

Bio-inspired Electrospun Fibre Structures - Numerical Model

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Abstract

A systems approach that integrates processing, structure, property and performance relations has been used in the design of multilevel-structured fibrous materials. For electrospun fibrous structure, numerical implementation of multiscale materials philosophy provides a hierarchy of computational models defining design parameters that are integrated through computational continuum mechanics. Electrospun micro/nano (multiscale) poly(ϵ -caprolactone) (PCL) fibrous scaffolds were studied. The fibrous structures were evaluated for their mechanical, morphological and cell attachment properties. The cell attachment studies showed that cell activity on multi-scale scaffolds was higher compared to micro-fibrous scaffolds. These results suggest that the combination of a micro- and nano-fiber hierarchical scaffold could be more beneficial for tissue engineering applications than for individual scaffolds.

Keywords: Electrospun PCL; Multiscale; Numerical Model

1 Introduction

The variety of materials and fibrous structures that can be electrospun allow for the incorporation and optimization of various nanofiber functions, either during spinning or through post-spinning modifications [1]. Electrospun nanofibers have more than ever received greater attention, primarily because nanoscaled structures can be easily fabricated by the simple electrospinning process. These non-woven structures show unique morphologies in nano- or micrometer scales according to various electrospinning conditions. The unique relationship between surface and mechanical properties that occurs at the nanoscale define features that form the basis of nanoscale fibres and their versatility [2-4]. The chemical interactions dominate at smaller scales while bulk mechanics at larger scales. The balance between them in the system is a determinant factor from the aspect of assembly, from shape to chirality to hierarchy. Complicated phenomena for fibrous structure operate at multiple material scales and are governed by varying degrees of network properties;

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thus, numerical models are a necessary tool to unravel the relationships among individual network components and the aggregate properties and functions of the whole system. For example, scaffold design structures, their fabrication and structural behaviour at different scales lead to numerous experimental and computational challenges. In particular, there is a need for modelling and test tissues at multiple scales to gain an insight into issues such as drug delivery, drug interaction and cellular–environment interactions. The modelling of bio-inspired materials, such as fibrous scaffold, involves the concepts of both forward and inverse modelling [5]. A forward problem is to simulate biological material properties and responses using internal microstructures already determined by nature. On the other hand, a bio-inspired design may be regarded as an inverse problem. Here the internal microstructures are not initially known and the aim is to design these structures that will provide the desired properties, which may be required to be superior to those of nature. An inverse problem is inherently difficult since the specified performance criteria might consist of multiple properties (high strength, high toughness, significant extensibility, etc.) and multi-physics properties (elastic stiffness, thermal conductivity etc.).

Learning from nature is a source of bio-inspiration for scientists and engineers to design multifunctional synthetic materials with multiscale structures. Hierarchical structures with extraordinary properties that exist are widespread in bio-systems, such as bone, skin, nacre (shell) etc. The lessons drawn from hierarchical biological materials could obviously help us to design new nanostructure engineering materials and products [6-8]. Hierarchy in a material system is represented by several structural quantifications. The first come from the multiscale nature, i.e., the system is built on different structural levels with gradual transition in sizes among them. This multiscale always brings multiple heterogeneity into the system where each phase occupies a relevant structure level. This current paper examines how such multi-scaling, hydrogenizing or multi-phasing are advantageous or beneficial to account for the associated unique functionalities in fibrous materials systems.

2 Hierarchical Nanofiber-based Structure

According to the present stage of technology [9], at least four different levels of organization (see Fig. 1) can be put together to form a nanofiber based hierarchically organized structure. At the first level (nanoscale), nanoparticles or a second polymer can be mixed in the primary polymer solution and electrospun to form composite nanofiber. With the incorporation of nano-objects into electrospun solution it is possible to create nanofibers with various properties such as conductive network, ultraporous fibers, and ultrastrong fabrics. Using a dual-orifice spinneret design, a second layer of material can be coated over an inner core material during electrospinning to create the second level organization. Rapid evaporation of the solvents during the spinning process reduces mixing of two solutions, thus forming core-shell nanofiber. Hollow nanofiber has many applications in drug transport, nanofluid devices, and nanofibre sensors. At the same level, various surface functionalization techniques may be used to introduce an additional property to the nanofiber surface. The third level organization is fibres oriented and organized to optimize structural performance. A multi-layered nanofiber fabric or mixed micro-nanofibers 3D structure can be fabricated *in situ* through selective spinning or using a multiple orifice spinneret design, respectively. There are various methods to produce a multiscale structure; one of them is to use modulation processing parameters during electrospinning and different setup constructions. Finally, the nanofibrous assembly may be integrated within a microfiber structure with various