MATSE-597 Final Project Report

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**Topic: Semi-supervised learning for the CT morphology and the mechanical properties of PP/CaSO4 composites**

**Background and motivation**

**Task:** Understand the relation between the morphology of PP/Gypsum composites and its mechanical properties response through semi-supervised learning

My present study investigates the tensile properties of Polypropylene (PP)/Gypsum composites. Multiple composites were prepared with the same composition as shown in Figure 1, but the tensile properties response varied significantly. For instance, as shown in Figure 2, the tensile stress-strain curves of three composites with the same compositions displayed distinct behavior. Further investigation utilizing X-ray micron computerized tomography (X-ray µ-CT) revealed significant differences in the inner morphology of the three composites, which potentially contribute to their differing mechanical properties response.

Diagram

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Figure 1. µ-CT images of PP/Gypsum composites

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Figure 2. Tensile stress-strain curve of PP/Gypsum composites

In the context of fracture mechanics, the sizes of gypsum domains across the width and thickness of the tensile bar gauge region, as illustrated in Figure 3, are crucial in determining the length of crack growth from the failure of gypsum domains. To investigate this further, we propose a semi-supervised learning approach to determine if the gypsum domain size is a pattern that can be learned by a model when predicting the mechanical properties response using µ-CT images of the composites.



Figure 3. Schematic of how gypsum domain size gets calculated

Literature review

1. Yang, Charles, et al. "Prediction of composite microstructure stress-strain curves using convolutional neural networks." *Materials & Design* 189 (2020): 108509.
2. Kim, Do-Won, Jae Hyuk Lim, and Seungchul Lee. "Prediction and validation of the transverse mechanical behavior of unidirectional composites considering interfacial debonding through convolutional neural networks." *Composites Part B: Engineering* 225 (2021): 109314.
3. Xu, Yangjian, et al. "A method for predicting mechanical properties of composite microstructure with reduced dataset based on transfer learning." *Composite Structures* 275 (2021): 114444.

All three papers utilized supervised learning techniques to predict the mechanical properties response of composites by analyzing microstructure images. Papers (a) and (b) focused on predicting the stress-strain curve of the composites, while paper (c) focused on predicting the modulus. The input data sets for all three papers were generated through finite element (FE) simulation.

**Dataset for this project:**

Input: CT images

A picture containing text, furniture, pillow, fabric

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Output: The ultimate tensile strength (UTS) of each image.

Image size: 424 \* 360 pixels

File size: 20 KB

Total number: 31 composites and each composites has 100 CT images. Total images: 3100 images.

**Method:**

The proposed method involves two steps.

Firstly, transfer learning is performed using a pre-trained convolutional neural network (CNN) model such as ResNet18(weights="IMAGENET1K\_V1") to predict the ultimate tensile strength (UTS) of the composites.

Secondly, PCA embedding is applied to the extracted features from the layer before the output layer. The principal components are then plotted against the pattern of composites, specifically the gypsum domain sizes which are hypothesized to have a high correlation with the mechanical properties response.

**Result & Discussion:**

**Feature extraction from pre-trained model:**

Initially, a pre-trained model was utilized for feature extraction to evaluate if the extracted features matched the patterns observed in the experiments. However, as illustrated in Figure 4 and Figure 5, while the pre-trained model performed well for classification, it failed to extract similar features to what was expected. The PCA embedding plot did not show any discernible trend, and the explained variances plot indicated that the first few PCA components did not capture a significant portion of the image features.

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Figure 4. Principal component analysis of extracted features from pre-train model

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Figure 5. Cumulated explained variance plot of PCA components.

**Do transfer learning from the ResNet18(weights="IMAGENET1K\_V1"):**

As the direct feature extraction from the pre-trained ResNet18(weights="IMAGENET1K\_V1") model failed to meet our project goals, transfer learning was used to develop a model that could predict the UTS response of the composites from the input image data. Firstly, data preprocessing was performed to combine the images, specific features of each image, and the UTS response of each image into a dataset. To train the model, the grouped dataset was converted into PyTorch data loader format. The final layer of the pre-trained ResNet18 model was replaced with a single value for regression, and the mean-squared error (MSE) was used as the loss function during training. To ensure unbiased training, the dataset was randomly split into 80% for training and 20% for validation.

As illustrated in Figure 6, the MSE of both training and validation decreased over the 10 epochs without overfitting. The trained model's performance was evaluated using a parity plot (Figure 7), which showed that both the training and validation data points were aligned with the reference line, indicating that the predicted UTS response of the model was similar to the true UTS. The model's R2 value was calculated to be 0.994, indicating high accuracy.

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Figure 6. Train-validation loss plot

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Figure 7. Parity plot of model prediction UTS and true UTS

**Do PCA embedding to visualize what the model learns:**

After the model training, it is shown that the model can highly predict the UTS response of the composite by looking at the microstructure images of the composite. It is crucial to understand what the information is we can learn from this well-trained model. In other words, we want to see if the morphology of the composite really determines the mechanical properties response and is the learned pattern of the model is similar to the perspective of fracture mechanism as our hypothesis assumption. Therefore, PCA embedding of the high dimension features from the model were projected into low dimension to compared with some characteristics of the composite.

In Figure 8, the cumulated explained variance of first two principal components reached around 60%. All data points are projected in principle component 1, 2 and the data was plot with the colormap that represent the average gypsum thickness or standard deviation of the gypsum thickness in the µ-CT cross section image as shown in Figure 9. From Figure 9(a), it is shown that the principle component 1 might related to some pattern that separate the really brittle material and others. When the PC1 is smaller than -5, the UTS response of the composites is really low and very brittle. From the Figure 9 (b), it is shown that the PC2 might related to the standard deviation of the gypsum thickness in the CT-images, which can differentiate the semi-brittle and ductile response of the composite. When the PC2 is at low value, the std of thickness is higher and the UTS response is lower. On the other hand, when the value of PC2 increase, std decrease, and the composite becomes more ductile. In Figure 9(c), the CT-images that located in their PCA locations also follow the above trend and observations.

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Figure 8. Cumulated explained variance plot of PCA components for trained model

(a)

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(b)

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(c)

Figure 9. PCA embedding plot. (a) plot with gypsum thickness as colormap (b) plot with standard deviation of gypsum thickness (c) draw the CT-images at their locations in the PCA space

**Conclusions and future work:**

This project aimed to explore the relationship between the morphology of composites and their mechanical response by utilizing semi-supervised learning techniques. Transfer learning was employed using the well-pretrained ResNet model with "IMAGENET1K\_V1" weights, which allowed for highly accurate predictions of UTS response based on the CT images of different composites. The parity plot displayed a strong alignment between the training and validation datasets, with an R2 value of 0.994, indicative of a robust model. To investigate the learned patterns within the model, PCA embedding was conducted. Notably, the model was never explicitly trained on gypsum thickness data; however, the first two principal components revealed that PC1 effectively separated brittle from other materials, while PC2 distinguished between semi-brittle and ductile materials based on the STD of gypsum thickness. This suggests that the model implicitly learned to relate these features to UTS response.

For this project, we have established a clear relationship between the ceramic domain size (gypsum thickness) and the UTS response, which is consistent with our experimental observations. However, there are still aspects of the model, such as other PCA components, where we are uncertain about what the model has learned. For example, we are unsure if there are any other patterns in the CT-images that are related to the young's modulus or elongation at break of the composite. Additionally, we would like to explore whether the model can predict the stress-strain curve of the composite, similar to what has been achieved in other papers in the literature review. To address these questions, we propose using a convolutional autoencoder in future work. This would enable us to learn a compressed representation from the latent space of the autoencoder and investigate whether other patterns can be identified in the CT-images.