Deep Learning Modelling for Composite Properties of PCB Conductive Layers

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Abstract

This paper presents the development of a novel modelling approach, based on the use of deep learning (DL), to predict the orthotropic composite properties of copper-patterned conductive layers of printed circuit boards (PCBs). This data is needed to assess the bulk PCB properties with existing methods for laminar composites. Image datasets of copper patterned artwork, required with this approach, are gathered and the composite (homogenised) orthotropic elastic modulus of the respective conductive layouts is evaluated through an automated, macro-script executed, finite element analyses. The modulus values are assigned as labels to each image of a copper layout in the dataset. A regression convolutional neural network is developed and optimised using a training dataset and validated using the test dataset.

The results show that the DL model can predict the orthotopic values of the elastic modulus of highly nonstructured copper patterns accurately, with the absolute errors of the predicted vs. true (FEA evaluated) property value being less than 3% of the composite propriety range for 99% of the patterns in the validation dataset. The advantages of the proposed machine learning solution over existing techniques are that it can be digitalised and made available to the end-user as an easy-to-use and computationally fast toolset. The modelling approach can enable design engineers effectively explore PCB design alternatives, with awareness of their thermo-mechanical properties and the effect they have on the assembly performance and components' reliability.

1. Introduction

In electronic assemblies, the thermo-mechanical reliability of components attached to printed circuit boards is impacted by the level of their stiffness and thermal expansion compliance. This dictates the need for material characterisations that are increasingly embedded in the product development flow, particularly for high-value, high-reliability, and high-performance electronic products. Printed circuit boards (PCBs) are an integral part of any electronic assembly and therefore are present in all electronic products and systems. PCBs are multi-layer composite structures, consisting of dielectric layers (typically glass fibre reinforced resins) and conductive metal layers (typically etched copper patterns), as schematically detailed in Fig. 1. PCBs have thermomechanical properties that depend on the properties of the individual layers in the stacked structure. Currently, the homogenised (effective) mechanical properties of composite structures such as fully stacked PCBs or constituent prepreg (fibre-loaded resins) laminates are evaluated mainly through physical testing using respective metrology instruments and characterisation techniques. Testing methods used include TMA, DMA, DIC, and others. These tests are expensive to undertake and require the use of specialised systems, often integrating different types of equipment, and can be done only by technicians and operators with relevant skillsets and training.



Figure 1: A schematic (bottom) and real example (top) of sheet layers of etched copper laminated onto and/or between sheet layers of a non-conductive material (fibreglass reinforced resin).

Rule-of-Mixture (ROM) methods such as Reuss and Voight, and similar semi-empirical elastic models (Halpin-Tsai, Nielsen, and Chamis), have been widely used to predict the effective properties of various multi-layered laminar composites, and particularly of fibre-reinforced resins [1,2]. These methods use the constituents' material properties and their volume fractions to estimate the effective properties of the composite system. But the use of these methods enables reasonable evaluation only of the bounds for the property value and works well only for material compositions that feature well-defined and structured layouts. In practice, none of these can be used to assess accurately the true orthotropic behaviour of real fibre-loaded resin laminates and particularly of PCB layers featuring complex patterns of conductive artwork.

For this task, a finite element (FE) simulation has been the only viable modelling option; but the challenge is in the complexity of the modelling task with this method and the unique and new finite element model that must be developed for each composite structure of interest [3]. This is evident from several investigations using finite element analysis that have been reported in the public domain. Khan et al. developed a simplified micromechanics model for calculating the mechanical properties of plain weave composites [4] and Sudheer et al. studied fibre-resin systems for varying percentages of fibre volume but limited their work only to very simple geometries [5]. Kim et al. demonstrated the application of large-scale finite element analysis using direct numerical simulation (DNS) which described explicitly the composite constituents and their interactions, for evaluating the mechanical properties of metal matrix composites, active fibre composites, crossply laminates, and 3-D orthogonal woven composites [6]. Other studies on fibre-reinforced polymers using finite element analysis reached a similar conclusion that the numerical simulation is superior to existing analytical methods and can generate a more comprehensive and accurate evaluation of the effective composite properties [7,8].

Recently, there has been an interest to exploit methods from the domain of computational intelligence to predict the properties of composite material systems [9-11]. Hamidi et al. presented a high-level general methodology that aimed at the use of machine learning models for predicting the properties of polymer composites using the composite constituents, but their approach has not been applied to electronics applications [9]. Barbosa et al reported a study on several laminate composites with a varying number of layers and angles of orientation employing machine learning models [10]. Research by Pathan et al [12] and Abueidda et al [13] deployed a similar machine learning modelling strategy, for predicting the composite properties of unidirectional fibre composite structures and two-phase, two-dimensional checkerboard composite, respectively, where the ground-truth data used in the training process are obtained from finite element analyses.

Unlike the extensive modelling of the composite thermo-mechanical properties of fibre-reinforced resins used as prepregs (dielectric layers) in a common PCB stack-up, very little work is reported on approaches and methods to derive the composite properties of conductive layers. One of the reasons is the geometric complexity of the conductive artwork resulting in highly unstructured patterns which, even for the same copper fraction in a representative cell volume, can have very different composite properties, hard to predict with any of the ruleof-mixture methods available for composite systems.

This work demonstrates the feasibility of integrating, digitalising, and applying methods from two computational domains - mechanics and intelligence (Machine Learning), to the domain of composite materials and their homogenised mechanical property characterisation. The modelling approach targets specifically the problem of predicting the homogenised orthotropic elastic modulus of conducive layers featuring realistic and highly nonstructures patterns as found in modern PCB multi-layer stack-up composites. A computational approach using deep learning models that use as input the image of the conductive pattern and information for the modulus of the layer's constituents is developed and demonstrated.

2. Methodology

The proposed methodology deploys an AI-based modelling approach, using data and supervised learning, which is fundamentally different from most of the current methods used for the task of composite material characterisation. It does not rely on physical testing and the use of metrology instruments, and unlike the analytical and physics-based modelling approaches has the potential to overcome their key limitations in evaluating the homogenised mechanical properties of composite material structures (e.g., compromised accuracy due to the approximations made, model complexity, computational time).

The proposed methodology is realised in several steps, detailed graphically in Fig.1, and involves certain data flow, model developments, and computations.



Figure 1: Methodology for development of AI-based modelling capability for homogenised properties of copper patterned layers used in printed circuit boards.

Step 1: Gather PCB design data and obtain layer characteristics. The metal patterned layers, typically copper (as in this study), are defined most with PCB Gerber or ODB files. The graphics file shows the 2D layout of the copper in each conductive layer of the PCB stack. Properties of constituent materials (copper and resin from the adjacent prepregs) are also obtained.

Step 2: Process the Gerber files and extract images with predefined pixel resolution/size of copper patterns. Process the images in binary greyscale format and save them in chosen pixel-based image file format (e.g. bitmap BMP).

Step3: Develop and use an automated process for the image-to-parametrised finite element model data flow and the high-fidelity analysis of the copper patterns given with each image in the dataset. Obtain the orthotropic thermomechanical property values of interest from respective simulated load cases. In the absence of experimental measurements, these values are taken as the ground truth.

Step 4: Create an expanded database where each image of a copper pattern is linked (labeled) with the respective composite property value obtained in the previous Step 3.

Step 5: Split the dataset randomly into (1) training data - used to build the deep learning model and (2) validation data - used to validate the accuracy and performance of the model. Define the deep learning model structure - for example, a convolutional neural network (CNN), the model parameter estimation algorithm, and any training parameters. Then train the CNN model. The model has as input the image of a copper pattern, with a predefined image size/resolution, and the output is the composite material property for which the model has been trained. Sperate models for each property of interest can be considered and constructed.

Step 6: Validate the deep learning model(s) developed in Step 5 by using the validation dataset. Analyze predictive power and accuracy. Iterate with Step 5 to optimise the model structure and parameters, if required.

3. Data and Modelling Developments

3.1 Raw Data of PCB Copper Artwork

The raw data in this study consisted of Gerber files providing conductive artwork images with size/resolution up to $4,000 \times 4,000$ pixels. Image processing was realised using resizing and multi-image cropping with varying steps to generate a substantially larger dataset of copper pattern images with the size of 100×100 pixels. The final dataset contained approximately 26,000 images. In terms of the image dataset used to develop and validate the machine learning model, the dataset size was increased 4X through a process of rotation of each image by 90, 180, and 270 degrees, respectively.

We consider the conductive layer of the PCB as a bimaterial composition (copper-resin) because during PCB lamination the resin of the prepreg fills the gaps of the conductive pattern thus forming a composite layer. The material properties of interest of the constituent materials making the PCB copper layer – copper and resin, are listed in Table 1.

Table 1: Mechanical properties of conductive layer constituents: copper and epoxy resin.

Elastic Properties	Symbol (unit)	Epoxy Resin	Copper
Young's Modulus	E (GPa)	3.0	110.0
Poisson's Ratio	v (-)	0.40	0.34

3.2 Composite Property Evaluation with FEA

Finite element analysis technology was deployed to evaluate the composite properties of the bi-material copper patterned layers. This is the only feasible and most accurate approach to evaluate the three values of the orthotropic elastic modulus, E_x , E_y , E_z , where X-Y defines the plane of the layer, and Z is the out-of-plane direction. To achieve this, a scripted macro for FEA using ANSYS APDL simulation software was developed to automate the analysis process for all images in the dataset. It should be noted that while for the deep learning with image data the rotated image variants of an original image are different data points, the FEA was required only for the original (non-rotated) copper patterns to obtain the respective orthotropic (X, Y and Z) properties. For the other three associated images with a pattern (90, 180, and 270 rotations), their orthotropic properties are specified through appropriate consideration of the axis orientation in relation to the un-rotated image.

A parameterised 3D model with a fixed mesh that has matched the pixel resolution of the images. The automated simulation-in-the-loop is executed over the entire (unrotated) set of images in the database. In each such iteration, one image is taken from the database and the binary material information is extracted on a pixel-by-pixel basis, and then transferred into the respective material specification for the mesh elements corresponding to the image pixels (see Fig. 2).



Figure 2: Example of (a) an image of copper pattern from a PCB Gerber file transferred onto (b) an equivalent finite element (FE) model. The FE model in (b) shows the load case boundary conditions for *X*-loading under the iso-strain condition at the boundary of the pattern.

Once the finite element mesh model for a given pattern is defined, the macro script defines sequentially several load cases, assuming iso-strain conditions as shown in Fig. 2, right) that simulate the mechanical responses of the composite pattern to loads, in X, Y and Z. The unidirectional displacement/elastic strain results can then be used to compute the equivalent homogenised modulus of the composite pattern in the respective X, Y and Zdirections. The load case settings, the respective load case analyses, and the extraction of FEA results (directional displacement, strain, and stress) along with the secondary calculations for the homogenised properties are also automated within each FEA iteration executed by the macro-script.

The FEA of the patterns in the dataset is performed in a shared memory mode (16 logical processors) on a serverspec Intel Xeon CPU@2.20 GHz processor and 10 physical cores. It has taken approximately 72 hours to assess all 26,000 copper patterns in the dataset with an image resolution of 100×100 pixels. Each analysis within the loop had additional load cases executed which, in addition to the three orthotropic (*X*, *Y* and *Z* direction) values of the composite Young's modulus, have provided also results to enable the prediction of the orthotropic values of the coefficient of thermal expansion and the ratio of transverse strain to axial strain (Poisson's ratio equivalent). The latter set of results is not discussed in this paper. At each iteration, the obtained properties of the composite pattern are exported and stored in a results file, with a link to the associated image in the database.

Figure 3 shows an example of results obtained from the load case used to evaluate the composite Young's modulus in $X(E_x)$. The load conditions are detailed in Fig. 2(b). The force applied in the X direction is represented as a load in the form of pressure P, and the X-displacement degree-of-freedoms on that side are coupled. The coupled displacement value in X at the boundary of the pattern is extracted from the FEA and used to calculate the equivalent properties.



Figure 3: Example of FEA prediction for *X*-displacement (mm) field of a copper pattern under

For the copper pattern illustrated in Fig. 2(b), the volumetric fraction of copper content is 0.321. The mechanical load response results, under the load case to derive Young's modulus in the *X* direction, are summarised in Table 2. For this copper pattern, similar results are obtained with the other load case loadings and informed that: $E_y = 10.068$ GPa, $E_z = 37.319$ GPa.

Table 2: Summary results obtained from FEA (examplecomposite pattern shown in Fig. FFF2).

X-displacement at the pattern's coupled UX side, UX (mm)	Force in X FX (N)	Normal Strain in X at pattern boundary: (ε_{xx})	Young's modulus in X, E_x (GPa) $=\frac{FX/Area}{\varepsilon_{xx}}$
0.878e-3	0.35	0.878e-3	11.390

All absolute predictions of the orthotropic modulus for the copper patterns in the dataset are normalised over the range 0 to1, with normalised value of 0 corresponding to 3 GPa (resin modulus, 0% Cu fraction) and 1 corresponding to 110 GPa (the copper modulus, 100% Cu fraction).

3.3 Deep Learning Modelling

The image dataset, now labeled with the respective composite values (normalised over the 0-1 range) of the orthotropic modulus, enables targeting the construction of a convolutional neural network (CNN) model [14]. Because of the image size and resolution, it is possible to attempt a CNN model with fewer layers and smaller convolution kernels sizes compared with standard deep learning neural network architectures. The latter would require substantially larger datasets to train compared to those available for this case study, given the highly nonlinear nature of the problem, and can take days of training time. Several CNN networks were built using different parameters for the model structure to achieve optimal predictive performance. The optimised convolutional neural network is composed of convolutional layers, maxpooling layers, a fully connected layer, and a softmax layer as detailed in Fig. 4. The pattern resolution of the dataset (100×100 pixels images) dictates the size of the 3-channel input data (third array dimension is 1 as grey image data is deployed, i.e. input size 100×100×1). This CNN is constructed as a regression model which means the output is a real scalar value.



Figure 4: Convolutional neural network (CNN) for the orthotropic material properties of copper-patterned composite layers.

The deployed CNN model structure has been designed with several modules.

- Input layer: The size of the input images is 100×100 with a single channel (greyscale image). For the problem of images representing different copper patterned composite layers, the images are binary (black and white, representing the copper and resin, respectively).
- Convolutional CNN module: This is a composition of neural network layers that includes:
 - Convolutional 2D layer: The convolutional layer uses a kernel (a matrix) of learnable weights

which is slid across the input image and multiplied by the input so that the output is enhanced in some aspect, thus extracting relevant features. The proposed CNN model contains six modules and hence there are six convolutional layers. The kernel size is 2x2 in all cases, but the number of filters is different across the layers - 8, 16, 32, 64, 128, and 128 for layers 1 to 6, respectively.

- Rectified Linear Unit (ReLU) layer: The ReLU is a non-linear threshold activation function. performed to each element of the input. The ReLU sets any value less than zero to zero and keeps any positive value unaltered. The use of ReLU layer helps avoid overfitting.
- Batch Normalisation (BN) layer: The batch normalization is an operation used to normalise the elements of the input to each layer by using the mean and variance for each mini-batch independently.
- Pooling layer: The pooling layer is used to reduce the dimensionality of the feature maps. The developed CNN model uses 2×2 pooling layers applied with a stride of 2 pixels. This provides a reduction of the size of each feature map by a factor of 2 and consequently is reducing the number of pixels (values) in each feature map to one quarter. The last CNN Module #6 in the proposed model does not have a pooling layer, and hence the output from the last convolutional layer is 128 feature maps with the size of 3×3 pixels.
- Dropout layer: The introduction of a dropout discards neurons in the fully connected layer with a certain probability to avoid the problem of over-fitting the solvable weights of the neural network. As a technique, it also gives the benefit of accelerating the training of the CNN model. The dropout probability value used in this model development is 0.2.
- Fully connected layer: Each neuron node of the fully connected layer is connected to each neural node of the upper layer, and the neuron nodes of the same layer are disconnected. The CNN model feeds the features of the last convolution layer to a fully connected layer with 1152 neurons. This fully connected layer is essentially a 1×1×1152 convolution operation on the output from the previous layer (kernel 3×3 and 128 feature maps).
- Regression output layer: The regression layer computes the mean-squared error (MSE) loss.

The CNN model structures for the three orthotropic values of Young's modulus are trained using the parameters detailed in Table 3. For each CNN model, the training process using MATLAB with 90,000 images takes approximately 130 minutes to perform on a GPU Nvidia Quadro P5000 graphics card and a 10-core Xeon CPU@2.20 GHz station.

Table 3: Parameter values used to design and train the convolutional network models.

Parameter	Value	
Number of epochs	150	
Batch size	256	
Optimisation	Adaptive Moment Estimation	
Algorithm	(ADAM)	
Learning rate	1e-3	
Loss function	Mean Squared Error	

4. Results and Discussions

To assess the predictive power and model accuracy of the developed CNN models, the following metric for accuracy is used:

Accuracy (%) =
$$\frac{N_{correct}}{N_{val}} \times 100$$
 (1)

where

$$N_{correct} = \sum_{i=1}^{N_{val}} F_{correct}(P_{CNN}(i), P_{FEA}(i), TD)$$
(2)

$$F_{correct}(P_{CNN}, P_{FEA}, TD) = \begin{cases} 0, & if |P_{CNN} - P_{FEA}| > TD \\ 1, & if |P_{CNN} - P_{FEA}| \le TD \end{cases}$$
(3)

and $P_{CNN}(i)$ is the CNN model predicted value (over normalised [0,1] range) for the composite property $P, P \in$ $\{E_x, E_y, E_z\}$ associated with an image (copper pattern) with index $i, P_{FEA}(i)$ is the true (normalised) value of the composite property, evaluated with a finite element analysis, TD is a threshold value, and N_{val} is the size of the validation dataset, in this investigation $N_{val} = 15,000$ images.

Table 4 details the performance metrics of the developed CNN models for Young's modulus E of the copper patterned composites comprising the validation dataset. The model accuracy value (in %, see Eq.1) measures the percentage of copper patterns (images) in the validation dataset for which the difference between the CNN-predicted and the true value of the property, both normalised in [0,1], is less than the respective threshold value TD. A summary of this performance metric for three different threshold levels is detailed. The TD values are taken as 0.01, 0.03, and 0.05. It can be noted that TD = 0.01 (or 1% of the normalised composite property range) is equivalent to approximately 1.07 GPa in absolute terms.

Table 4: Summary of the prediction accuracy of the CNN models for the composite orthotropic Young's modulus (in-plane E_x and E_y , and out-of-plane E_z).

<i>TD</i> Ref	TD	CNN Model Accuracy (%) (Eq.1)		
	value	E_x	Ey	Ez
TD1	0.01	80.86	81.39	89.75
TD3	0.03	98.60	98.86	99.99
TD5	0.05	99.89	99.90	100.0

It is observed that the in-plane modulus $(E_x \text{ and } E_y)$ of a composite pattern has a clear non-linear dependency on the copper content and that the stiffness of the structure is very sensitive to the spatial layout of the copper. The CNN models were still capable to capture very well the relationship between the copper layout pattern and the associated composite Young's modulus in the data, and show a very good predictive capability for such a complex task. The CNN models for the in-plane modulus can predict the property value with an error less than 1 GPa (approximately) for about 80% of all copper patterns in the validation dataset. The accuracy increases substantially, above 98.5%, if the accuracy threshold loosens to about 3 GPa. Figure 5 details the CNN model predicted values for E_x and E_y versus the ground truth (FEA obtained) values of the property.



Figure 5: CNN predicted values vs. ground truth FEA values of the [0,1]-normalised in-plane orthotropic Young's modulus E_x and E_y of PCB conductive copper patterns in the validation dataset (size 15,000 patterns). Red dotted lines represent the ±5% error band.

The CNN model for the out-of-plane modulus E_z features better accuracy: 90% of the validation patterns have the predicted composite property value with an error less than 1 GPa (approximately) compared to the true

value, and practically 100% of the copper patterns have predicted E_z values with an error less than 3GPa. The reason is that in the out-of-plane direction (Z) the copper and the resin materials form a bi-material composition that results in a strictly longitudinal (parallel) composite configuration. Hence the composite modulus E_z is dependent on the fraction of copper. The CNN model for E_z shows an improved predictive power because of the ability to establish this dependency and the associated relationship between the stiffness and the copper fraction. Figure 6 illustrates in a similar format, CNN predicted vs. true E_z values, the accuracy of the constructed model.



Figure 6: CNN predicted values vs. ground truth FEA values of the [0,1]-normalised out-of-plane orthotropic Young's modulus E_z of PCB conductive copper patterns in the validation dataset (size 15,000 patterns). Red dotted lines represent the $\pm 5\%$ error band.

4. Conclusions

learning-based, А novel, machine modelling methodology utilising deep learning neural networks to predict the orthotropic composite properties of PCB conductive layers was developed. The investigation has demonstrated the application of this approach for predicting the effective elastic modulus of copper patterns with complex layouts. The convolutional neural network models were found to be a feasible and advantageous alternative to experimental testing or high-fidelity finite element analysis for assessing the properties of composite layers. Unlike the latter methods, once developed the deep learning models can be used to assess any composite pattern in a cost and computationally efficient manner. They require a simple input from the user in the form of an image of the pattern which is readily available from PCB design specifications.

The CNN models reported in this paper featured the following absolute error performances:

- Accuracy of 1% of the composite property range or better with 80% of the composite conductive patterns.
- Accuracy of 3% of the composite property range or better with at least 98.5% of the composite conductive patterns.

It has been found that the orthotropic properties associated with the out-of-plane direction can be predicted by a CNN model very accurately, explained by the fact that in that direction the layout of the copper and the resin represents a parallel composition of the two materials. The in-plane composite properties are predicted with less accuracy because of the strong sensitivity, in a non-linear manner, of the composite property to the actual 2D layout features of the pattern and because of the weaker dependence on the copper volume fraction.

The use of a CNN model enables fast prediction and unlike the FEA approach does not require special skillsets and toolsets to use. With an expanded and patterndiversified dataset, there is a realistic prospect that the CNN models can improve their performance and prediction accuracy. This can also allow for increasing the size/resolution of the images and building more advanced CNN model structures. The machine learning technology discussed in this paper is also applicable to the problem of designing redistribution layers (RDLs) for advanced IC packaging with desired composite properties.

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