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MECHANICS OF NANOSCALE FIBER NETWORKS AND THEIR COMPOSITES: A THREE-DIMENSIONAL MULTISCALE STOCHASTIC MODELLING STUDY

By

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Abstract

Three-dimensional fiber networks and their composites are commonly observed as bird nests in nature, collagen in biological systems, papers, respiratory face masks filters, water filter cartridges, and air purification meshes, etc. In this study, two different fiber network systems: electro spun silica nanofiber mats (stand-alone networks) and carbon nanotube (CNT) reinforced nanocomposites (network-based composites) are considered. The overall properties and mechanics of fiber networks are governed by the morphological parameters such as fiber length, diameter, orientation, waviness, agglomeration, and inter-fiber interactions. In addition, as CNT networks are embedded in a matrix medium, their mechanical properties are further influenced by CNT-matrix interfacial properties. Most of the available literature assumes idealized network parameters, perfect interphase, and two-dimensional modelling approaches. In this study, we have proposed a unique Python-based modelling approach which can incorporate above-mentioned parameters and their stochastic variations towards the construction of a three-dimensional model. Size-dependent mechanical properties of silica nanofiber are evaluated using Molecular Dynamics simulations, which are then input in the finite element model. Atomistic simulations are used to study the CNT/epoxy interfacial region. Future guidelines to enhance current modelling technique to study the failure properties of these materials are discussed.