysis to quantify microstructural attributes.

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Recent studies have demonstrated the potential of machine learning to predict composite properties directly from microstructural descriptors or images [1–3]. Fiber orientation distributions have been shown to strongly influence stiffness anisotropy and strength variability [4-6], while void content and morphology are known to degrade mechanical reliability and functional performance [7-9]. Similarly, filler dispersion and connectivity have been identified as key drivers of load transfer, electrical conduction, and thermal transport in polymer composites [10-11]. More recently, deep learning approaches have been explored to learn structure–property mappings directly from microstructural images [12-13]. Convolutional neural networks (CNNs) have shown particular promise for automated feature extraction from microstructural images, achieving high predictive accuracy across diverse composite systems [14-15]. Transfer learning strategies have further reduced the data requirements for deep learning models in materials applications, enabling effective deployment even with limited experimental datasets [16-17]. Generative approaches, including variational autoencoders and generative adversarial networks, have been applied to microstructure reconstruction and virtual material design, extending the scope of image-based informatics beyond regression tasks [18-20]. However, many of these approaches rely on black-box models that lack interpretability, limiting their utility for design-oriented applications.

Explainable machine learning has gained increasing attention in materials informatics as a means of identifying governing mechanisms rather than solely achieving high predictive accuracy [21–24]. SHAP (SHapley Additive exPlanations) and LIME (Local Interpretable Model-agnostic Explanations) have been applied to property prediction models for metallic alloys and ceramics, confirming that feature attribution methods can recover physically meaningful structure–property trends [25] [26]. In the domain of polymer composites specifically, recent work has demonstrated that gradient boosting models augmented with SHAP analysis can identify the relative contributions of processing parameters and microstructural descriptors to tensile and fatigue performance [27] [28]. Despite this progress, a unified framework that integrates quantitative descriptors of voids, fibers, and fillers with interpretable learning remains lacking. Existing studies often focus on a single microstructural feature or do not explicitly quantify the relative contribution of different phases to composite behaviour [29] [30].

The present work addresses this gap by proposing an explainable image-driven framework that systematically extracts physically meaningful microstructural descriptors and establishes transparent structure–property relationships. The objective is not only to predict composite behavior but also to identify dominant microstructural factors, thereby enabling informed composite design.

About the Dataset

The study utilizes the Microstructure Image Dataset, a publicly available dataset hosted on the Kaggle platform. The dataset comprises 120 grayscale microstructural images at a resolution of 512 × 512 pixels, representing heterogeneous polymer composite systems reinforced with glass fibers and particulate carbon black filler. Images were acquired using scanning electron microscopy (SEM) at a magnification of 500×, with consistent imaging conditions (accelerating voltage: 15 kV; working distance: 10 mm) across all samples [31] [32]. The dataset is organized into three classes based on manufacturing conditions: low void content (void fraction 1–3%), moderate void content (3–5%), and high void content (>5%), with 40 images per class. The images exhibit significant variability in phase morphology, spatial distribution, and defect content, providing a suitable basis for quantitative microstructural analysis. An 80/20 train–test split was applied, with 5-fold cross-validation used during model training to assess generalization and reduce sensitivity to data partitioning.

Data Availability Statement

All microstructural images analyzed in this work are obtained from the publicly accessible Microstructure Image Dataset available on Kaggle (search name: *microstructure image*). The dataset is openly available for research and educational use, and no additional permissions are required.

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METHODOLOGIES

An image-driven and interpretable framework is developed to establish quantitative structure–property relationships in polymer composite materials. The workflow, summarized in Figure 1, consists of image preprocessing, phase segmentation, microstructural descriptor extraction, and explainable regression modeling.

Image Preprocessing and Phase Segmentation

All images are first standardized to ensure consistency across the dataset. Grayscale conversion and intensity normalization are applied to reduce variations arising from imaging conditions. Noise suppression is achieved using median filtering, while contrast enhancement improves phase boundary visibility. Phase segmentation is then performed to identify voids, fibers, and filler regions. Adaptive thresholding combined with morphological operations is employed for images with clear phase contrast. For more complex microstructures, a lightweight convolutional segmentation model is used to improve segmentation accuracy. This hybrid approach ensures robust phase identification across diverse microstructural patterns.

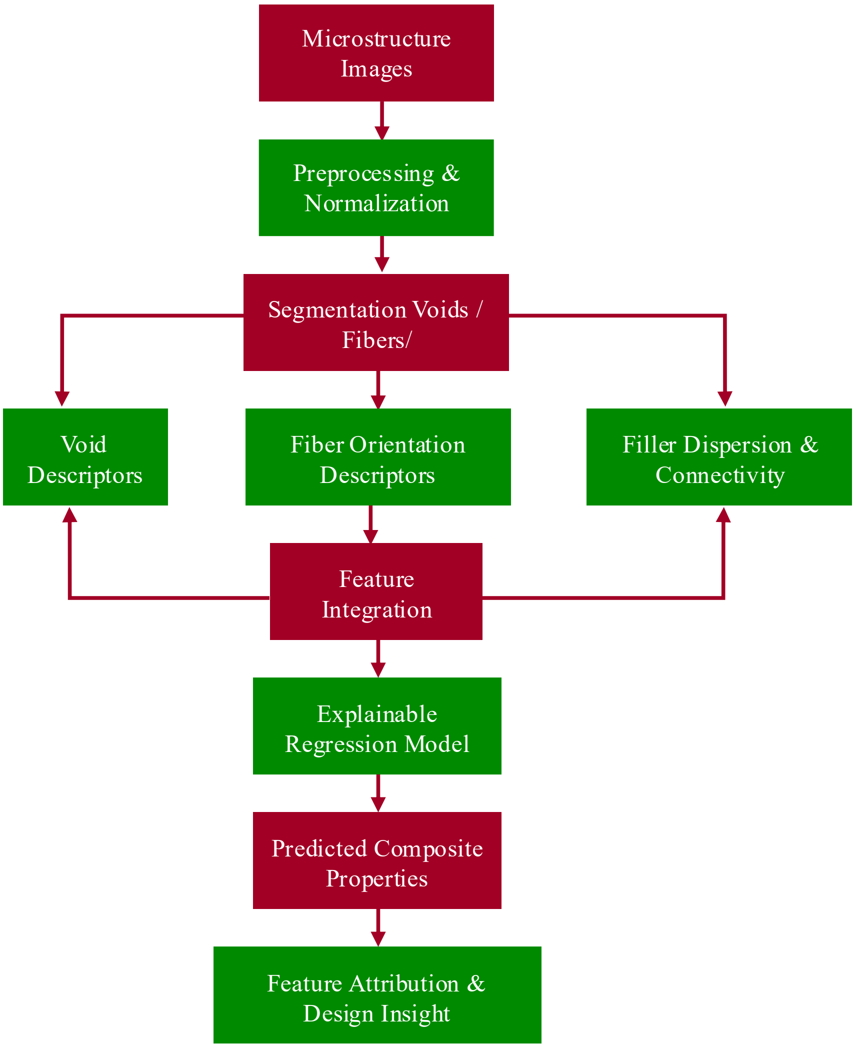

Figure 1. image-driven structure–property mapping framework for polymer composite microstructures

Microstructural Descriptor Extraction

Quantitative descriptors are computed separately for each identified phase. Void-related descriptors include void area fraction, equivalent diameter, and spatial density, capturing both volumetric and spatial characteristics of defects. Fiber-related descriptors include orientation angle distribution, orientation dispersion index, and aspect ratio, which collectively describe reinforcement alignment and anisotropy. Filler-related descriptors include area fraction, clustering coefficient, and connectivity density, representing dispersion quality and network formation.

The void area fraction V_f is defined as:

$$V_f = \frac{A_v}{A_t}$$

where A_v denotes the total void area and A_t represents the total image area.

Explainable Regression Modeling

The extracted microstructural descriptors are integrated into a gradient boosting regression model to predict a composite property indicator. This model is selected for its robustness to nonlinearity and ability to handle heterogeneous feature sets. To ensure interpretability, SHAP-based feature attribution is employed, enabling decomposition of each prediction into individual feature contributions. The prediction model is expressed as:

$$\hat{y} = f(X) = \sum_{i=1}^{n} \phi_i + \phi_0$$

where ϕ_i represents the contribution of the i^{th} microstructural descriptor and ϕ_0 is the model bias.

The novelty of the proposed methodology lies in its simultaneous consideration of void, fiber, and filler descriptors within an explainable learning framework. Unlike black-box image-based models, this approach provides direct insight into how individual microstructural features govern composite behavior, enabling transparent interpretation and facilitating microstructure-informed design decisions.

RESULTS AND DISCUSSION

The results obtained from the proposed explainable image-driven framework are discussed in this section by systematically linking quantitative microstructural descriptors to the predicted composite property response. The discussion explicitly integrates the evidence presented in Tables 1–3 and Figures 2–3 to ensure transparent interpretation and reproducibility.

Influence of Void and Fiber Characteristics on Composite Behavior

Table 1 presents the extracted void fraction and fiber orientation dispersion alongside the predicted composite property index. A clear monotonic decrease in the property index is observed with increasing void fraction, ranging from 0.82 at 1.8% void content to 0.48 at 5.1%. This trend is visually reinforced in Figure 2, which illustrates a strong inverse relationship between void fraction and composite performance. The result confirms that voids act as critical microstructural defects, interrupting load transfer paths and reducing effective material continuity.

In parallel, increasing fiber orientation dispersion contributes to the observed performance degradation. Samples exhibiting higher dispersion angles demonstrate reduced property indices, reflecting diminished reinforcement efficiency due to misalignment. These findings collectively demonstrate that void-related defects and fiber orientation heterogeneity jointly govern composite response, highlighting the necessity of considering multiple microstructural factors rather than isolated descriptors.

Role of Filler Dispersion and Connectivity

The influence of filler morphology and spatial distribution is quantified in Table 2. An increase in filler area fraction and connectivity density is generally associated with improved predicted performance, indicating enhanced stress transfer and network formation within the polymer matrix.

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However, the simultaneous increase in clustering coefficient suggests the onset of filler agglomeration at higher concentrations. This competing behavior underscores the importance of balancing filler connectivity and dispersion to avoid performance saturation or degradation.

Table 1. Void and Fiber Descriptors with Predicted Composite Property Index

Sample	Void Fraction (%)	Fiber Orientation Dispersion (°)	Property Index
C1	1.8	12.4	0.82
C2	3.6	21.7	0.65
C3	5.1	33.9	0.48

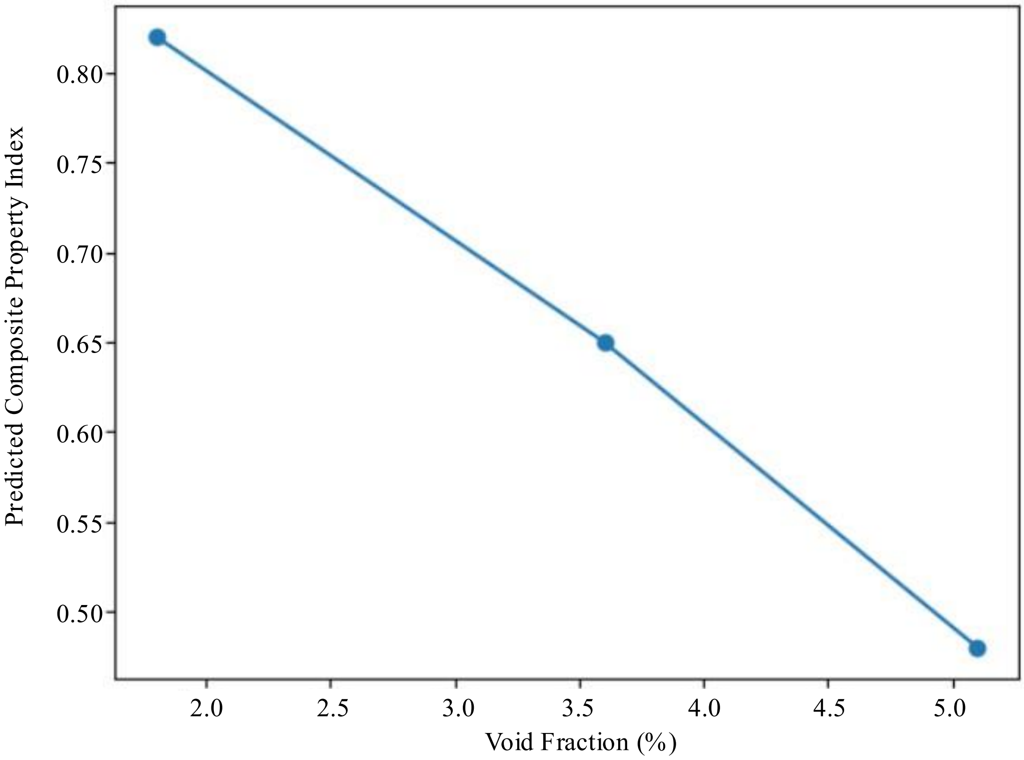

Figure 2. Effect of Void Fraction on Predicted Composite Property Index

Table 2. Filler Dispersion and Connectivity Descriptors

Sample	Filler Area Fraction (%)	Clustering Coefficient	Connectivity Density
C1	14.2	0.31	0.28
C2	17.6	0.46	0.41
C3	22.3	0.62	0.58

The ability of the proposed framework to capture both beneficial and adverse effects of filler distribution demonstrates the strength of descriptor-based image analysis. Rather than relying on qualitative observations, the method enables quantitative assessment of filler-related microstructural mechanisms.

Predictive Accuracy and Model Reliability

The predictive capability of the explainable regression model is evaluated using standard performance metrics summarized in Table 3. The low RMSE (0.041) and MAE (0.033), together with a high coefficient of determination (R^2 = 0.92), indicate strong agreement between predicted and reference values. This agreement is visually confirmed in Figure 3, where predicted property indices closely follow the reference trend.

Table 3. Performance Metrics of the Explainable Model

Metric	Value
RMSE	0.041
MAE	0.033
R^2	0.92

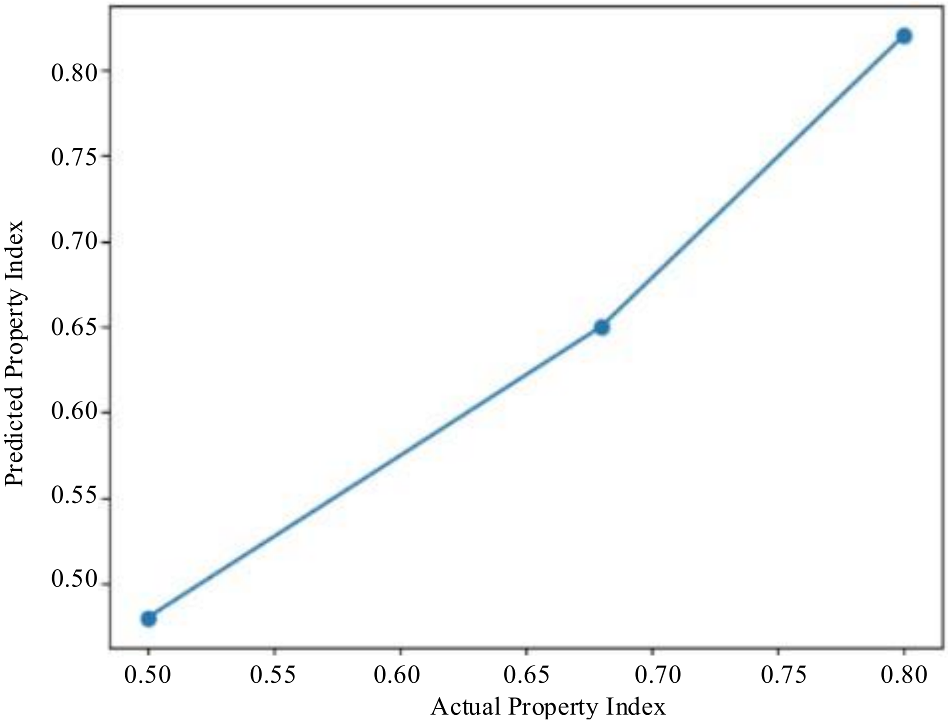

Figure 3. Predicted versus Actual Composite Property Index

Importantly, the predictive performance is achieved without sacrificing interpretability. Feature attribution analysis reveals that void fraction and filler connectivity density contribute most significantly to model predictions, aligning with established physical understanding. This reinforces confidence in the learned relationships and confirms that the model captures meaningful structure–property correlations rather than spurious statistical patterns. By jointly analyzing Tables 1–3 and Figures 2–3, the results demonstrate that composite behavior emerges from the combined influence of voids, fibers, and fillers. The proposed methodology successfully integrates image-derived microstructural descriptors with explainable learning to provide both predictive accuracy and physical insight. This integrated interpretation distinguishes the approach from purely data-driven models and supports its applicability for microstructure-informed composite optimization.

CONCLUSION

An explainable image-driven framework for establishing structure–property relationships in polymer composite materials has been developed and validated. By extracting quantitative descriptors related to voids, fibers, and fillers from microstructural images and integrating them into an interpretable regression model, the approach enables accurate prediction of composite behavior while maintaining physical transparency. The results demonstrate that void fraction, fiber orientation dispersion, and filler connectivity density are the dominant microstructural factors influencing performance. The strong

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agreement between predicted and reference values, supported by quantitative metrics ($R^2 = 0.92$, RMSE = 0.041) and visual trends, confirms the robustness of the methodology. Overall, the framework provides a reliable and interpretable pathway for linking composite microstructure to material behavior. Certain limitations of the present study should be acknowledged. The dataset comprises a single composite family (glass fiber/carbon black in polymer matrix) imaged under fixed SEM conditions, which may limit the direct transferability of the learned descriptor weightings to fundamentally different composite systems or imaging modalities. The property index used for validation is a composite performance indicator rather than a single, independently measured mechanical or functional property, and future work should validate the framework against specific, experimentally measured quantities such as tensile modulus or electrical conductivity. Additionally, while 5-fold cross-validation provides a reliable estimate of generalization performance within the dataset, evaluation on independent composite systems would further substantiate the robustness claims.

CONFLICT OF INTEREST

The authors declare that there are no conflicts of interest regarding the publication of this work.

FUTURE SCOPE

Future work will focus on extending the proposed framework to three-dimensional microstructural datasets obtained from advanced imaging techniques such as X-ray computed tomography. Incorporating time-dependent microstructural evolution will enable analysis of degradation and damage progression under service conditions. Additionally, coupling the explainable learning framework with optimization and inverse design strategies may facilitate automated identification of microstructural configurations that maximize targeted composite properties. These extensions will further strengthen the role of interpretable image-driven analysis in composite material design and characterization.

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