

# MULTISCALE FE MODELLING AND NEURAL NETWORK TO PREDICT THE RATE-DEPENDENT INELASTIC DEFORMATION RESPONSE OF NON-CRIMP FABRIC COMPOSITES WITH MANUFACTURING DEFECTS

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**Keywords:** *UD-NCF composite, Multiscale modelling, Microstructural features*

## ABSTRACT

FRP composites with unidirectional non-crimp fabrics (UD-NCFs) are gaining traction for energy-absorbing vehicle structures, but optimizing their properties poses challenges due to their strain rate-dependent nonlinear deformation response and unique microstructural features. Manufacturing defects, like variations in tow position and shape, fiber misalignment, non-uniform fiber distribution, and curing discrepancies, can lead to mechanical property variations within parts. Therefore, understanding and predicting the influence of these defects on microstructure and properties are crucial. This study investigated the impact of UD-NCF-FRP composite microstructure on its inelastic deformation response. A numerical finite element (FE) modeling approach predicted inelastic behaviors of impregnated tows, considering constituent properties, geometry, and defects. Neural Network (NN) models, trained on microscale FE simulations, accelerated predictions without compromising accuracy.

## 1 INTRODUCTION

High-performance fiber-reinforced plastic (FRP) composites with unidirectional non-crimp fabric (UD-NCF) layers are increasingly utilized in automotive and wind energy sectors. UD-NCF reinforcements offer excellent drapability and serve as a cost-effective option for reinforcing liquid composite molded parts. Typically, these reinforcements consist of evenly spaced parallel fiber tows bonded with a warp-knitted polyester stitch, supported by orthogonally oriented low-density glass fiber yarns (Fig. 1) [1]. Compared to UD tape composites, liquid molded UD-NCF composites display unique microstructures and are susceptible to process-induced defects that may undermine their mechanical performance. These defects often involve non-uniform fiber dispersion within the tows, variations in tow position and shape, crimping of tows in the out-of-plane direction, and misalignment of fibers within the plane (Fig.2) [2]. Misalignment of fibers due to inter-tow stitching loops cannot be remedied and must be taken into consideration when forecasting the mechanical properties of UD-NCF composites [3, 4]. The stitching in UD-NCF composites has been shown to have a detrimental impact on their mechanical properties [5]. According to Rouf et al. [3], a carbon fiber UD-NCF composite with a warp-knitted tricot stitching pattern exhibited maximum fiber misalignment angles of 19° in the in-plane direction and 5° of tow crimping in the out-of-plane direction. Suratkar [6] has shown that local cracks initiate at the stitching sites when the same UD-NCF composite was subjected to transverse tensile loading.

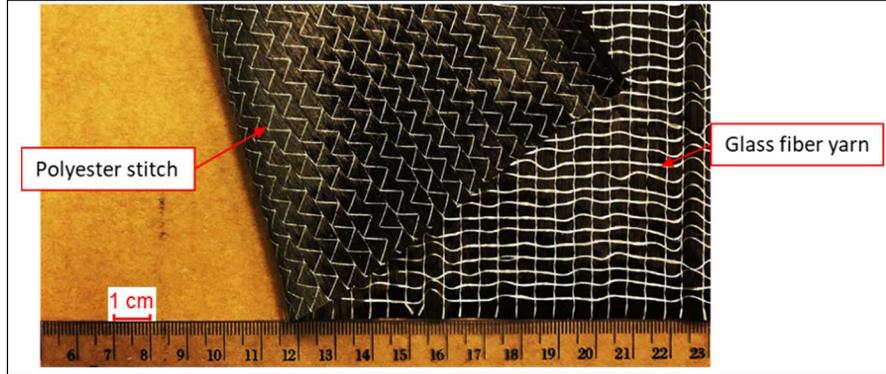


Figure 1. Typical unidirectional non-crimp carbon fabric [7].

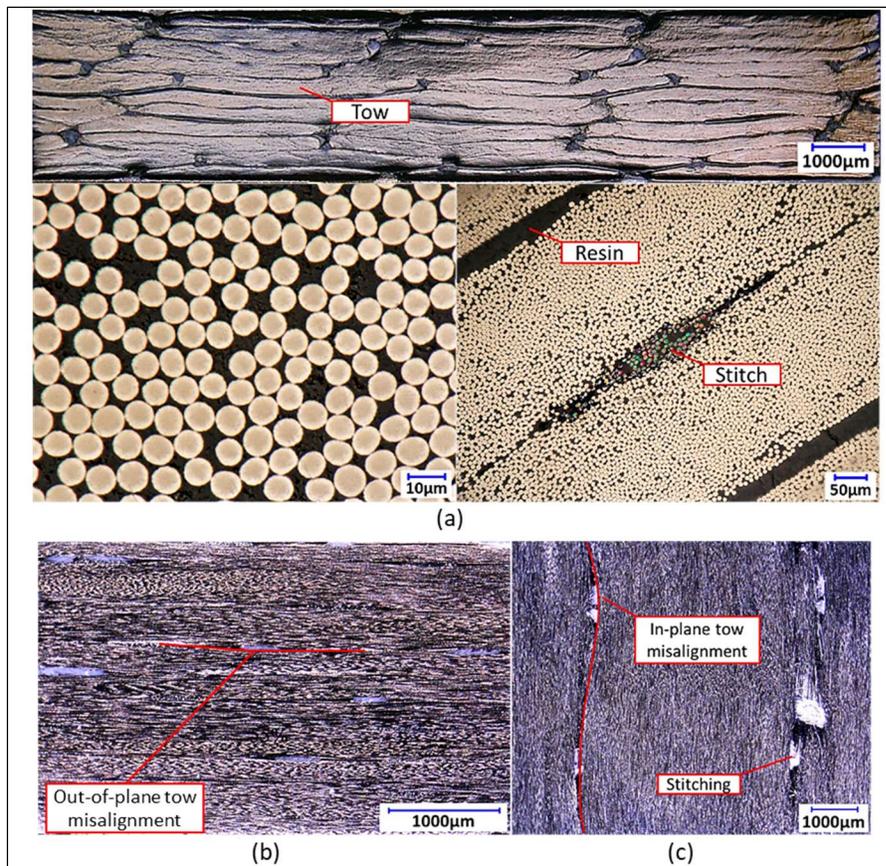


Figure 2. Images of the UD-NCF composite along: (a) the fiber direction; (b) the transverse direction; and (c) out-of-plane direction [8]

The complexity of UD-NCF composite parts, influenced by material microstructure and preforming deformation, poses challenges in accurately predicting their performance via finite element (FE) simulation or virtual testing methods. Therefore, there is an imperative to develop a reliable tool capable of precisely forecasting the local mechanical properties of UD-NCF composites, while considering defects like fiber misalignment. Several studies have explored numerical multiscale models for this purpose. González et al. [9] introduced a 3D FE representative

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unit cell (RUC) model to predict the effective in-plane stiffness properties of UD-NCF laminates, revealing that fiber crimping reduced tensile modulus of both the tow and the lamina. Rouf et al. [3, 10] proposed a hierarchical dual-scale modeling framework to predict strain rate-dependent nonlinear deformation behavior in UD-NCF composites, achieving satisfactory agreement with experimental results. Machine learning (ML) algorithms also are increasingly utilized in FRP composites research for various applications, including nonlinear constitutive modeling, accelerating FE simulations, damage detection and prediction, and optimization techniques [11]. Studies by Lefik et al. [12, 13] and Le et al. [14] demonstrated the effectiveness of neural networks (NN) in characterizing elastic properties and constructing constitutive models for nonlinear elastic heterogeneous materials, significantly enhancing efficiency. Additionally, Logarzo et al. [15] developed a method to generate strain and stress histories from FE representative volume element (RVE)s, facilitating the training of specialized NN models for sequence data.

To date, there's been limited use of multi-scale models in predicting the inelastic deformation response of UD-NCF composites, especially regarding process-induced defects, and ML algorithms haven't been explored for UD-NCF materials. This study aims to fill these gaps by employing computational multiscale models to generate data for training NN models. These models will then swiftly predict material parameters for selected inelastic constitutive material models for UD-NCF composites at the lamina level, accounting for diverse microstructures and defects. Additionally, the research examines how the microstructure of UD-NCF-FRP composites affects their inelastic deformation response, utilizing numerical FE modeling to predict effective inelastic deformation behaviors of impregnated tows, integrating constituent properties, geometric parameters, and defect specifics.

## 2 Method

### 2.1 Material system

The material system utilized PX35-UD300 stitch bonded UD-NCF (ZOLTEK™ Corp) (Fig. 1) along with a fast-curing three-part epoxy system. The UD-NCF comprised aligned tows containing 50,000 continuous PX35 carbon fiber filaments bonded by a polyester stitch in a tricot pattern, with additional support from transversely aligned low density glass fiber yarns. The epoxy material included EPIKOTETM Resin TRAC 06150, EPIKURETM Curing agent TRAC 06150, and HELOXYTM Additive TRAC 06805 (Westlake Epoxy) mixed at a ratio of 100:24:1.2 parts by weight, respectively. Flat composite panels were manufactured via high-pressure resin transfer molding (HP-RTM) at a constant temperature of 120°C and a cure pressure of approximately 91 bar for 5 minutes per Ref. [7]. Each panel consisted of 11 aligned UD NCF layers.

### 2.2 Multi-scale Modelling

Hierarchical FE models, comprising microscale and macroscale components, were developed for the UD-NCF composite (Fig. 3). The microscale FE model accurately predicted inelastic deformations of impregnated tows. Using a customized Python script, microscale RVEs were generated in Abaqus/CAE 2020 (Dassault Systèmes®), incorporating features like fiber diameter variations and nonuniform spatial distribution of fibers. These RVEs assumed an infinitely strong bond between fiber and matrix, with 3D hexahedral elements for meshing. Periodic boundary conditions were automatically applied via custom code due to periodic geometry of RVEs. A mesh sensitivity analysis investigated global mesh sizes ranging from 0.25-2  $\mu\text{m}$  (results not shown). Similarly, an RVE size sensitivity study established dimensions of  $70 \times 70 \times 10 \mu\text{m}$  (with an approximate fiber diameter of 7.5  $\mu\text{m}$ ). Effective properties of microscale RVEs were computed for in-tow fiber volume fractions ranging from 20% to 70%, with carbon fiber modeled as transversely isotropic elastic material and resin represented by a strain-rate-dependent elastoplastic model (Drucker-Prager).

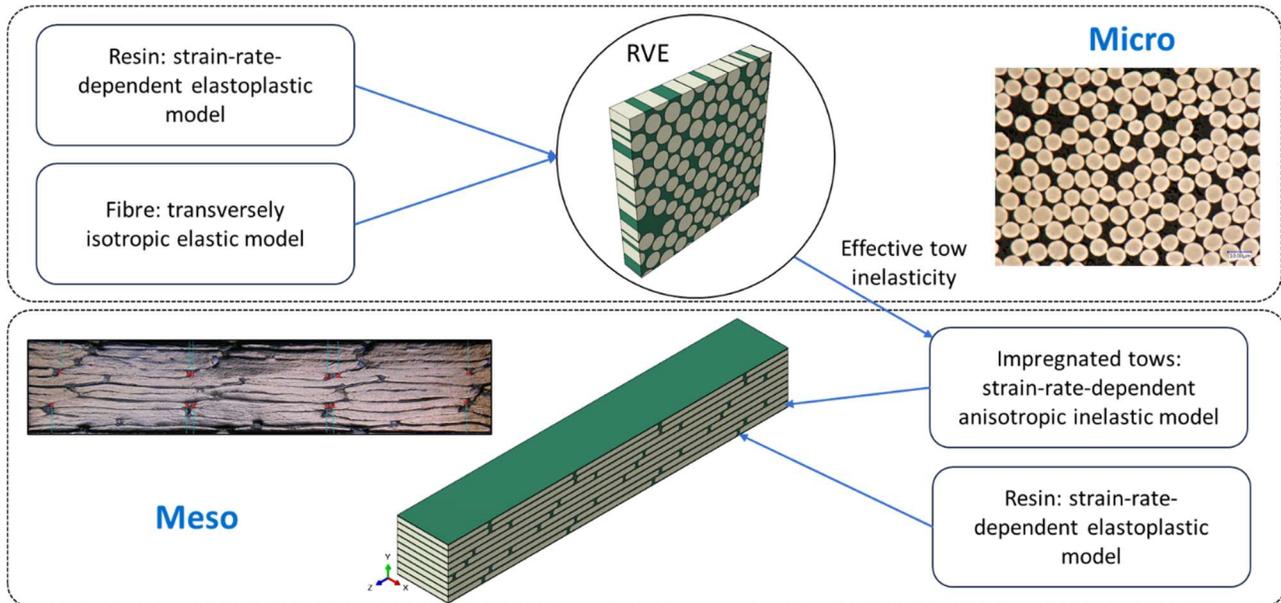


Figure 3. Dual-scale hierarchical FE model was developed for the UD-NCF composite

The mesoscale model extrapolated effective properties of UD-NCF composite laminae using impregnated tow properties from the microscale model and matrix properties. Mesoscale RVEs were crafted to capture impregnated tow geometry, distribution, and in-plane misalignment. A Python script, informed by microscopic assessment data, generated mesoscale RVEs with key features such as periodic boundary conditions, varying tow sizes, nonuniform spatial distribution, in-plane fiber misalignment, and adjustable tow volume fraction (see Fig. 3). In-plane misalignment was managed by rotating the local coordinate system of RVE elements, with random misalignment within specified tow areas. Validation of generated tow patterns was conducted through statistical analysis. A mesoscale RVE size sensitivity study set dimensions to  $10 \times 3 \times 3$  mm. A methodology was developed within the mesoscale RVE to derive material coefficients of chosen Hill's anisotropic elastoplastic models, from predicted strain-stress curves for impregnated tows. These coefficients and models could subsequently be applied to mesoscale FE RVEs to predict the inelastic deformation behaviours of the UD-NCF composite laminae.

### 2.3 NN Models Estimator

A Neural Network model, trained on microscale FE simulation data, was devised to predict local inelastic deformation of impregnated tows, accounting for microstructure variation (Fig. 4). Implemented in Python with PyTorch, it employed feedforward neural networks (FFNNs) for this purpose. The dataset, generated via microscale FE simulations, encompassed random variations in fiber volume fractions and strain rates (e.g., 20% to 70% fiber volume fraction) to mimic inelastic deformation behaviors of impregnated tows. Ensuring minimal manual intervention and randomness in data generation was critical due to the extensive simulations required. Notably, NN models typically excel in interpolation rather than extrapolation, underscoring the importance of generating training datasets covering the desired domain of interest for accurate predictions. Given computational constraints, present research concentrates on data generation for microscale inelastic simulation, with detailed exploration of NN model architecture slated for subsequent papers.

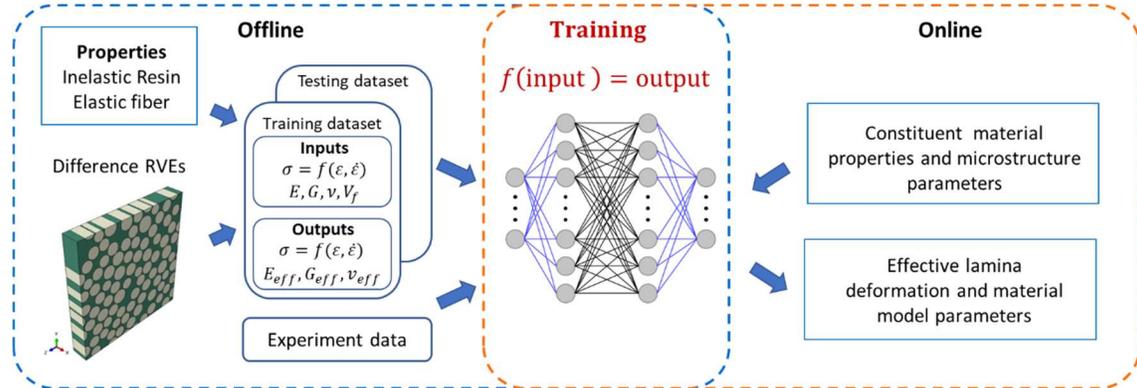


Figure 4. Dual-scale hierarchical FE model to generate training and testing data for the NN models

### 3 Results and discussion

Five repetitive tests were conducted on microscale FE RVEs with 65% fiber volume fraction and random fiber dispersion to predict impregnated tow deformation under various loading modes (Fig. 5). These tests aimed to assess the impact of random fiber dispersion on microscale inelastic simulation results, as the script generated fiber locations randomly. Results showed limited influence of random fiber dispersion on inelastic deformation in longitudinal and transversal tension, as well as in-plane shear modes owing to the relatively high fiber volume fraction. A 12.5% discrepancy was observed in the out-of-plane shear mode, attributed to resin-rich regions, though this did not affect subsequent calibration of the Hill's material model. Hill's model relies on a basic hardening curve, typically derived from the in-plane shear curve, with adjustments for other modes based on yield strength ratios. Following verification of microscale simulation results, the next step involved scripting to standardize results for calibrating the Hill's model for mesoscale FE simulation.

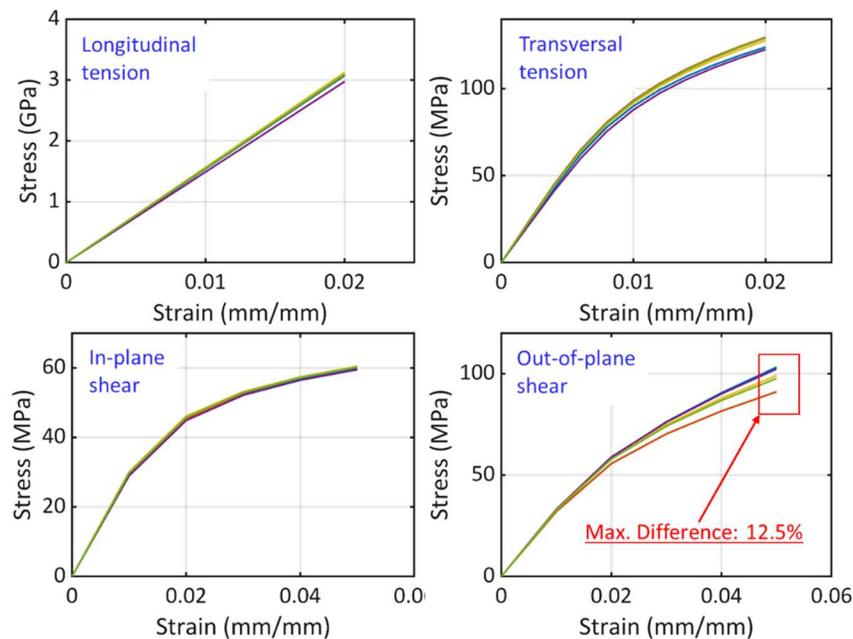


Figure 5. Repetitive tests for RVEs with 65% fiber volume fraction and random fiber dispersion

## 4 Conclusion

This study proposes a multiscale FE modeling approach to predict effective inelastic deformation of UD-NCF composites at micro and meso levels, taking into account the manufacturing-induced defects. An automated script was developed to generate FE RVE models for predicting corresponding effective inelastic deformation of UD-NCF laminae, aiming to produce reliable training and testing data for NN models. These NN models establish relationships between inputs (constituent properties and material structure parameters) and outputs (laminae effective properties), significantly reducing prediction time compared to multiscale FE models while maintaining accuracy. Future tasks include conducting additional simulations to generate ample training and testing data for microscale inelastic NN models. The development of mesoscale NN models awaits availability of a mesoscale dataset for training and testing. Ultimately, integrating microscale and mesoscale NN models into a larger network will enable rapid prediction of effective inelastic deformation of UD-NCF laminae, considering constituent properties and manufacturing defects.

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