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# Modeling effects of fiber rigidity on thickness and porosity of virtual electrospun mats

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ABSTRACT

Despite the widespread applications of electrospun fibers, there is still no accurate method to measure the thickness or porosity of thin electrospun mats. The current study is devised to develop a modeling approach toward solving this problem by simulating the 3-D structure of nanofiber mats. The uniqueness of our algorithm is in its ability to capture how the fibers conform to the geometry of the surface on which they deposit. This feature is important for predicting how the thickness of a nanofiber mat grows as fibers continue to deposit on the collector. Our algorithm is implemented in a C++ computer program, and is used to study the effects of fiber rigidity, fiber diameter(s), and fiber orientation on the thickness and porosity of electrospun mats. Contrary to the common belief, it was shown that reducing fiber diameter, while maintaining the total weight of the material constant, does not necessarily lead to an increase in the thickness and porosity of the resulting mat. The thickness and porosity of electrospun mats were shown to depend on fibers' tendency to bend at the fiber–fiber crossovers, which may vary depending on the properties of the fibers and the electrospinning process conditions.



## 1. 1. Introduction

Electrospinning has been the focus of countless studies for the past decades for applications such as aerosol filtration, tissue engineering and catalysis. Electrospinning is a one-step process for producing submicron fibers—fibers one or two orders of magnitude smaller than traditional textile fibers. To date, there is no accurate method for measuring the thickness, and consequently the porosity of a nanofiber mat (see e.g., [1,2]). This is because the available measurement techniques are mostly suitable either for nano-scale dimensions (e.g., AFM microscopes) or for measurements on scales greater than say 10 μm (e.g., profilometers or indenters), leaving a thickness range of about 1 to 10 μm hard to measure accurately, especially when working with soft and compliant materials like fibrous mats. Accurate determination of the thickness of a nanofiber mat is very important for most applications that take advantage of such materials. Obviously, one cannot know the performance of a nanofiber mat (for particle/fluid separation, for instance) without knowing its most intrinsic properties such as thickness and porosity.

In a typical electrospinning process, a liquid jet (a single filament) is ejected from the surface of a charged polymer solution (or melt) and then driven by the electrostatic forces toward a collector. The charged filament experiences a so-called whipping process in which it follows an erratic trajectory before depositing on a collector [3–6]. The instabilities in the filament are due mainly to the effects of electrostatic repulsions of the charges in the filament and the coulombic forces caused by the electric field [3–7]. It is possible that the electric charges in the filament may become dissipated in the ambient air due to humidity or other factors during the electrospinning process. However, depending on the polymer structure and the process conditions, it is also possible that some charges remain in the fibers after the fibers are deposited on the collector [8–9]. Unfortunately, the effects of these residual charges on the morphology of a nanofiber mat have not yet been established. One can expect that the residual charges generate some attraction forces between the fibers and the collector as well as some repulsion forces among the fibers. It is not yet known if such attraction forces can play a role in further compressing the fibers together, and thereby decreasing the thickness of an electrospun mat. Given the number of unknowns affecting the formation of an electrospun nanofiber mat, the current study is devised to perhaps shed some light on the possible relationships between the thickness (and porosity) of a nanofiber mat and the properties of its constituting fibers. As such, this work is only a first step in developing a mathematical means for predicting the thickness and porosity of an electrospun mat. As will be discussed later in this paper, our focus in the current study is on the influence of fiber bending characteristics on the morphology of a fibrous mat.

In the remainder of this paper, we first describe how a mass-spring model is used in our work to represent a fiber in Section 2. We then present our algorithm for depositing such fiber on top of one another to form a mat in Section 3. We present a comparison between the predictions of our model and the Fourier solution of the Vibrating String

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**Nomenclature**

*Variables*

| | |
|---|---|
| $c$ | speed of the wave in a string |
| $d$ | fiber diameter [μm] |
| $\overrightarrow{f}_{i,j}$ | force exerted on the $i$th point-mass by the $j$th point-mass [N] |
| $\overrightarrow{f}_{i}^{\Sigma}$ | resultant force acting on $p_i$ [N] |
| $k_d$ | damping constant $[\mathrm{N}\cdot(\mathrm{m}\cdot\mathrm{s}^{-1})^{-1}]$ |
| $k_s$ | spring constant $[\mathrm{N}\cdot\mathrm{m}^{-1}]$ |
| $l_r$ | un-stretched length of a spring [μm] |
| $l$ | fiber length [μm] |
| $l_{fil}$ | filaments center-to-center distance [μm] |
| $m_i$ | mass of a point-mass $i$ [kg] |
| $n$ | fiber number fraction |
| $p_i$ | point-mass $i$ |
| $\overrightarrow{p}_i$ | position vector of the point-mass $i$ |
| $\overrightarrow{p}_i^{t}$ | position vector of the point-mass $i$ at time $t$ |
| $R_{cf}$ | coarse-to-fine fiber diameter ratio |
| $u$ | initial velocity of the string $[\mathrm{m}\cdot\mathrm{s}^{-1}]$ |
| $\overrightarrow{u}_i$ | velocity vector of point-mass $p_i$ $[\mathrm{m}\cdot\mathrm{s}^{-1}]$ |
| $v_i$ | velocity of point-mass $p_i$ at time $t$ $[\mathrm{m}\cdot\mathrm{s}^{-1}]$ |
| $x$ | x-coordinates of the string [μm] |
| $x_i$ | x-coordinate of point-mass $p_i$ at time $t$ [μm] |
| $z(x,t)$ | deflection of string in the $z$-direction for any point $x$ at time $t$ [μm] |
| $\Delta z$ | maximum deflection of fiber in the $z$-direction [μm] |
| $\rho_f$ | fiber density $[\mathrm{g}\cdot\mathrm{cm}^{-3}]$ |
| $\theta$ | standard deviation about a zero-mean |

*Superscript*

| | |
|---|---|
| $c$ | coarse fiber |
| $f$ | fine fiber |
| $t$ | time step |

*Subscript*

| | |
|---|---|
| $c$ | coarse fiber |
| $f$ | fine fiber |
| $fil$ | filament |
| $i$ | counter |
| $j$ | counter |

problem for validation in Section 4. Our results and discussion are given in Section 5 followed by the conclusions in Section 6.

## 2. Problem formulations

Our group has been active in developing modeling methods for simulating the 3-D structure of fibrous mats for the past decade [10–12]. Our previous structure simulations were specifically designed to provide a computational domain for simulating the transport of fluid and particles through a fibrous material. Such virtual structures need only to be developed on scales comparable to the dimensions of the fibers —about 25 times greater than the diameter of the fibers. On such small scales, one can assume the fibers to remain rigidly straight (modeled as rigid cylinders) across the entire length of the simulation domain. On the other hand, to simulate how the thickness of a fibrous mat grows as fibers continue to deposit on the surface, one needs to consider simulation domains with in-plane dimensions much greater than the fiber diameter. However, in such large domains (accommodating long fibers) a rigid-cylinder may no longer provide an accurate representation of a real fiber and how it interacts with other fibers in the mat. A new modeling approach is therefore needed to capture both the in-plane (if needed) and the through-plane curvature of the fibers. In the current study therefore, we have assumed the fibers to be made up of a continuous array of beads connected to one another by structural and flexion springs and dampers (see Fig. 1a). Our approach to simulate a nanofiber mat here is to treat the fibers as linear viscoelastic materials. The most common linear viscoelastic models are the Maxwell model, in which springs and dampers are connected in series, and the Kelvin–Voigt model, where springs and dampers are connected in parallel [13]. In these methods, the springs and dampers resemble the material's elasticity and viscosity, respectively. The Maxwell model is more suited for a fiber in the liquid/melt state whereas the Kelvin–Voigt is more appropriate for a solid fiber (the case here). This model allows an efficient representation of a fiber's motion through solving the balance of mechanical forces acting on each bead $p_i$. These forces are due to the structural and bending springs and dampers (neglecting gravitational forces), as shown in the free body diagram in Fig. 1b. For instance, the spring and damping forces between beads $p_i$ and $p_{i+1}$ can be written as

$$\overrightarrow{f}_{i,i+1}^{s} = -k_s\left(\left\|\overrightarrow{p}_i - \overrightarrow{p}_{i+1}\right\| - l_r\right)\frac{\left(\overrightarrow{p}_i - \overrightarrow{p}_{i+1}\right)}{\left\|\overrightarrow{p}_i - \overrightarrow{p}_{i+1}\right\|} \tag{1}$$

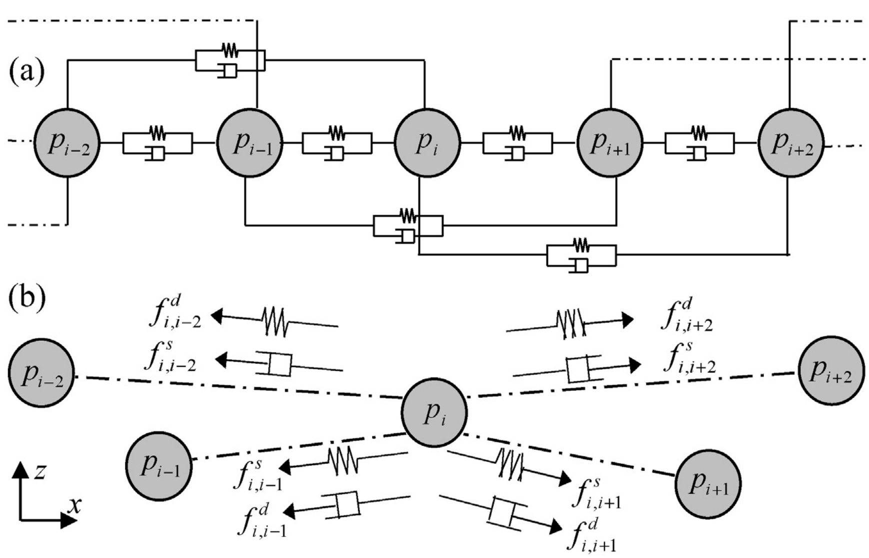


**Fig. 1.** (a) The mass-spring-damper model representation of a fiber, (b) free body diagram of a point-mass, $p_i$.