Nondestructive Testing Integrated with Data-Driven Metamodeling to Predict Microstructure-Property Relations in Woven Fabrics

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ABSTRACT

Multi-scale properties of fabric-reinforced composites are commonly modeled via numerical and experimental methods, which are often time-consuming and complex. In this paper, a nondestructive, materials informatics-based approach has been presented to link the meso-level properties such as fibers orientation and distribution to the effective Young's modulus of a typical glass woven fabric. The learning dataset is generated using radiographs of micro-computed tomography as the input, and the Young's modulus of the samples as the output. Reduced-order quantification of the fabric microstructure is established using 2-point spatial correlations and the principal component analysis. Finally, a machine-learning model is successfully applied to predict the fabric's microstructure-property relationship.

KEYWORDS: *fabrics, 2-point statistics, materials informatics, micro-computed tomography*

1 INTRODUCTION

Finding structure-property relationships is an increasingly important area of materials science, since understanding the underlying micro-level characteristics of different materials can lead to their design optimization and also discovering new materials with customized properties of interest(Rajan, 2005). Nonlinearity and high dimensionality of such relationships, however, makes it challenging to ensure reliable linkages between the materials micro-structural patterns and properties of interest. Agrawal and Choudhary (Agrawal & Choudhary, 2016) introduced four paradigms of science for development of material characterization over the centuries. The first paradigm conducts experimental tests to understand the material property which can be expensive and time consuming. After that, is the paradigm of theoretical models which formulate various phenomena by introducing physical laws and mathematical equations, which can be very intricate and still time consuming. Then, numerical models are established as the third paradigm with the development of computers, which are deemed less time consuming but still computationally expensive. Finally, in the last few years, data-driven metamodeling has become very popular in materials science which integrates the first three paradigms in a more practical and cost-effective manner. This new approach is called 'materials informatics'. In essence, materials informatics is the field of applying high-throughput data-driven techniques in materials science by predicting based purely on past data rather than by direct experimentation or simulations (Ramprasad, Batra, Pilania, Mannodi-Kanakkithodi, & Kim, 2017).

Rajan (Rajan, 2005) published a paper that described the profound influence of informatic strategy on elucidating structure-property relationships in both materials design and discovery applications. Rajan listed cluster analysis, predictive modelling, association analysis, and anomaly detection as different data mining tasks that can be applicable for understanding materials behaviour; he also introduced some widely used machine learning algorithms and statistical methods that are proved to be successful in this field. More recently, in their review of the topic, Ramprasad et al. (Ramprasad et al., 2017) pointed out key elements of machine learning within materials science. In machine learning terminology, the term "input" here refers to material structure and the term "target" or "output" refers to property. The first step of this methodology is to collect reliable data. Input data is usually a real image of the material or a synthetic model. Output data can be collected experimentally or by simulations. The next step is numerical representation of the material structure which Ramprasad et al. describe as "fingerprinting". Fingerprints or descriptors transform the input data into a quantitative scheme. They must be selected by a thorough understanding of the material morphology. Descriptors are referred to as features in machine learning language and should be invariant to transformation, rigid translation or rotation of the material image. Finally, supervised learning algorithm enables a mapping between the fingerprinted input and output property. The size of dataset highly effects the choice of learning algorithm. Depending on the application, unsupervised learning can be applied just using the fingerprints for classification or dimensionality reduction purposes.

One of the successful attempts in this field is a framework to extract high fidelity structure-property linkage using data science approach established by Kalidindi and co-workers(Gupta, Cecen, Goyal, Singh, & Kalidindi, 2015). In this methodology, they have utilized n-point spatial correlation to rigorously quantify complex material microstructures. In the next step, because of the large number of spatial correlations in the microstructure image, they applied dimensionality reduction methods to the spatial correlation of microstructure; finally, they linked the reduced-order microstructure and the property of interest (which they obtained from FE models) using a regression algorithm. Gupta et al. (Gupta et al., 2015) applied this technique to predict the mechanical properties of a non-metallic inclusion/steel composite system. They generated 900 two-dimensional synthetic microstructures with different particle sizes, shapes and spatial configurations. Effective yield strength, effective strain hardening exponent, and localization propensity were three output properties that were extracted from a 2-D micro-mechanical FE model. After that, a 2-point statistics autocorrelation map was used as the fingerprint of each microstructure followed by a dimensionality reduction step using PCA. Then, numerous regression analysis was performed to optimize model hyperparameters using leave-one-out cross-validation and find the best surrogate model to establish structure-property linkage. At the end, the writers compared the results of this approach and conventional methods to the simulation results and proved robustness and reliability of the data science framework. In a recent work from the same research group, Cecen et al. (Cecen, Fast, & Kalidindi, 2016) suggested a computationally efficient strategy for finding 2-point spatial correlation using Fast Fourier Transform. They also studied some challenging cases like microstructures with non-periodic boundaries, regions with no information or bad quality in the microstructure, and large datasets. Finally, they examined their method for the case of a three-dimensional micro-CT image of reinforced polymer composite and observed distribution of the fibre orientations in the contour plots of the calculated autocorrelations.

In a more recent study, Cang et al. (Cang et al., 2017) utilized convolutional deep belief network for feature extraction and reconstruction of microstructure images. They applied their method to four material systems and could achieve an efficient representation of the microstructures via a Convolutional Neural Network with four layers of feature extraction and one layer of dimensionality reduction. In a follow-up study by the same group (Cang, Li, Yao, Jiao, & Ren, 2018) , Convolutional Neural Network was used to develop a predictive structure-property model as well as two other networks for artificial microstructure creation and feature extraction. They showed improvement in the prediction performance of their model compared to the results of another method on predicting the Young's modulus, diffusion coefficient, and permeability coefficient of sandstone microstructure.

In all the above previous studies, upon materials informatics the input data is generated by modelling and the output data is provided by simulations. The purpose of this investigation is to apply the materials informatics framework of Kalidindi(Gupta et al., 2015) to woven fabric composites using real (experimental) data collected from non-destructive evaluation tests. Woven fabric composites are widely used in aerospace, transportation, and construction industries owing to their superior properties such as high strength-to-weight ratio. In virtue of hierarchical structure, modelling of these heterogeneous materials such as composites requires multiscale simulations. At the macro-level, large geometrical parameters, such as fibre volume fraction, as well as effective mechanical properties along with some simplifications (e.g. lack of crimp in the weave) are considered. Properties of the yarns and the fabric architecture are dealt with at the meso-level which is often referred to as the most important length scale to analyse (Komeili & Milani, 2012). The micro-level is characterised by the arrangement of fibres within the yarn and matrix, along with their interactions. Finally, at the lowest scales (e.g. at the nano-level), detailed interaction between constituent properties (e.g. including their surface properties) may be modelled (Bostanabad et al., 2018; Komeili & Milani, 2012). In this study, the microstructure of a woven glass fibre reinforced polymer was collected using micro-computed tomography highlighting the meso-level specification of the composite. Then, the low-dimensional representation of the microstructure was determined by employing 2-point statistics and principal component analysis. Finally, material microstructure is linked to the results of a macro-level tensile test by regression algorithm to explore effect of the meso-scale structure of material on the effective mechanical properties of the woven fabric composite using the materials informatics approach.

2 INPUT DATA COLLECTION AND DIMENSIONALITY REDUCTION

The primary step of each materials informatics study is collecting an ensemble of material microstructure. In the current study, 7 woven glass-PP prepreg plates were consolidated in a hot press with a maximum temperature of 180 ºC. Accordingly, 8 samples of 25 × 140 mm in size, with different fibre orientations were cut from each plate, creating 56 samples in total. The microstructures of the samples were captured by a MicroXCT-400 (Composite Research Network, Kelowna, Canada). After optimization of the scan parameters, the X-ray tube voltage and current were set to 40 kV and 500 µA, respectively. Because of the small thickness of the consolidated fabric, only 2D radiographs of the samples were captured to indicate the meso-level structure of the composite. The scans were carried out with a 1x focal lens with the pixel size of 11.63 µ. Because of the device's window size limitation, each sample full image was created by stitching together 18(3×6) small images, as exemplified in **Figure 1**(a). After that, each integrated image was cropped into 25 mm × 65 mm size (**Figure 1** (b)). Next step was binarizing images in order to have two phases: black phase as fibre and white phase as matrix. The result of a histogram-derived thresholding using "intermodes" method is shown in **Figure 1**(c). ImageJ software was used for stitching, cropping, and thresholding operations.

Following the binarization, the fingerprint of images was obtained utilizing 2-point correlation function. 2-point correlation function can be illustrated by a square image with the size equal to the width (minimum dimension) of the original image as shown in in **Figure 1**(e). The number assigned to each pixel in this image is calculated by finding the vector connecting centre to this point (red vector in **Figure 1**(e)). Then vectors with the same size and direction are put within the whole microstructure (**Figure 1**(d)). Probability of finding both head and tail of these vectors in black phase is called 'auto-correlation' of black(Gupta et al., 2015). In **Figure 1**(d), red vectors have both their head and tail in black phase, but green vectors have either head or tail or both in the white phase. The probability is computed for all other vectors in colormap and these values are presented as colours. In the case of auto-correlation of a specific phase, the value in the centre of this image indicates the percentage of pixels in that phase, since the probability of finding head and tail of a vector of size zero in the same phase is one. For cross-correlation, however, the centre value is zero because the probability of finding head and tail of a vector of size zero in different phases is zero. To assess the capability of 2-point statistics, several case studies with various fibre volume fraction, fibre orientation and waviness were examined. The cases were compared while changing only one parameter at a time and accordingly, the above statistical feature extraction method is proved to capture fibre volume fraction, fibre orientation and waviness, successfully.

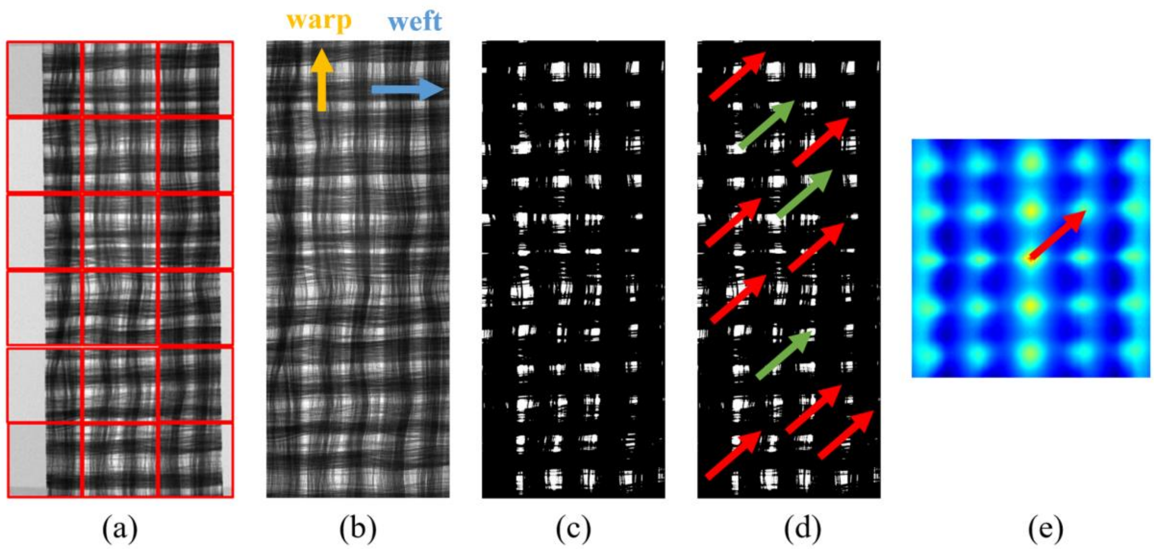


Figure 1: Processing input images: (a) stitching small images, (b) integrated image, (c) binarized image, (e)&(d) 2 point auto-correlation of black pixels

Although 2-point statistics is extracting important features of woven fabric in meso-scale, the correlation matrix still has more than 4 million dimensions which is extremely large for carrying out a learning algorithm. In an attempt to reduce the dimensions of these data, principal component analysis (PCA) was employed. PCA is an eigenvector-based multivariate technique that uses an orthogonal transformation to convert correlated features in a dataset to a set of linearly uncorrelated variables called principal components in a way that the first principal component has the largest variance in the original dataset(Rajan, 2005). In order to decide how many principal components are sufficient to describe the data, the percentage of variance retained for different number of principal components is presented in **Figure 2** as dashed line. It was found that by using the first 15 principal components, 91% of variance could be retained; in other words, the reconstructed microstructure is 91% similar to the original microstructure.

3 OUTPUT DATA COLLECTION

Output parameter, Young's modulus, was obtained by performing tensile tests following the ASTM D3039/3039M for obtaining tensile properties of polymer matrix composite materials (ASTM, 2008). **Figure 3**(a) shows sample size for the test and **Figure 3**(b) compares stress-strain curve of three samples with warp fibre orientations 0º, 20º, and 45º. The fibre orientation refers to the smallest angle between fibre direction of one family of yearns (warp) with the uniaxial load direction; while the second family of the yearns (weft) remain perpendicular to the first one, as shown in **Figure 1**(b). Tensile behaviour of the tested balanced glass fibre/polypropylene woven composite is shown in **Figure 3**(b). According to (Ogihara & Reifsnider, 2002) as well as (Panthapulakkal & Sain, 2007), woven fabric composites demonstrate nonlinear elastic stress-strain relations. This nonlinearity intensifies as the initial fiber angle rises and gets to its maximum at 45 degrees. Nonlinear elastic behaviour is in fact caused by the presence of shear strain on the matrix in the lamina. As it is shown by Vaziri et al. (Vaziri, Olson, & Anderson, 1991), tensile stress-strain curve of the [±45º] laminate has a very similar shape to the pure shear stress-strain curve of the [0º/90º] cross-ply laminate. As shown in **Figure 3**(b), mechanical response of the woven composite is dominated by brittle fibres in the 0º configuration. On the other hand, it is apparent from this figure that in the 45º arrangement of fibres, no fibre connects the bottom edge of the sample to the top; so, fibres are taking a minor part in carrying the load and the shape of the stress-strain curve is very close to the thermoplastic ductile matrix stress-strain curve.

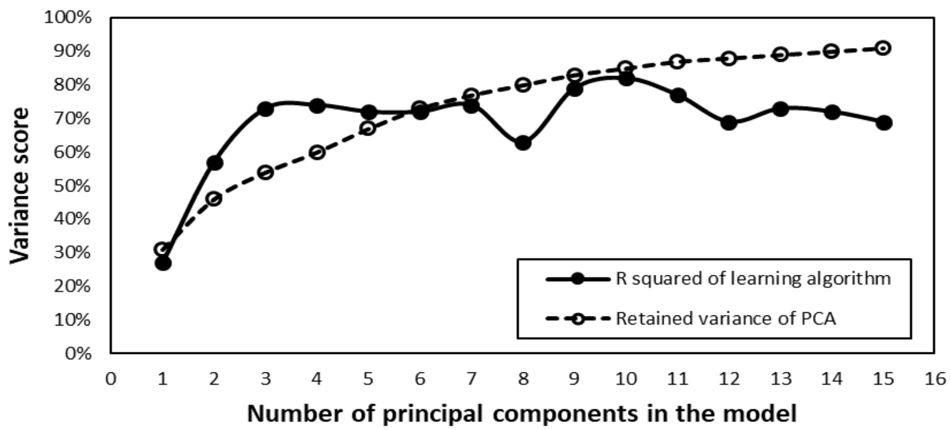
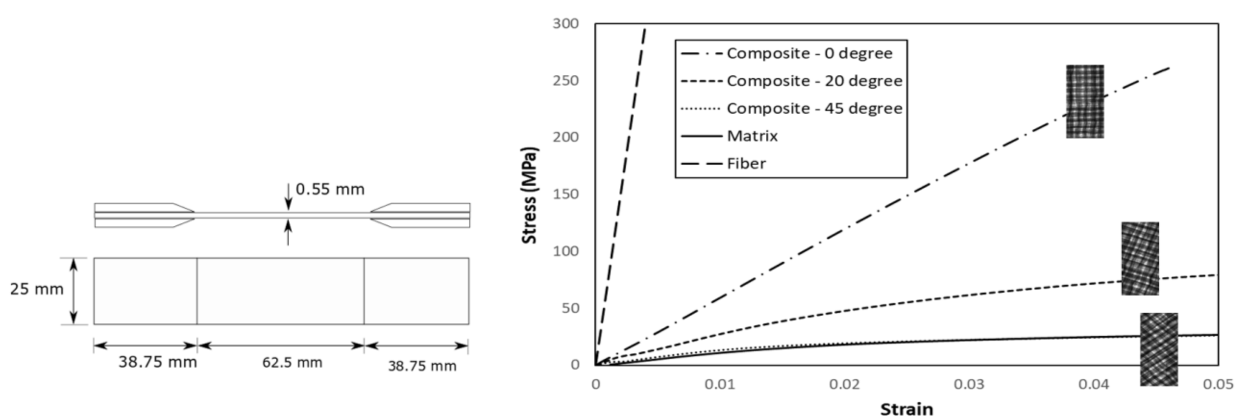


Figure 2 : The effect of number of principal components on the retained variance of PCA and resulting R^2 of the regression

As a linear elastic material, the Young's modulus of all cases with 0º orientation was obtained by estimating the slope of stress-strain curve. For off-axis reinforcement cases, the initial slope of the nonlinear curve was taken as the (initial) Young's modulus. In addition to fibre orientation factor, the number of yarns in loading direction was deemed as another source of observed macro-level response differences in the Young's modulus of samples, especially for the repeated samples with 0º orientation.



(a) (b)

Figure 3: (a) Sample size employed for the tensile tests; (b) Stress-strain curve of fiber, matrix, and composite with different fiber orientations; notice that in the 45º configuration, the composite response becomes nearly fully dominant by the matrix (Panthapulakkal & Sain, 2007).

4 STRUCTURE-PROPERTY LINKAGE

After generation of calibration dataset, the standard regression analysis was carried out to establish a linkage between reduced representation of the microstructure and measured Young's modulus of the woven composite samples. Among 56 samples, 48 of them were considered as training and 8 samples were randomly chosen as test set (while including all different fiber orientations). To evaluate the impact of dimensionality reduction on materials informatics predictions, multiple regression analyses were performed with retaining different number of principal components in the model. Solid line in **Figure 2** shows the R^2 of regression model for the first 15 principal components. Surprisingly, increasing the number of principal components did not always lead to a better prediction. This result suggests that cross validation techniques must be used to find the optimum value of this hyperparameter. In order to better illustrate the accuracy of regression model, the measured Young's modulus was compared to the predicted results (while retaining the first 10 principal components) as shown in **Figure 4**. Accumulation of points near the 45-degree line in this figure proves a fair accuracy of the prediction. This is deemed a significant machine learning result for such a small dataset (56 samples) of a glass/PP woven composite with different fiber orientations and non-uniform fiber geometry distribution (misalignments) within and between samples.

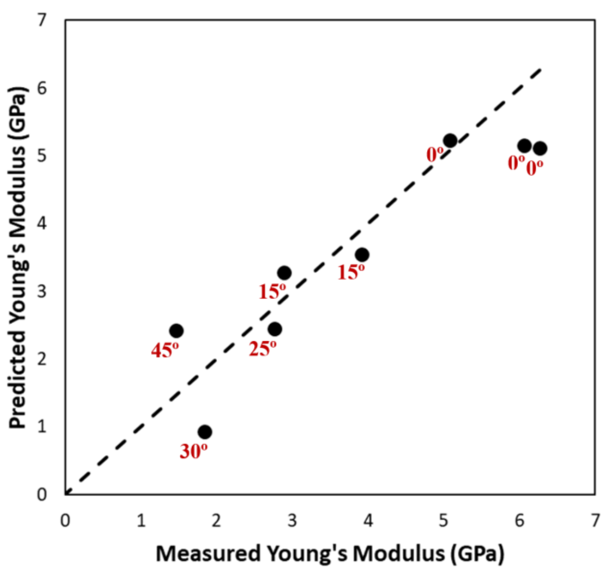


Figure 4: Measured versus the predicted Young's modulus of the test set using the first 10 principal components; the numbers beside each point shows fiber orientation.

5 CONCLUSION

This study aimed to establish a framework for data-driven metamodeling to predict microstructure-property relations of woven fabric composites using micro-CT. 2-point statistics linked with principal component analysis could reduce the large dimensionality of scanned images from more than 4 million pixels to 10. A simple regression algorithm was then used to build a basic machine learning framework to predict the Young's modulus of the composite from the images (i.e. non-destructively). The predictive model had a significant accuracy given the small training dataset of size 48. The scope of the developed model was limited to specific weave pattern, fiber and matrix material, and 2-dimensional microstructure. Data with a greater diversity can be gathered in a future study in order to establish a broad-based materials informatics model for textile composites. Also, further research could consider more input parameters such as processing parameters to increase the accuracy of predictions.

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