MECHANICS OF NANOFIBER NETWORKS AND YARNS

by

Yong Liu

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Yong Liu, Ph.D.

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Adviser: Yuris Dzenis

Continuous nanofibers (NFs) are among the most promising types of advanced nanomaterials due to their unique mechanical and functional properties, extreme surface to mass ratio, and ultrahigh strength/toughness coupled with extreme flexibility. Continuous nanofiber networks (NFNs) and yarns are being developed for applications in advanced composites, filtration, tissue engineering, electronic and optical devices, and other fields. Mechanical behavior of NFNs is complex and not yet sufficiently understood, despite its critical importance for most applications. Existing models of NFNs often lack consideration of structural details, complex contact conditions, and non-linear mechanical properties of NFs. The objective of this dissertation was to perform comprehensive analysis of mechanical behavior of NFNs and yarns based on novel numerical models with explicit nanofiber and contact representation.

Three-dimensional geometric models of NFNs were generated by mimicking nanomanufacturing process resulting in networks with random or preferred nanofiber orientation. NFs were represented as beams with non-linear elastic-plastic properties obtained from experiments. Different contact conditions such as friction and bonding between nanofibers were realized. The developed models were used to simulate large deformations of NFNs under various loadings through failure. Mechanisms of non-linear deformation and failure, such as nanofiber plastic deformation, nanofiber reorientation

under loading, and nanofiber and contact breaks accumulation were extracted and analyzed. A comprehensive analysis of the effects of input parameters on NFNs stiffness, strength and toughness was performed. Variations of nanofiber diameter, density, orientation distribution, and nanofiber contact strength and friction were simulated and analyzed for the first time and the relative importance of these network parameters was evaluated and compared. Effects of nanofiber diameter, mechanical properties, contact friction, and the pitch angle in nanofiber yarns were also studied. Significant enhancement of yarn properties over individual NF properties was predicted and the mechanisms of such enhancement were explained.

The results provide better understanding of the mechanics of NFNs and yarns and can be used for design and optimization of novel nanofilamentary materials for applications.

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