Supplementary Material

An Integrated Experimental-Computational Investigation of the Mechanical Behavior of Random Nanofiber Networks

HyeongJu Lee [a], Mithun K Dey [b], Kathiresan Karunakaran [a], Catalin R Picu *[b] and Ioannis Chasiotis *[a]

[a]Aerospace Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, U.S.A.

[b]Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, NY, U.S.A.

*Corresponding Authors: chasioti@illinois.edu, picuc@rpi.edu

S1. Effect of Near-field Electrospinning Parameters on Nanofiber Morphology

Near-field electrospinning mainly involves four process parameters: the applied voltage, the distance between the polymer solution droplet and the collector, the polymer concentration, and the collector speed. Among these, the collector speed plays a critical role in determining the shape of the nanofibers that are deposited on the collector. The polymer jet velocity that is controlled by the applied field must be balanced by the collector speed in order to lay straight fibers on the collector. A collector velocity that is lower than the jet velocity would result in meandering nanofibers, while a collector velocity that is higher than the jet velocity would result in fiber stretching and potentially discontinuities. Figure S1 demonstrates this balance between the collector velocity and the jet velocity for Polyethylene Oxide (PEO) nanofibers. As shown in this figure panel, a collector velocity of at least 31 mm/s is required to lay straight fibers.

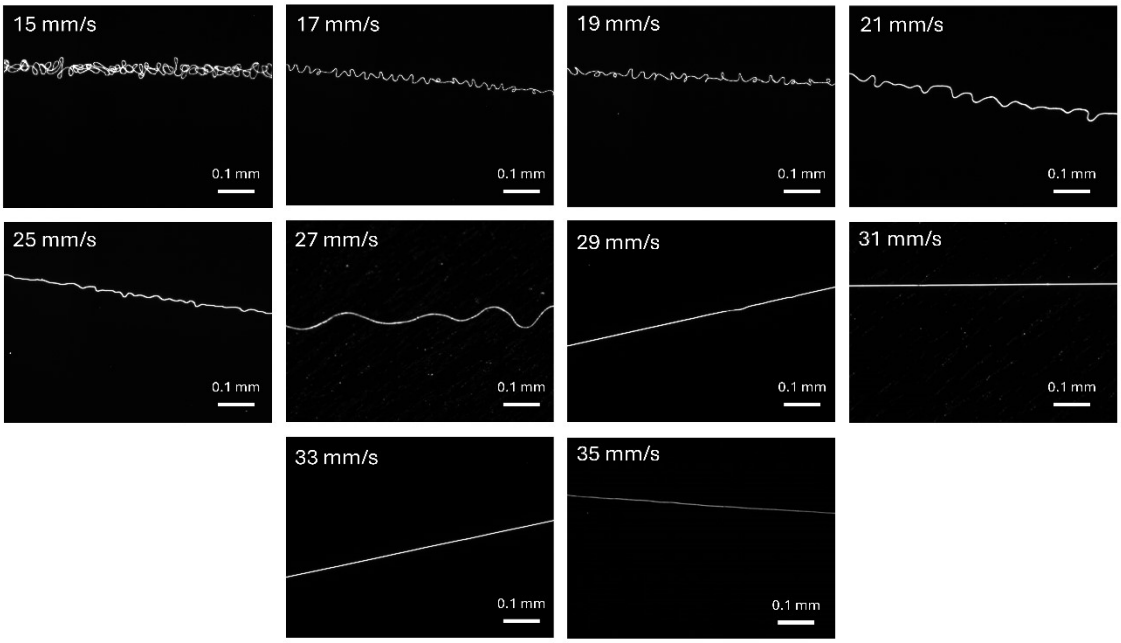

Figure S1. Nanofiber shapes for different collector speeds.

In the example in Figure S1 the applied voltage was 800 V, the distance of the polymer solution droplet from the collector was 0.5 mm, and the polymer solution concentration was 10 wt.%. These electrospinning parameters were determining by a parameter study that aimed at depositing continuous PEO nanofibers with uniform diameter. Towards this goal we varied the applied voltage in the range of 600 V to 1000 V, the polymer solution concentration from 6 to 12 wt.%, and the polymer solution droplet-to-collector distance from 0.3 to 1.0 mm to assess. The lower range of applied voltage values resulted in electrospraying, while large voltage values occasionally resulted in arcing. Low concentrations of the polymer solution (e.g. 6 wt.%) did not allow for a stable jet to form fibers on the collector. Also, dilute polymer solutions resulted in deposition of "wet" fibers that adhered more strongly to the collector surface. On the other hand, high polymer concentrations (e.g. 12 wt.%) resulted in high solution viscosity and large nanofiber diameters. Finally, large spacing between the polymer solution droplet and the collector (~1 mm) provided longer times for solvent evaporation, resulting in consistent fiber diameters of ~250 nm. In contrast, very short spacing (e.g. 0.3 mm) led to an unstable jet and increased nanofiber diameter due to insufficient travel time for solvent evaporation before reaching the collector. Based on these results a polymer solution droplet-to-collector distance of 0.5 mm was selected for all PEO nanofiber networks printed in this work.

S2. Mesh Convergence of Finite Element Model

Our mesh convergence tests considered six cases of mesh refinement with decreasing element size ranging from 50 to 0.5 µm. In each case, fiber segments (defined by two successive crosslinks along a given fiber) shorter than the specified element length were eliminated by merging the respective crosslinks and nodes. Convergence of the effective stress vs. stretch ratio curves, Figure S2, was achieved for a minimum element size of 1 µm which was used in all simulations presented in this work. This element size ensured a balance between computational accuracy and cost.

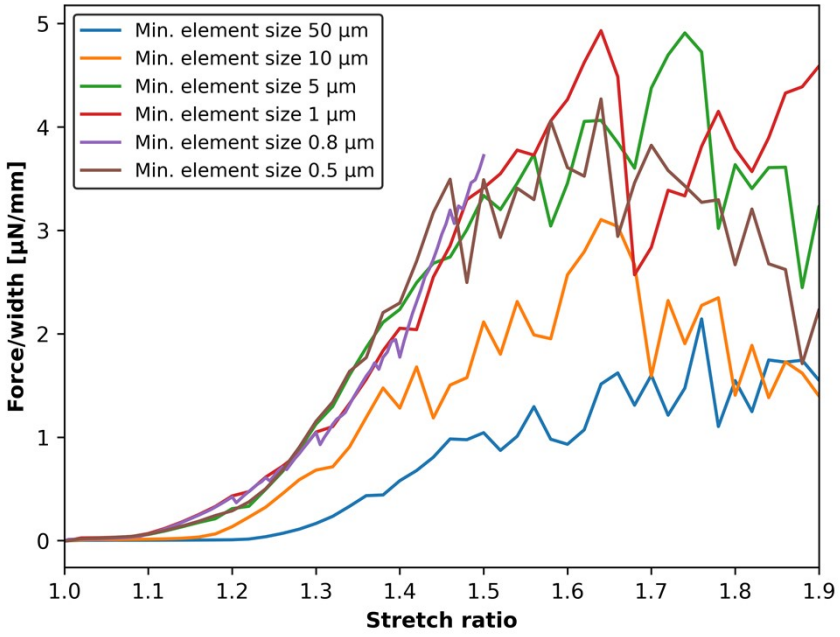

Figure S2. Mesh convergence for different element sizes.

S3. PEO Nanofiber Diameter Distributions in Networks with Different Structural Parameters

The PEO nanofiber diameter distribution was independent of the network density. As derived from the distributions shown in Figures S3(a-d), the average nanofiber diameters for the four different networks with N=500, 1000, 3000, and 5000 were 242 ± 20 nm, 237 ± 18 nm, 246 ± 21 nm, and 259 ± 24 nm, respectively, thus showing no systematic trends. In general, the nanofiber diameter depends on the electrospinning parameters, namely, the applied voltage, the polymer solution droplet-to-collector distance, and the concentration of the polymer solution.

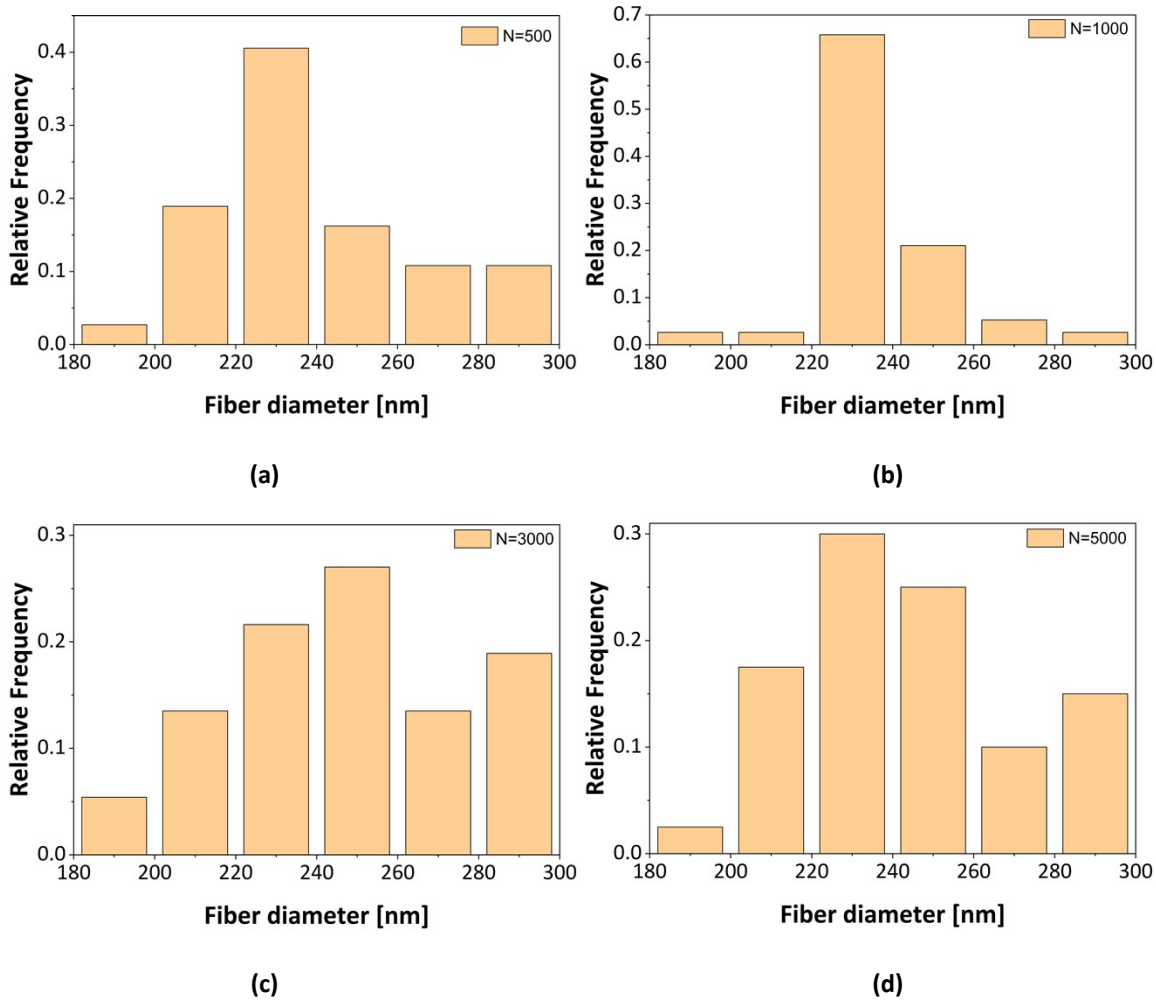

Figure S3. Fiber diameter distributions for four network densities.