Novel Experiments and Models for the Nanomechanics of Polymeric and Biological Nanofibers

NSF NIRT Grant DMI #0532320

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The mechanical response of biological materials reflects deformation mechanisms occurring within a hierarchical architecture extending over several length scales. This research program aims at filling the void in quantitative experimental/computational mechanics of soft nanofibers in the range of 10-200 nm that will help to predict and mitigate bone fracture, design improved synthetic bone replacements, ligaments and tendons, and lay the ground work for bioinspired and hierarchically structured multifunctional composite materials.

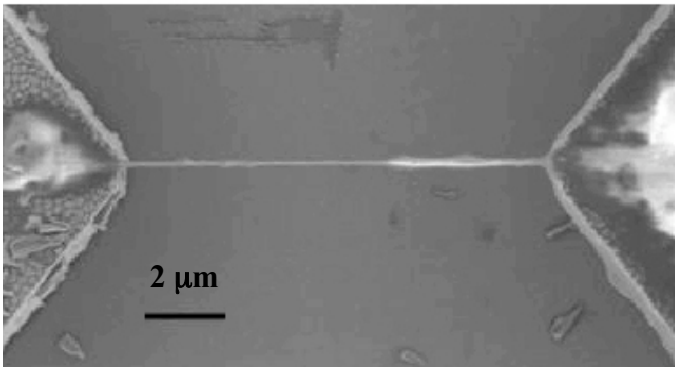


Figure 1. Collagen nanofibril loaded in tension by a MEMS mechanical testing platform [1].

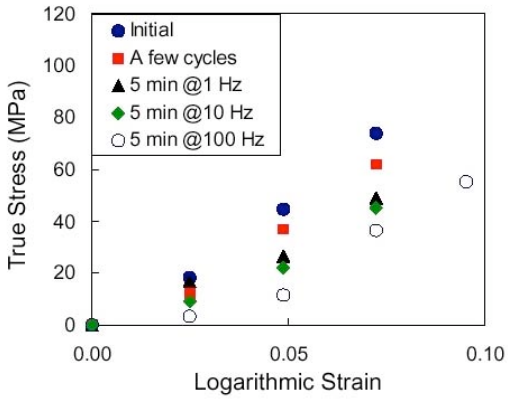


Figure 2. Stress-strain curve of a collagen nanofibril showing decreasing stiffness upon cyclic loading [1].

A microelectromechanical (MEM) platform for mechanical property measurements was designed and fabricated to *obtain the first stress-strain (σ-ε) curves of type I collagen nanofibrils* isolated from the sea cucumber *Cucumaria frondosa* [1], as seen in Figure 1. Sea cucumber fibrils are similar to those found in vertebrates having the same length, assembled with the same repeat period, possessing the same gap/overlap ratio and the same cross-linking chemistry. The challenge to manipulate isolated collagen nanofibrils onto the MEMS test platform was overcome by labeling the nanofibrils with fluorescently tagged antibodies. This procedure provided punctate staining concomitantly allowing for measuring the strain distribution along the fibril. The elastic moduli at small and large strains were estimated by converting the load-displacement data to true stress - logarithmic strain. At low strains, the nanofibrils displayed tangent moduli in the range 0.26-0.30 GPa. The true stress-logarithmic strain curves suggest a

tensile strength of individual nanofibrils that may be greater than 1.0 GPa [1]. Furthermore, our data show that cyclic loading of fibrils for progressively larger number of cycles and at successively higher strain rates decreases the fibril modulus, indicating that even these nanoscale substructures are susceptible to a form of fatigue (Figure 2). Fundamental information of degradation mechanisms at the scale on single nanofibrils is key in determining the origins of bone damage and in devising therapeutic methodologies and restorative approaches.

This nanoscale mechanical property characterization approach is being employed to measure the mechanical properties of soft polymeric nanofibers as a function of their fabrication parameters. This part of the project investigates the relations between manufacturing of soft electrospun polymer nanofibers and their viscoelastic and fracture response before they are implemented in large-scale materials and structures. Polyacrylonitrile (PAN) polymer nanofibers, prepared by collaborators of this NIRT team, are the test material. The PAN nanofibers have 150,000 average molecular weight and diameters between a few tens to a few hundreds of nanometers. We developed a method to isolate, manipulate and place segments of these nanofibers onto the MEMS testing platform seen in Figure 3(a). Then, the fibers are secured using a small amount of epoxy adhesive that provides sufficient bonding onto the test device, Figure 3(b). This MEMS device will be operated under an AFM to collect images of the deforming nanofiber, Figure 3(c), from which the strain and displacement fields on the fiber will be resolved by Digital Image Correlation analysis [2].

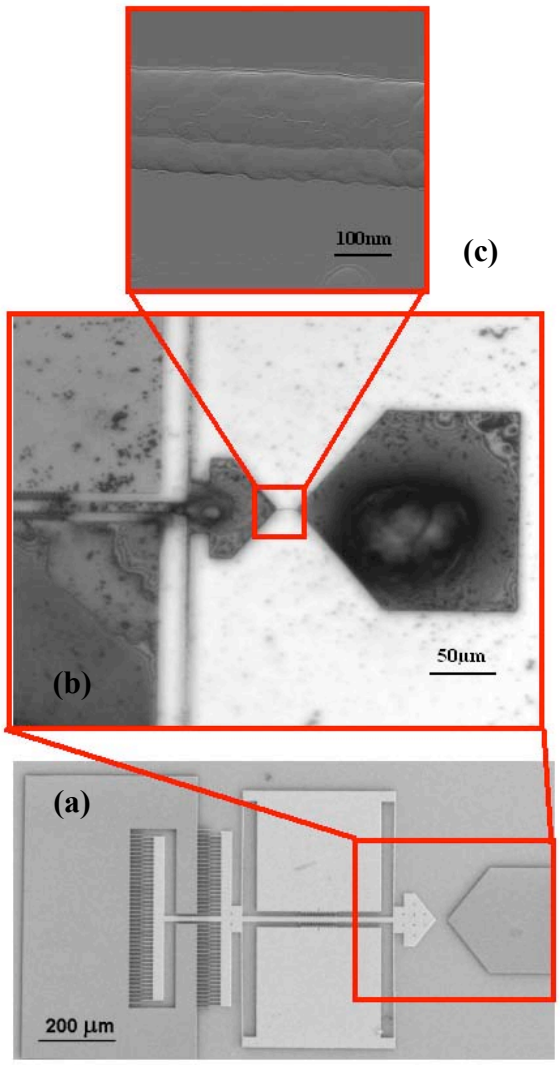
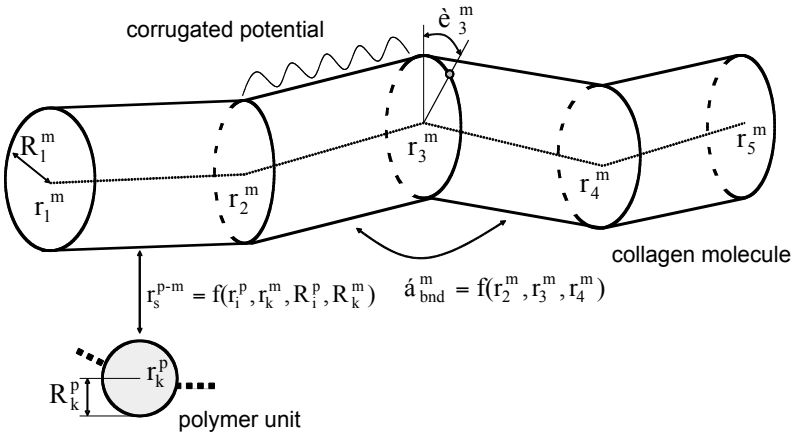


Figure 3. (a) MEMS platform for testing individual nanofibers, **(b)** a polymer nanofiber mounted on the microtesting device, **(c)** AFM image of the electrospun nanofiber.

The experimental data will be coupled with mesoscale and finite element models to shed light into the constitutive behavior of the biological building blocks and the polymeric nanofibers. The NIRT team is developing a coarse-grained computational model for simulations of polymeric and collagen fibers at a mesoscopic level [3]. This entails a novel shape-based mesoscopic force-field model for simulation of either a collagen molecule within a

nanofibril or a fibril within a microfiber. Figure 4 provides a description of the model parameters.



Independent variables: $\vec{r}_i^{\,m}, \vec{r}_k^{\,p}, R_i^m, R_k^p, \theta_i$

Figure 4. Shape-based mesoscopic force-field model for simulation of either a collagen molecule or a fibril.

In order to disseminate the results of this work, an Internet web page has been created at a UIUC server [4]. The page is updated as results from this NIRT research program become available.

References

[1] S. J. Eppell, B. N. Smith, H. Kahn, R. Ballarini, "Nano measurements with microdevices: mechanical properties of hydrated collagen fibrils," accepted in Journal of the Royal Society Interface (2005)

[2] S.W. Cho, I. Chasiotis, T.A. Friedman, and J. Sullivan, "Direct Measurements of Young's Modulus, Poisson's Ratio and Failure Properties of ta-C MEMS", Journal of Micromechanics and Microengineering 25 (4), pp. 728-735, (2005)

[3] L. V. Zhigilei, C. Wei, and D. Srivastava, Mesoscopic model for dynamic simulations of carbon nanotubes, Phys. Rev. B 71, 165417, 2005 [also in the Virtual Journal of Nanoscale Science & Technology 11 (16), 2005]

[4] For further information about this project link to <http://www.ae.uiuc.edu/NIRT>