NUMERICAL SIMULATION OF POLYMERIC COMPOSITE NANOFIBER MAT

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Abstract. Polymeric composite nanofiber mats have attracted considerable interest due to their unusual features, which include a large surface area, high porosity, and excellent mechanical strength. Numerical simulation is an essential tool for understanding and optimising the behaviour of these nanofiber mats. This research provides a detailed investigation of numerical simulations of polymeric composite nanofiber mats, with particular emphasis on the computational methods used to predict their mechanical characteristics. Tensile testing allows for quick and easy evaluation of the performance of nanofiber composites. To further understand this increase in the mechanical characteristics of polymeric nanofiber composite systems, a finite-element model was built. Using the experimental data of the publicly available authors and an analytical model, the model is evaluated and compared. To compare the numerically and experimentally determined values of the elastic modulus of the nanofiber composite, the Rule of Mixture (ROM) and Tsai-Pagano models were used. Using the experimental data, Representative Volume Elements (RVE) were built, and the elastic modulus was predicted using RVE. In comparison to an additional analytical model, the RVE model that makes use of numerical simulation predicts an elastic modulus that is very nearly identical to the value that is practically observed. In this work, a technique for forecasting the elastic modulus is proposed using a numerical simulation of the nanofiber composite mat.

Keywords: nano composites, nanofiber, mat, elastic modulus, RVE.

Introduction

Nanofiber composite mats have received a great interest due to their exceptional features, including a large surface area, mechanical strength, and porosity [1-4]. Nanofibers offer numerous options to change things physically and chemically during or after the fabrication process to give them novel properties [5-7]. This makes them interesting materials for a variety of applications, including tissue engineering [8; 9], medication delivery [10; 11], water filtering [12-14], and smart textiles [15-17]. However, understanding and optimising their mechanical behaviour is essential for effective use of these materials in various applications [18].

Numerical simulation has become an indispensable tool for understanding and forecasting the mechanical behaviour of polymeric composite nanofiber mats [19-21]. These simulations provide the study of complicated material behaviour at many sizes, from molecular to macroscopic. They also allow the examination of the impact of numerous characteristics, such as the polymer type, fibre diameter, and interfacial adhesion, on the properties [22].

This research focuses on numerical modelling of the mechanical behaviour of polymeric composite nanofiber mats using the finite element analysis (FEA). FEA is a commonly employed approach for simulating the behaviour under different loading circumstances [22; 23]. Experimental data and analytical models were used to create a representative volume element (RVE) for the FEA model generated in this work [25]. Polyacrylonitrile (PAN) and polyamide 6 (PA6) were the components of the polymeric composite nanofiber mats studied in this article. PAN is a synthetic polymer with high mechanical qualities, such as high modulus, whereas PA6 is a well-known engineering thermoplastic with outstanding thermal and chemical resistance [25-27]. The combination of PAN and PA6 in the composite matrix results in better mechanical characteristics due to a synergistic effect [28; 29]. The interfacial bonding between nanofiber mats plays a vital role in defining the mechanical behaviour of the composite [23].

The RVE model was created to replicate the microscale mechanical behaviour of the composite. It comprises a unit cell that repeats and captures the complex shape as well as the interfacial bonding between the two nanofiber mats. The RVE model was used to forecast the elastic modulus, an important mechanical parameter that influences the stiffness of the material [30].

Comparing the predictions of the RVE model with publicly available experimental data [31] served to verify and confirm the validity of the model. The findings of this work indicate that the RVE model is a useful tool for forecasting the mechanical behaviour of nanofiber composite polymeric mats [32].

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The findings might contribute to the creation of polymeric composite nanofiber mats with enhanced mechanical characteristics for diverse applications.

Modelling and boundary conditions

The FEM model has been included in ANSYS software. The following is a description of the CAD model, material attributes, and boundary conditions. Fig. 1 depicts the RVE model of the nanofiber mat based on the assumption that the entire nanostructure is fully filled, and the nanofiber mat contains no voids. The material is assumed to be isotropic and linearly elastic.

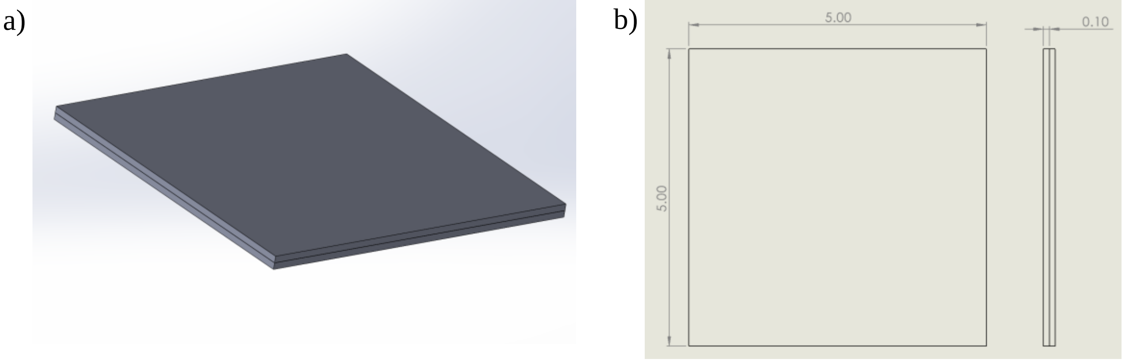

Fig. 1. **RVE of nanofiber composite mat of PAN and PA6:** a – 3D model;
b – 2D model with dimension in mm

Table 1 represents the experimental data of the authors and the material properties used for the numerical simulation.

Table 1

Average mechanical properties of PAN, PA6, and composite nanofiber mat [31]

Materials	Tensile Strength at Break, MPa	Young’s Modulus E, MPa	Strain, %
PAN nanofiber mat	19.1 ± 1	1510 ± 11	3.5 ± 0.2
PA6 nanofiber mat	14.9 ± 2	405 ± 6	11.2 ± 0.5
Composite nanofiber mat	13.1 ± 1	917 ± 8	2.8 ± 0.3

Many assumptions are used in order to compute the elastic modulus of a composite material using a representative volume element (RVE). RVE is considered homogeneous, which means that the material properties are constant throughout the volume. It is presumed that RVE is continuous, meaning that there are no voids or other flaws that might impair the material properties. The material is assumed to be linearly elastic, indicating that the stress-strain relationship within the elastic range is proportionate and reversible. The material is considered isotropic, meaning that its characteristics are identical in all directions. There is no contact between the phases of the composite material. This means to be expected that there is no sliding or debonding between the layers. These assumptions allow the elastic modulus of a composite material to be calculated from RVE using the conventional equations of elasticity and linear elasticity theory.

Boundary conditions: in the FE model, boundary conditions were applied to the face of the unit cell to create stress. The nodes on one of the two opposing sides were prevented from out-of-plane displacement and rotation, while the nodes on the other face were allowed to freely move along the plane. This constraint was overcome by requiring each face to have a frictionless support. In the direction perpendicular to the faces of the limited face, the opposite faces were evenly shifted by 0.1 mm. The surface displacement of 0.1 mm on the right face normal to the right plane was defined for the longitudinal Y direction, as represented in the preceding figure. Both the bottom and the left surfaces serve as friction-free supports. A boundary condition is stated to guarantee that the stress is uniformly distributed over the geometry and that the geometry maintains its symmetries. The model employs a fine mesh, because it enables the resolution of small-scale features and phenomena that would be overlooked with a coarser mesh. This is relevant because small-scale characteristics can have a substantial effect on the overall behaviour of the simulated system.

Results and Discussion

Figs. 2 and 3 depict the average stress and strain values of the composite. The maximum stress on the provided displacement face is 98.83 MPa, while the minimum value is 7.5 MPa. Using the mean value of the stress and the initial known displacement, the elastic modulus of the composite nanofiber mat has been determined as 913 MPa. The estimated elastic modulus of the nanofiber composite mats corresponds to the experimentally determined value of 917 ± 8 MPa. The results obtained reflect the same results as those obtained with electrospun composite laminates and nanofibers in textiles [15].

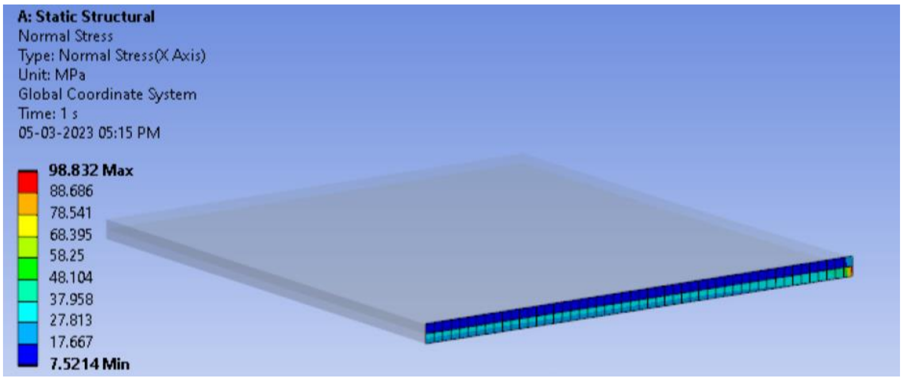
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Fig. 2. **Stress in the normal direction along the longitudinal axis**

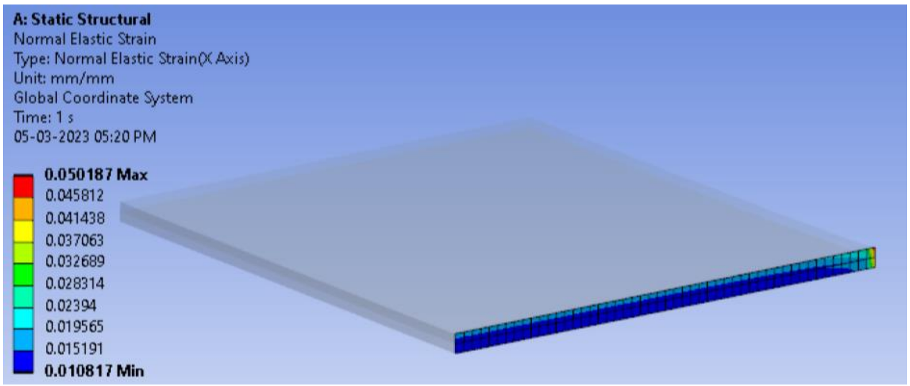
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Fig. 3. **Strain in the normal direction along the longitudinal axis**

Fig. 4 shows a comparison of numerical findings using experimental data and analytical models, using ROM and the Tsai-Pagano model [33]. The experimental value of the elastic modulus of a nanofiber composite mat was 917 ± 8 MPa, while numerical simulation predicted a value of 913 MPa. The ROM model predicted an elastic modulus of 957.5 MPa, and the Tsai-Pagano model underestimated the value by 758.24 MPa [31].

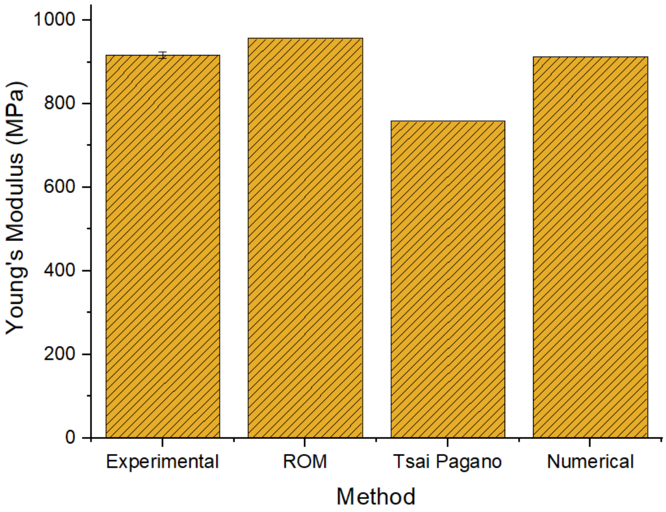

Fig. 4. **Comparison of the calculated Young's modulus with different methods**

Conclusions

Based on the results given, it can be concluded that the numerical simulations using the ROM model and the Tsai-Pagano model provided predictions for the elastic modulus of the nanofiber composite mat, but the precision of the predictions differed significantly; namely, the ROM model predicted an elastic modulus of 957.5 MPa, which is closer to the experimental value of 917 ± 8 MPa, while the Tsai-Pagano model significantly underestimated the value with a value of 758.24 MPa.

The predicted value of 913 MPa from the numerical simulation is very close to the experimental value, but the ROM model gives a more accurate prediction of the nanofiber composite mat's elastic modulus. However, it is worth noting that the accuracy of these models may vary depending on the specific properties of the nanofiber mats being tested and the conditions of the experiment for collecting the nanofibers.

Overall, these results suggest that numerical simulation can be a useful tool for predicting the properties of nanofiber composite mats and can provide accurate predictions of the elastic modulus when compared to experimental data. Further research could explore the use of other models and experimental techniques to improve the accuracy of these predictions.

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Authors' contributions

Conceptualization, J.V.S; methodology, J.V.S; software, J.V.S., S.P.K., and U.K.; validation, J.V.S.; formal analysis, S.P.K. and U.K.; investigation, S.P.K. and U.K.; data curation, S.P.K. and U.K. and J.I.; writing – original draft preparation, J.V.S.; writing – review and editing, J.V.S., S.P.K. and V.B.; visualization, J.V.S.; funding acquisition, J.V.S. and S.P.K. All authors have read and agreed to the published version of the manuscript.

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