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Finite Element Modelling for Fracture of Multilayer Fibrous Networks

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Abstract: Tissue engineering involves three-dimensional scaffolds to support cell culture activities and provide mechanical support. One of the potential scaffolds used in tissue engineering is an electrospun scaffold consisting fibres ranging from nano- to micrometer scales deposited on layer stack. The finite element models have been used to study the in-plane deformation of two-dimensional single layer fibrous networks. The two-dimensional models do not consider the out-of-plane deformation of layer structured of electrospun scaffolds through the scaffolds thickness. In this study, three-dimensional finite element model was constructed to investigate the fracture of multilayer fibrous networks. The three-dimensional results were compared with the fracture on two-dimensional single layer fibrous network. The result shows that these two models had identical fracture behaviour and similar deformation at the crack-tip region, where the fibres are rearranged and reoriented with similar stress distribution. The work here concludes that two-dimensional single layer fibrous network model is a simple yet effective model for the study of homogeneous fibrous networks.

Keywords: Fibrous networks, multilayer, fracture

1. Introduction

Electrospinning technique is a simple technique to produce fibrous materials with fibers ranging from nano- to micrometer scales that deposited on layer stack [1-2]. The simplicity and diversity of electrospinning technique attract the use of electropun scaffolds in various applications. One of the applications is to act as scaffold in tissue engineered construct. The microstructure architecture of fibrous scaffolds is designed to meet a certain requirement of tissue engineering. Sufficient mechanical property is required in tissue engineering to support loading applied on the tissue engineered constructs [3].

In recent years, the approach to understand the mechanical behavior of fibrous networks has been intensive. These approaches are done by either experimental samples or computational models [4–13]. The current approaches to generate computational model for fibrous networks are based on multiscale simulation combining microscopic and macroscopic models [6], post processing of SEM images [14, 15], fiber deposition method and dynamic analysis of fibrous networks [16, 17].

The priority for a computational model is to develop a simple and effective model to study the mechanical properties of fibrous networks under different loading condition. Hence, a certain assumption is usually found in computational models. One of the assumptions is treating a fibrous network as a two-dimensional single layer fibrous network without considering out-of-plane deformation [18]. The two-dimensional models are often modelled with large thickness and assume that the networks deform in in-plane condition. This leaves an interesting question on the effect of this projected thickness on two-dimensional model. Further, it remains unclear on how significant the out-of-plane

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deformation affects the mechanics of thin scaffolds. The study on out-of-plane deformation require a three-dimensional multilayer fibrous networks model that consider other parameters like torsional stiffness of fibers.

The objective of this work is to compare the fracture behavior of two-dimensional (2D) single layer fibrous network and three-dimensional (3D) multilayer fibrous networks. Both 2D and 3D consist identical network architecture of an electrospun scaffold. Further, a study on the effect of projected thickness on 2D single layer fibrous network was constructed. Such findings suggest a simple and effective computational model for the study of homogeneous fibrous networks.

2. Methodology

2.1 Modelling of Fibrous Networks

MATLAB code from previous work [16] was used to construct 2D single layer fibrous networks. Fibrous networks were generated in MATLAB 2017b software by placing random line at random positions with random angles. These random lines were then extended to model boundary and were randomly bonded at the same node depending on user-defined cross-link percentage (*i.e.* the ratio between the sum of bonding points and the sum of fiber intersection points). The fiber density (*i.e.* the sum of fibers per unit area) and cross-link density (*i.e.* the sum of bonding points per unit area) of fibrous networks were calculated. In this work, 2D fibrous networks were constructed with fiber density of 6403.6 mm^{-1} and were cross-linked at cross-link percentage of 15 % and 50 %. The fiber density is defined as the sum of fiber length per unit area. The fibers were modelled with rectangular profile with the width of 300 nm and thicknesses of 1 m [18], 1 mm, 10 μm and 1 μm. The thickness was defined as model thickness in this paper.

The 3D multilayer fibrous networks were generated by using MATLAB 2017b software. The networks were constructed layer by layer with 2D model construction method. Each layer was constructed by sequence and connected to each other. The networks were cross-linked within layer by intralayer cross-link and bonded between layer to layer by interlayer cross-link. Fig. 1 shows multilayer fibrous networks that consists of 3 layers of fibrous networks, which are bonded between layers at the thickness of *a*. In this study, 3D multilayer fibrous networks were constructed in 3 and 5 layers and with constant fiber density of 6558.01 ± 124.03 mm^{-1} for each layer. The networks were cross-linked within layer and between layers at cross-link percentage of 15 %. The total cross-link density of multilayer fibrous networks are made of the sum of intralayer and interlayer bonding points for the first network layer. The fibres were modelled with circular profile with diameter of 300 nm.

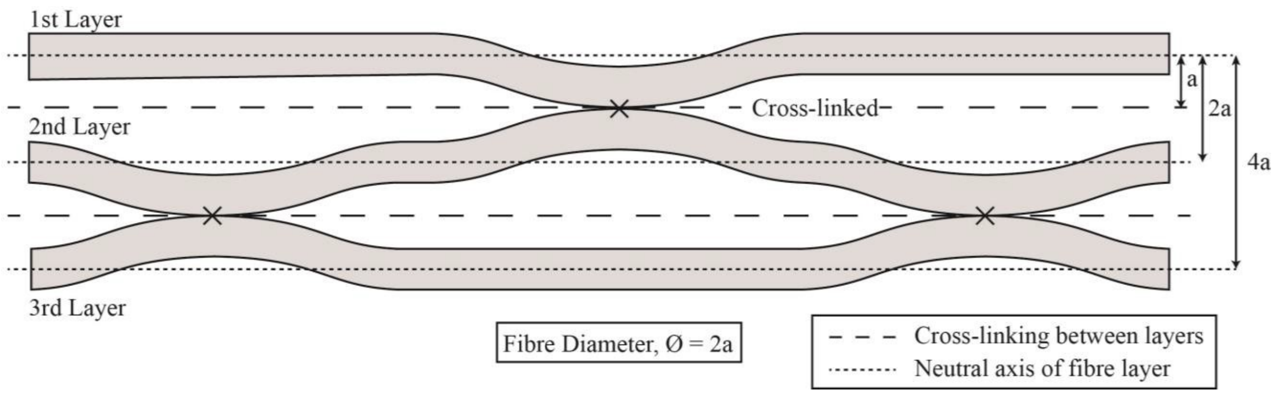

Fig. 1 - Schematic illustration of the finite element model of a multilayer fibrous network

All the networks models were imported into finite element software, ABAQUS 2017 and were analyzed by using nonlinear finite element analysis, which considers large strain and rotation. The fibers were defined with Young's modulus, *E* of 100 MPa and fracture strength, σ_f of 30 ± 4 MPa [18].

2.2 Fracture Analysis

The 2D and 3D fibrous networks were constructed in a circular unit with 75 μm radius and with a 75 μm notch length. The boundary conditions were subjected to the displacement field associated with the macroscopic crack tip field for a homogeneous and isotropic materials. The boundary conditions were calculated from the equations obtained in Kanninen and Popelar [19]:

$$u_1 = \frac{1}{2}\sqrt{\frac{r}{2\pi}}\frac{K_1}{G}\left[\kappa - 1 + 2\sin^2\frac{\theta}{2}\right]\cos\frac{\theta}{2} \quad (1)$$

$$u_2 = \frac{1}{2}\sqrt{\frac{r}{2\pi}}\frac{K_1}{G}\left[\kappa + 1 - 2\cos^2\frac{\theta}{2}\right]\sin\frac{\theta}{2} \quad (2)$$

Where (u_1, u_2) are the displacements for x and y directions at the model boundary, r is the distance of the node from the crack-tip, θ is the angle between node and crack-tip and K_I is the stress intensity factor for mode I. The fibrous network models were expected to have plane stress condition, where $\kappa = (3-v)/(1+v)$ with Poisson's ratio, v of 0.3. The shear modulus of fibrous network, G was assumed to be 4 MPa [16]. The fracture toughness was characterized by measuring stress intensity factor (SIF) once failure criterion met. The network was assumed to fracture once the first fibre exceeded its fracture strength.

3. Results

3.1 Fracture of 2D Single Layer Fibrous Network

The 2D fibrous networks were constructed to study the effect of model thickness on fracture behavior of fibrous networks. Fig. 2 shows the stress intensity factors for 2D single layer fibrous networks with various model thicknesses. The result shows that the networks have consistent stress intensity factor for model thickness ranging from 1 µm to 1 m. Moreover, the deformation of networks at the crack-tip is similar for all the networks. The critical failure location of these networks are found at the same fiber and location. The result indicates that 2D fibrous network with model thickness ranging from 1 µm to 1 m has similar fracture behavior. This indicates that the 1 µm thickness is large enough to allow the networks deform in in-plane manner.

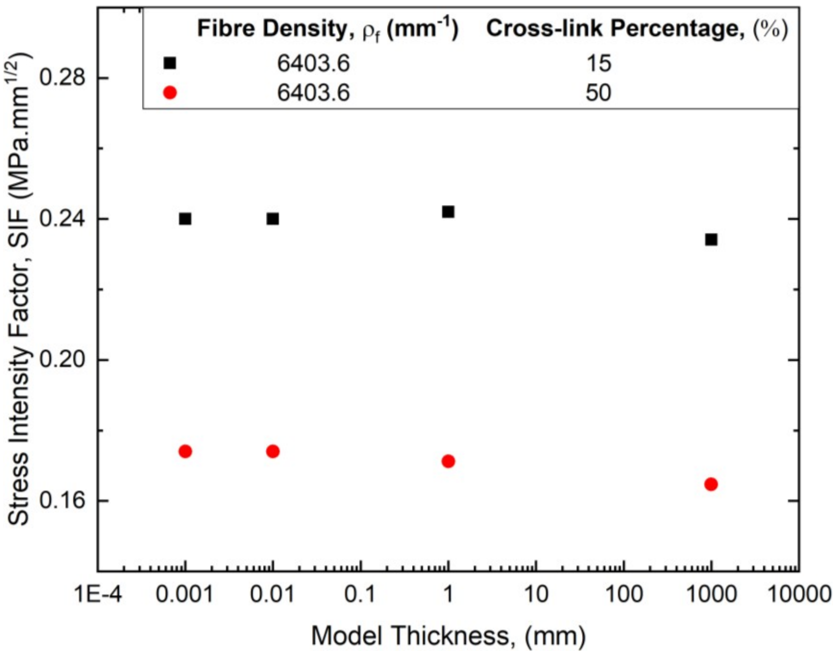

Fig. 2 - Stress intensity factor of 2D single layer fibrous networks constructed with various model thicknesses

3.2 Fracture of 3D Multilayer Fibrous Networks

The 3D multilayer fibrous networks were constructed to study the effect of out-of-plane deformation on thin scaffolds. Fig. 3 shows the comparison of the stress intensity factor for 2D single layer fibrous networks modelled with model thickness of 1 m and 3D multilayer fibrous networks modelled with circular cross-section. The result shows that 3D multilayer fibrous networks constructed with 3 and 5 layers have comparable stress intensity factor to 2D fibrous network with cross-link percentage of 50 % instead of 15 %. This is attributed to the additional interlayer cross-link from 3D fibrous networks that act towards each network layer. The total cross-link density of multilayer fibrous networks were now close to the cross-link density of 2D fibrous networks that constructed with cross-link percentage of 50 %. Further, the deformation of these networks at the crack-tip is found to be similar, where the fibres are rearranged and reoriented with similar stress distribution (Fig. 4).

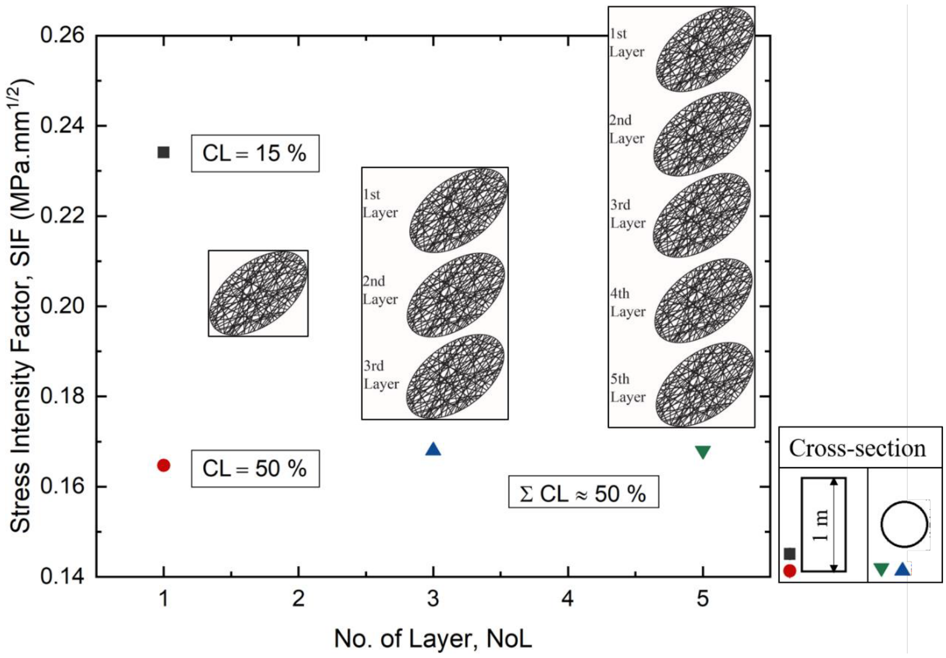

Fig. 3 - Comparison of the stress intensity factor for 2D single layer fibrous networks and 3D multilayer fibrous networks

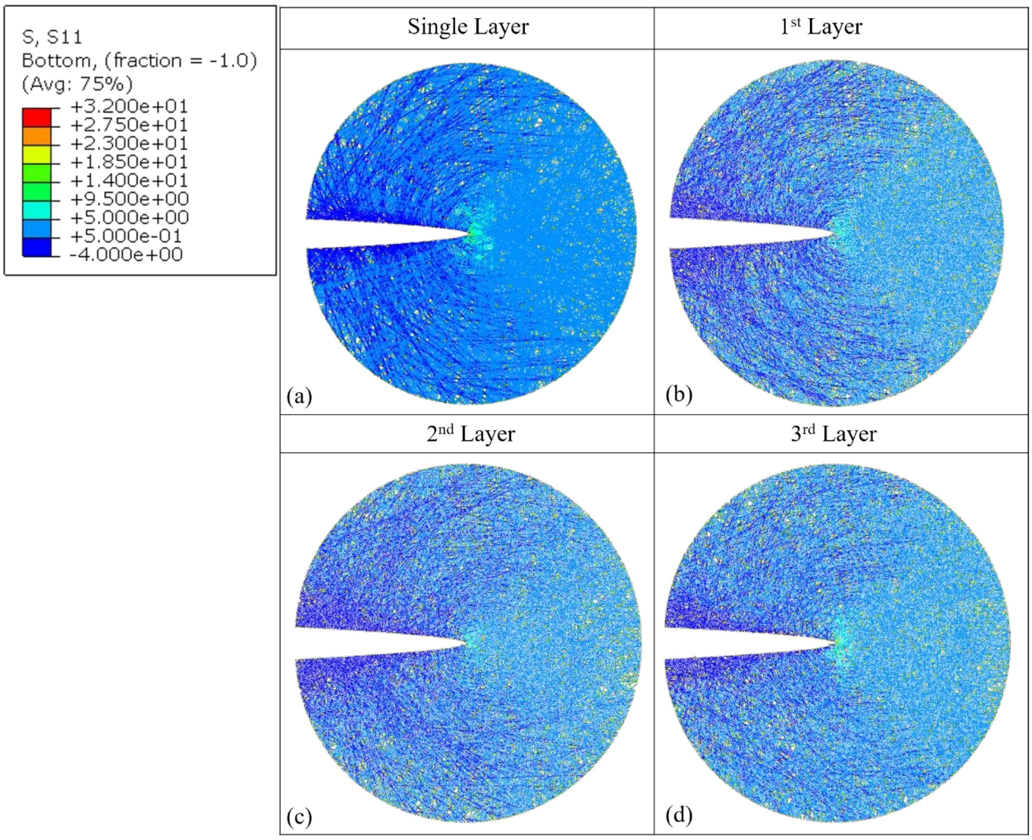

Fig. 4 - The stress distribution for (a) 2D single layer fibrous network with cross-link percentage of 50 % and (b-d) 3D multilayer fibrous networks

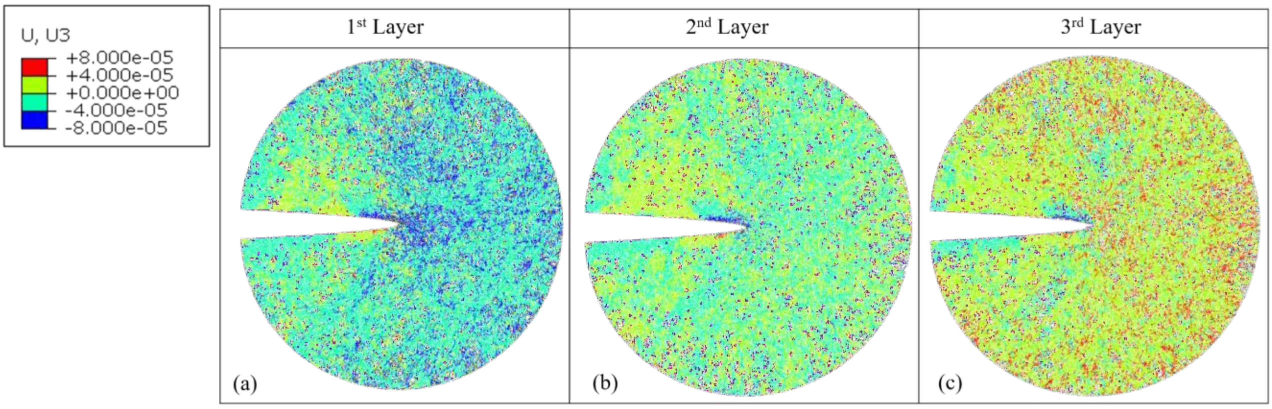

Fig. 5 - The out-of-plane deformation for (a) first layer, (b) second layer and (c) third layer of 3D multilayer fibrous networks

Fig. 5 shows the out-of-plane deformation for each network layer of 3D multilayer fibrous networks. The finite element result shows that 3D fibrous networks deform along the thickness of networks, where the first and the last layer of networks deformed towards the mid-plane of networks (*i.e.* second layer of networks). The out-of-plane deformation of each network layer are relatively small as compared to the thickness of networks. The network layers deform with a maximum out-of-plane displacement of 80 nm as compared to the networks thickness of 600 nm.

4. Discussion

Multilayer fibrous networks are often simplified into 2D fibrous networks that consider only in-plane deformation. The out-of-plane deformation of multilayer fibrous networks considers other parameters like torsional stiffness and bending stiffness and could possibly affect the fracture of fibrous networks. In this work, 2D and 3D models having homogeneous fibrous networks are shown to have identical stress intensity factor. To explain these results, analysis on the out-of-plane deformation, deformation mechanism and stress distribution of multilayer fibrous networks were considered. The relatively small deformation of each network layer along the thickness indicates that multilayer fibrous networks deform mainly in in-plane condition with minimum influence from out-of-plane deformation. The deformation mechanism of multilayer fibrous networks at the crack-tip region are similar to 2D fibrous network, which involves of fiber rearrangement and reorientation. This shows that the toughening mechanism of both models are similar. The 2D studies had highlighted the importance of fiber rearrangement and reorientation on the fracture of fibrous networks [16, 20, 21]. Further, the stress distribution of multilayer fibrous networks at the crack-tip region are identical to 2D fibrous network. Both 2D and 3D models had highest stress at the crack-tip and the stress are progressively distributed to the far-field. The result suggests that 3D multilayer fibrous networks can be reduced to 2D single layer fibrous network without any significant impact in simulating the fracture of homogeneous fibrous networks. The assumption of in plane deformation however relies on the thickness and consistent distribution of fibrous network structures. The homogeneous fibrous networks investigated here had uniform random fibrous networks throughout the thickness. The 2D models require further validation for the fibrous materials having non-uniform microstructures [24-25]. In general, finite element analysis is an effective tool to study mechanical behaviors of medical devices under different loading conditions [26].

5. Conclusion

The computational models for fibrous networks are often treated as a 2D single layer fibrous network with projected thickness. This work demonstrated that such model is an appropriate fracture model, where the fracture behaviour and deformation at the crack-tip region are similar to 3D multilayer fibrous networks. In addition, the work here suggests that 2D single layer fibrous networks modelled with projected thickness ranging from 1 µm to 1 m predict similar fracture behaviour. The work here demonstrates the suitability of 2D finite element models in simulating the fracture of homogeneous fibrous networks.

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