Effects of electrospinning conditions on microstructural properties of polystyrene fibrous materials

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The mathematical model developed by Reneker *et al.* [J. Appl. Phys. **87**, 4531 (2000)] and Yarin *et al.* [J. Appl. Phys. **89**(5), 3018–3026 (2001)] for modeling filament formation in electrospinning is combined in this work with the structure generation algorithm of Venkateshan *et al.* [Mater. Des. **96**, 27–35 (2016)] to simulate the effects of electrospinning parameters on microstructural properties (i.e., fiber diameter, thickness, and porosity) of the resulting electrospun materials. The model is calibrated using the experimental data obtained from electrospinning polystyrene (PS) fibers. The computational tool developed in this work allows one to study the effects of electrospinning parameters, such as voltage, needle-to-collector distance (NCD), or PS concentration, on the thickness and porosity of the resulting fibrous materials. For instance, it was shown that increasing the voltage or decreasing the NCD in electrospinning polystyrene results in mats with thicker fibers but smaller dimensionless thickness (or lower porosities), in agreement with experimental observations reported in the literature. In addition to serving as a characterization tool for the electrospun materials, the computational model developed in this work can be used to create accurate representations of the surface morphology or the internal geometry of fibrous materials used in a variety of applications, such as particle filtration or droplet separation. *Published by AIP Publishing.* https://doi.org/10.1063/1.5049128

I. INTRODUCTION

Electrospinning is a popular method for producing fine fibers ranging from about 0.05 μm to about 10 μm in diameter, and it has been the focus of countless studies for the past few decades for applications, including but not limited to tissue engineering,[1,2] filtration,[3–6] catalysis,[7] self-cleaning,[8–10] drug delivery,[11,12] and sensor manufacturing.[13,14] While it is quite easy to set up an electrospinning unit, it is very difficult to predict the outcomes of an electrospinning experiment in terms of fiber diameter, mat thickness, or mat porosity. This is mainly due to the complicated physics of fiber formation in electrospinning and also the minuteness of the resulting fibers.[15–17] For instance, there is no accurate method of measuring the thickness, and consequently the porosity, of an electrospun fiber mat. This is because such mats are generally very thin, and at the same time, very soft (tend to deform during measurement) (see, e.g., Refs. 18 and 19). Regarding this concern, our group has recently developed a mass-spring-damper (MSD) model to simulate the morphology of electrospun materials and thereby predict their thickness and porosity.[20] This model treats the fibers as arrays of beads connected to one another with springs and dampers, and it is therefore capable of realistically modeling the mechanical interactions between the fibers during mat formation. More importantly, our MSD model can realistically simulate curvature of the fibers at fiber–fiber crossovers without allowing the fibers to penetrate into one another—a major advantage over the previous fiber-mat generation methods.[21–36] Obviously, for the fiber-to-fiber interactions to be accurate, the MSD model requires material-dependent values for the stiffness of the springs and dampers that are used to simulate the rigidity of the fibers. Such fiber-level information is not always available, and therefore as it will be discussed later in this paper, we calibrated our MSD model using the experimental data obtained from electrospinning polystyrene (PS) mats. In addition, our MSD mat generation algorithm requires fiber diameter and fiber deposition velocity as inputs. These factors are both process- and polymer-dependent parameters, i.e., they vary with electrospinning parameters such as voltage, needle–collector distance (NCD), and solution concentration, among many others. To overcome this limitation and improve the usability of the MSD model as a design or characterization tool for electrospinning, we have coupled the electrospinning filament formation model of Refs. 37 and 38 with our MSD model in the current study. The pioneering mathematical formulations developed in Refs. 37 and 38 allow one to simulate the formation of a filament in an electrospinning process starting from the needle all the way to the collector. This allows us to obtain the necessary input values for the MSD mat generation model and thereby relate the properties of an electrospun mat to the electrospinning conditions for the first time.

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