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Geometric characterization and simulation of planar layered elastomeric fibrous biomaterials

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ABSTRACT

Many important biomaterials are composed of multiple layers of networked fibers. While there is a growing interest in modeling and simulation of the mechanical response of these biomaterials, a theoretical foundation for such simulations has yet to be firmly established. Moreover, correctly identifying and matching key geometric features is a critically important first step for performing reliable mechanical simulations. The present work addresses these issues in two ways. First, using methods of geometric probability, we develop theoretical estimates for the mean linear and areal fiber intersection densities for 2-D fibrous networks. These densities are expressed in terms of the fiber density and the orientation distribution function, both of which are relatively easy-to-measure properties. Secondly, we develop a random walk algorithm for geometric simulation of 2-D fibrous networks which can accurately reproduce the prescribed fiber density and orientation distribution function. Furthermore, the linear and areal fiber intersection densities obtained with the algorithm are in agreement with the theoretical estimates. Both theoretical and computational results are compared with those obtained by post-processing of scanning electron microscope images of actual scaffolds. These comparisons reveal difficulties inherent to resolving fine details of multilayered fibrous networks. The methods provided herein can provide a rational means to define and generate key geometric features from experimentally measured or prescribed scaffold structural data.

1. Introduction

Many important biomaterials are composed of multiple layers of networked fibers. Elastomeric fibrous scaffolds used in engineering soft tissues are a prime example [1]. Since soft tissues undergo large deformations [2,3], the constituent fibers must have elastomeric characteristics and undergo large macroscopic deformations as a result of large rotations and strains. These characteristics allow the scaffolds to duplicate many of the salient characteristics of the soft tissues they are intended to replace [4]. The scaffolds are also expected to have multiple functions, including facilitation of cell attachment and support of de novo tissue synthesis and stress transfer [1]. To meet these multifaceted demands, one must develop a fundamental understanding of the underlying physical processes occurring within the scaffolds across multiple scales [1].

Currently, electrospinning is a common process for elastomeric scaffold fabrication [1,5]. This process results in very long, often undulated "continuous" fibers that form dense networks with layered structures. Other approaches focus on reconstituted collagen or fibrin gels [6]. Regardless of the methodology used to create the scaffold structures, it is well established that the fiber geometry significantly influences the macroscopic mechanical response [7,8]. Accordingly, there has been a considerable amount of effort devoted to characterization of the fibrous geometry, with the focus on measuring an in-plane fiber orientation density function and establishing its relations with mechanical anisotropy [5,9–13].

Generally, current approaches to simulating fibrous network geometries are based on: (i) generating Voronoi diagrams [14]; (ii) generating assemblies of straight fibers with prescribed orientations [15]; (iii) using method (ii) to generate a network that is used as the initial state of a dynamics simulation in which the fiber positions and orientations evolve, and crosslinks are formed [16];

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and (iv) direct post-processing of scaffold images [10]. While all four approaches have been successfully used for predicting the macroscopic mechanical response in terms of fiber stiffness and volume fraction, the generated geometries simply do not consistently resemble the actual ones and involve somewhat subjective, empirical rules. Most importantly, the geometric parameters necessary for modeling and simulation of other aspects of mechanical behavior of fibrous networks are yet to be defined.

Herein, we rely on methods of geometric probability to develop theoretical estimates for the mean linear and areal fiber intersection densities for 2-D fibrous networks. These densities are expressed in terms of the fiber density and the orientation distribution function, both of which are relatively easy-to-measure properties. Secondly, we develop a 2-D random walk algorithm capable of generating realistic geometric models of fibrous network layers. This algorithm can greatly benefit further studies concerned with micromechanical modeling by generating geometries that resemble actual ones. We further present simulation results aimed at validating the assumptions underlying the theoretical development, testing the algorithm performance and establishing the minimum specimen size necessary for capturing macroscopic properties. Finally, we show how the theory and simulations can complement the use of experimental observations to more accurately determine important features of the material's microstructural geometry.

2. Methods

2.1. Derivation of key geometric relationships for planar fibrous networks

The materials considered in the present work can be idealized as a set of multiple, connected planar 2-D networks of long, curved fibers. This has been shown to be a very good idealization for electrospun polyester urethane urea (ES PEUU) scaffolds (Fig. 1), as well as many other important biomaterials. Our approach is thus restricted to layered networks, which can be treated as an assembly of 2-D monolayers. We introduce basic quantities that characterize 2-D fibrous geometries, the linear and areal intersection densities for planar fibrous networks, and develop simple expressions in terms of the fiber density and orientation density function. These quantities allow estimation of a characteristic segment length between neighboring fiber intersections. The derived expressions significantly simplify the task of microstructural characterization, since the intersection densities are difficult to measure directly.

We begin with a simplified model, in which a fibrous layer is represented as a 2-D network the building blocks of which are short, straight line segments. First, we establish some results for such networks of disjoint segments, then we extend those results to networks of long, curved fibers composed of connected segments. In the process, we adopt minimal assumptions required to establish simple expressions for the linear and areal intersection densities in terms of the linear fiber density and the orientation density function (ODF). The mathematical problem considered in this section can be classified as a generalization of the classical Buffon's needle problem [17]. In this problem, a needle of known length is dropped onto a floor composed of many parallel floor boards of known width, and we seek the probability that the needle lands on a boundary line between the adjacent floorboards. This problem represents the beginning of the field of geometric probability [18].

Let us consider a domain in Euclidean space $\Omega \in R^2$, the area of which is equal to A. The domain contains m straight line segments, each of length s. We suppose that $m \gg 1$ and assign to the segments an ODF $f(\varphi)$ such that the probability that any given segment has an orientation between φ and $\varphi + \Delta\varphi$ is $\Delta p = f(\varphi)\Delta\varphi$. The ODF is periodic, such that $f(\varphi) = f(\varphi + \pi)$, and therefore the angle φ can be restricted to the interval $[0, \pi)$. The segment centers are uniformly distributed in Ω following a Poisson's process [19]. It is expedient to assume that Ω is a unit cell of a periodic structure. Accordingly, the segments protruding outside of Ω can re-enter it from the opposite side.

Let us consider a randomly placed test straight line segment $\mathcal{T}$ of length L_t cutting through some of the m segments in Ω and oriented at an angle φ. Then a segment $\mathcal{S}$, oriented at an angle between φ' and $\varphi' + \Delta\varphi'$, intersects $\mathcal{T}$ if and only if the center of $\mathcal{S}$ is located inside the parallelogram $\mathcal{P}$ with edges of length L_t and s, and angle $|\varphi - \varphi'|$ (Fig. 2).

Since the area of $\mathcal{P}$ is equal to $sL_t \sin|\varphi - \varphi'|$, the probability that $\mathcal{S}$ is oriented at an angle between φ' and $\varphi' + \Delta\varphi'$, *and* intersects $\mathcal{T}$ is equal to

$$\Delta p = \frac{sL_t \sin|\varphi - \varphi'|}{A} f(\varphi')\Delta\varphi' \tag{1}$$

Accordingly, the probability that any segment, regardless of its orientation, intersects $\mathcal{T}$ is equal to

$$p(\varphi) = \frac{sL_t}{A} \int_0^{\pi} \sin|\varphi - \varphi'| f(\varphi') d\varphi'. \tag{2}$$

Let n denote the number of intersections along $\mathcal{T}$; the corresponding probability density function is denoted by $g(n)$. Since the position and orientation of each segment are independent of the positions and orientations of all the other segments, the intersections with $\mathcal{T}$ are independent events. This is a classical setting leading to the binomial distribution with the probability density function

$$g(n) = \frac{m!}{n!(m-n)!} p^n (1-p)^{m-n} \tag{3}$$

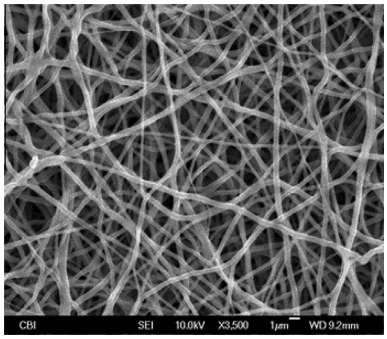

Fig. 1. Scanning electron microscope image of the top layer of an ES PEUU scaffold [10]. The fiber diameter is approximately 1 micron.

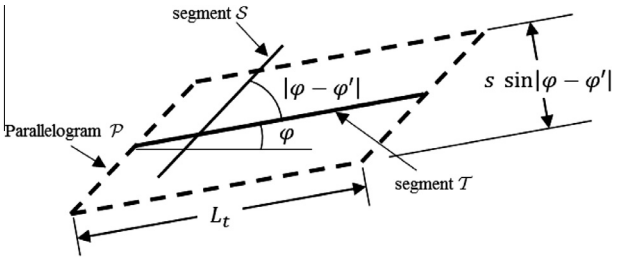

Fig. 2. An arbitrary segment $\mathcal{S}$ having length s and orientation angle φ' intersects the test segment $\mathcal{T}$ having length L_t and orientation angle φ if its center lies within the parallelogram $\mathcal{P}$ designated by the dashed lines.