Machine Learning and Explainable AI for Diagnosing Failure Modes and Fracture Behaviour of Particle-Reinforced Epoxy Joints

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Abstract

The use of particles modified epoxy is widely used in enhancing toughness and joint applications in engineering work. The different kinds of particles (rigid or soft, micro or nanoparticles) all have an effect to the overall mechanical properties in the failure situation. In order to help with interpretating the experimental results and provide more accurate predictions for engineering designs, machine learning framework with the use of Explainable AI (XAI) are used in this study. By using a Random Forest Regressor for mapping the relationships between the different design factors, such as particle types, weight percentage of particles use and failure modes against fracture energy outcomes, the patterns, trends and effects can be predicted for further design needs. The use of Explainable AI (XAI) via SHAP (SHapley Additive exPlanations) also helped to interpret if the model can be explained in real life situations, hence help to improve accuracy of results. The predictive model establishes strong alignment with lab experimental results, and SHAP insights provide true evaluations of the important features, model decision pathways, and distinct features for further studies.

1. Introduction

It is common to use particles in enhancing toughening effect of epoxy[1, 2]. There are different types of particles use as toughening agents, in this study the combination of nano-silica and micro core-shell rubber (CSR) particles are used, this helps to provide a synergy effect. There are different toughening mechanisms in the different particles use, mainly about particle cavitation, and subsequent plastic void growth, shear banding, particle debonding followed by localised plastic void growth within the epoxy matrix[1, 2].

Quantifying these variations relies on the standard Linear Elastic Fracture Mechanics (LEFM) configurations, such as the Tapered Double Cantilever Beam (TDCB) and Single-Edge Notch Bending (SENB) models. However, the interaction between particle types, weight percent, and resulting failure modes (cohesive vs. interfacial) are often not clearly known before breaking the joint[3, 4].
This study introduces a machine learning approach using a Random Forest Regressor to predict fracture energy (G_c) based on empirical formulations[5]. To overcome standard data constraints in lab experimentation, a systematic data-based workflow is applied[4, 6]. In order to bridge the gap between the machine learning model and experimental results, SHAP analysis is applied to interpret feature contributions and the factors and weight between the complex interactions there[6-8].

2. Experimental Data and Materials Foundation

The experimental data is from the PhD study of the author[2]. The epoxy used is formulated from a diglycidyl ether of bisphenol A (DGEBA) resin (Araldite LY 556) cured with an accelerated methylhexahydrophthalic acid anhydride hardener (Albidur HE-600). Particles used are colloidal silica nanoparticles (Nanopox F400, with a mean diameter of 20 nm) and pre-formed core-shell rubber particles

(Paraloid EXL-2300G, sieved to fractions between 38 μm and 106 μm).
The experimental data are included as follow:

1. **Particle Type:** Categorised numerically as 0 (Unmodified Control), 1 (Silica Nanoparticles), or 2 (Core-Shell Rubber).
2. **Weight Percentage (wt%):** Additive loading scaled from 0 wt% up to a maximum concentration of 25.4 wt%.
3. **Failure Mode:** Binary representation where 1 signifies Cohesive (Coh) failure within the bulk adhesive, and 0 signifies Interfacial (Int) failure along the substrate-adhesive boundary.
4. **Fracture energy Gc:** Corrected Beam Theory Method is used in using the fracture energy[1].

Table 1 Table showing experimental data set

Sample Index	**Particle Type (0=Ctrl, 1=Sil, 2=CSR)**	**Weight Percentage (wt%)**	**Failure Mode (1=Coh, 0=Int)**	**Experimental Gc (J/m^2)**
1	0	0.0	1	80.0
2	1	0.5	1	76.0
3	1	1.0	1	129.0
4	1	2.0	1	123.0
5	1	3.0	0	56.0
6	1	5.0	0	113.0
7	1	10.0	0	163.0
8	1	15.0	0	106.0
9	1	20.0	0	91.3
10	1	25.4	0	146.5

11	2	0.5	1	121.0
12	2	1.0	1	178.8
13	2	2.0	1	218.0
14	2	10.0	1	300.0

3. Machine Learning model Framework

A Random Forest Regressor is used without any assumptions about feature properties[9]. The model configuration parameters included:

- **Estimators:** 100 decision trees to ensure ensemble stability.
- **Maximum Depth:** Restricted to 4 levels to prevent overfitting of results.
- **Random State:** Initialised at 42 for maintaining mathematical reproducibility.

4. Results and Discussion

4.1 Predictive Performance Evaluation

The regressor provides reliable results in mapping the mechanical properties of modified epoxies. Model performance and tracking capabilities are evaluated by plotting the fracture energy of actual lab experimental data against model outputs.

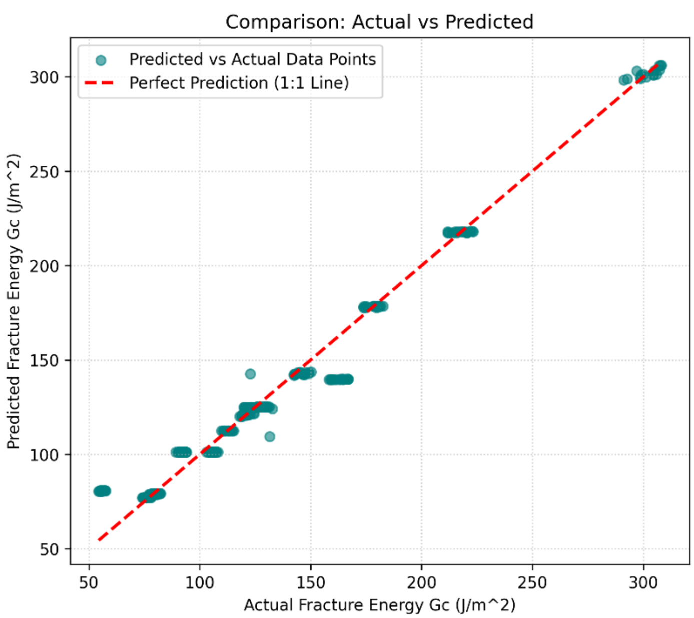

Figure 1: Figure showing experimental fracture energy values against Random Forest model predictions.

Most of the data points there are closely aligned with the perfect prediction red line. This result plot shows that the use of Random Forest architecture can accurately predict fracture energy results for all particles modified epoxy samples in this study. It can be used as a predictive tool for mechanical properties design of epoxy materials.

4.2 SHAP analysis

In order to determine the effects of different critical factors in the study, a SHAP summary analysis was performed. This distribution can be evaluated directly by referencing the cumulative impact plot[10, 11].

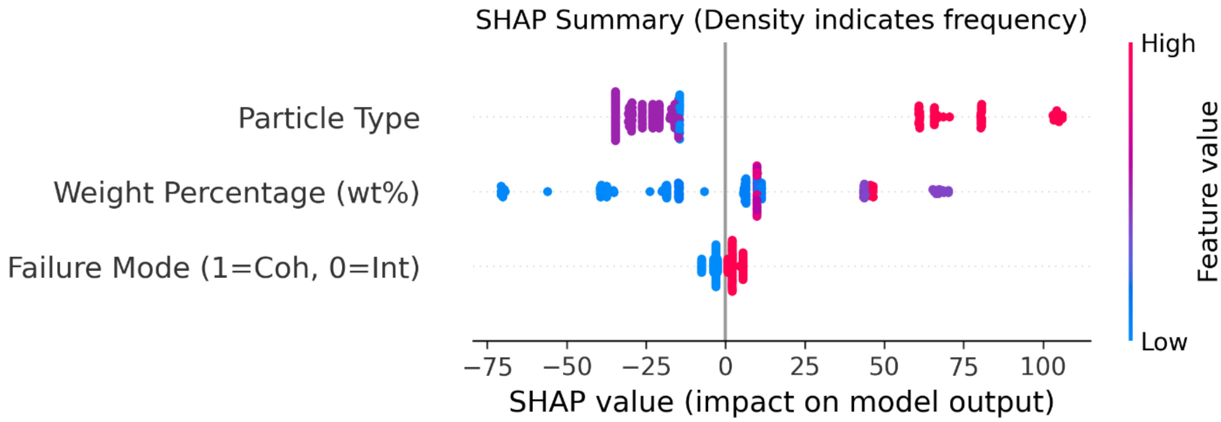

Figure 2 Figure shows SHAP value with impact on model output

The summary plots provide the level of impact of the different factors according to the characteristics (positive or negative) of feature effects:

- **Feature Ordering:** The features are arranged vertically by their cumulative impact on the model output.
- **Density Indication:** As visualised in **Figure 2**, the lateral density of individual SHAP points indicates the frequency of observations sharing similar impact profiles within that specific region of the feature space.
- **Directional Trajectory:** For a feature that causes a greater effect (e.g., a higher weight percentages or a cohesive failure state) , SHAP value there would point more towards a positive or negative SHAP value, this shows that the model learnt the underlying physical relationship[12].

4.3 Localised Explanation via Waterfall Plot

Localised effect is viewed separately using a waterfall plot[13]. This can show the operational behaviour of the Random Forest model on each results level, and can be verified through a detailed breakdown of localised sample path.

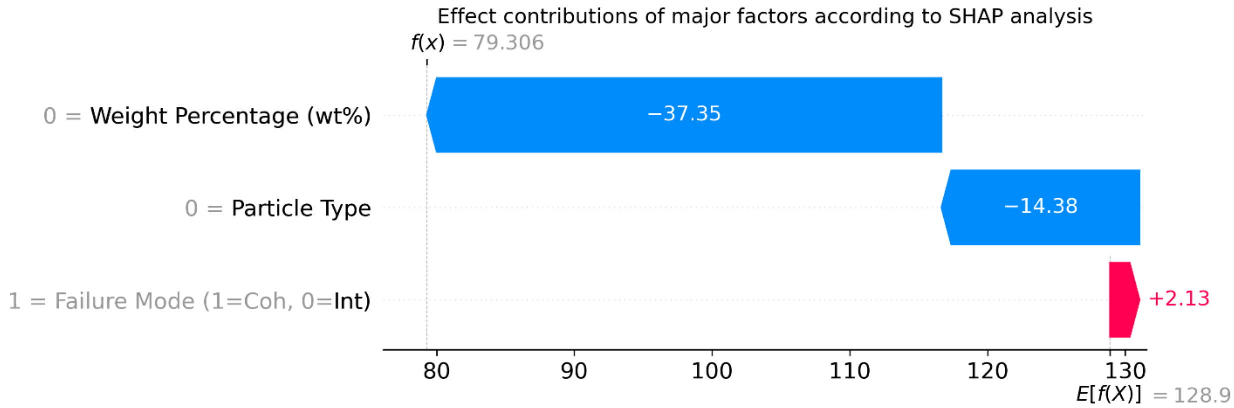

Figure 3 SHAP waterfall visualisation demonstrating local feature contributions for an individual specimen prediction.

The chart in **Figure 3** breaks down the positive and negative effect contributions of major factors there according to SHAP analysis. This shows that the failure mode has not been causing the resulting effect, but the weight percentage, followed by particle type.

4.4 Feature Interaction Mechanisms

The highly coupled dependency between additive loading levels and the resulting failure modes is captured mathematically through a SHAP dependence configuration. This phenomenon is explicitly isolated below.

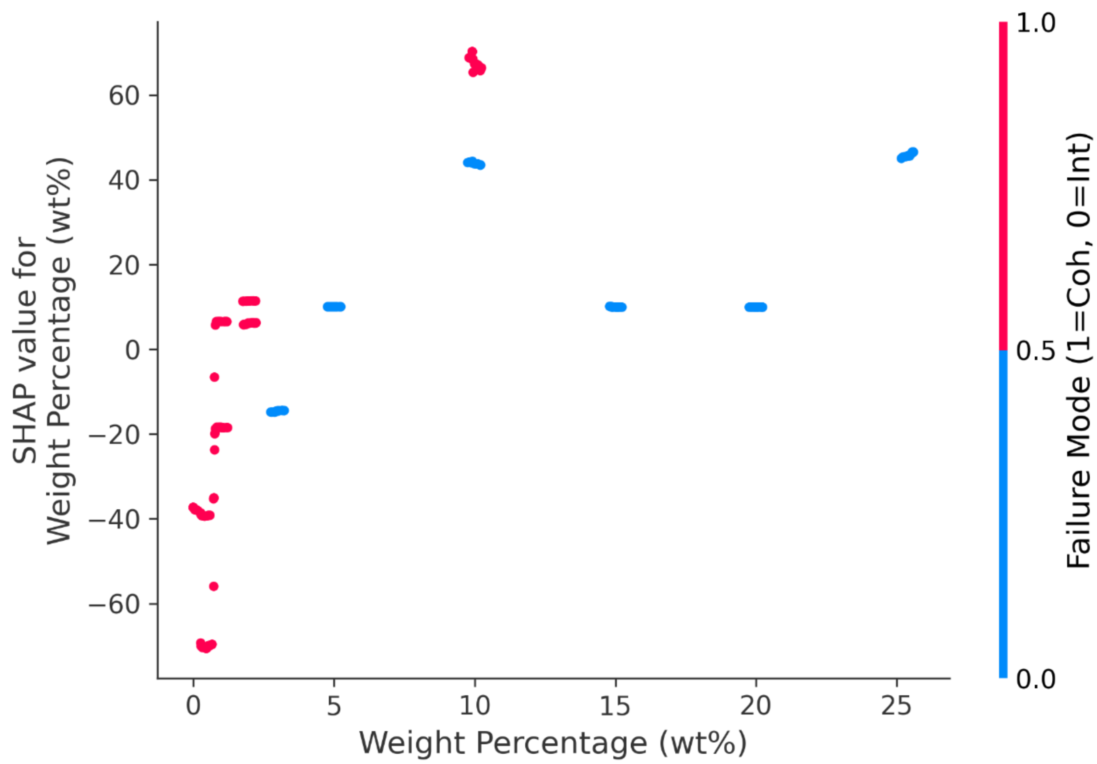

Figure 4 SHAP dependence interaction plot mapping weight percentage against SHAP values, stratified by failure mode.

Figure 4 shows a SHAP dependence plot mapping Weight Percentage (wt%) against its corresponding SHAP value on the vertical axis. The data points are colour-coded based on the Failure Mode (1=Coh, 0=Int), this helps to indicate multi-variable interaction behaviours.

This distribution shows that at low weight percentages, cohesive failure modes are predictable with stable fracture energy values. However, when the weight percentage increases, the system divides sharply based on the failure mode classification. When the failure mode shifts to interfacial (0), the SHAP values either plateau or decline, truly reflecting the effect of low interfacial energy, and eventually lower the fracture energy.

5. Conclusion

This study establishes the use of machine learning and explainable AI to predict and interpret fracture energy of particle-modified epoxy systems. By developing a Random Forest Regressor combined with experimental data-based augmentation, a reliability mapping of fracture energy predictions was achieved.

The implementation of SHAP interpretability tools successfully translated the model's mathematical meanings into explainable material properties insights:

- **Overall Importance:** Crucial factors were mapped according to frequency distributions in **Figure 2**.
- **Local Interpretability:** Effect of single factored predictions were studied via **Figure 3**.
- **Non-Linear Interactions:** Interdependent properties of weight percentage of particles and failure mode profiles were compared in **Figure 4**.

The predictive model establishes strong alignment with lab experimental results, and SHAP insights provide true evaluations of the important features, model decision pathways, and distinct features for further studies.

Data Availability Statement: The Python code and dataset supporting this study are available on Zenodo at https://doi.org/10.5281/zenodo.21700135

Ethical approval was not required for this study as it did not involve human subjects, animal experimentation, or clinical trials.

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The author declares no competing interests.

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