Effects of structural parameters of nanotube networks on mechanical properties and fracture mode of carbon nanotube thin films and fibers

Alexey Volkov*†1 and Saeed Siahtiri

1University of Alabama (UA) – Tuscaloosa, AL 35487, United States

Abstract

In carbon nanotube (CNT) films and fibers, individual nanotubes form networks of bundles. In the present work, the effect of structural parameters of the CNT network, such as porosity, bundle thickness, degree of internal connectivity in bundles, and density of bundle-bundle interconnects, on the elastic and inelastic properties as well as fracture mechanisms of thin CNT films and fibers are studied in systematic coarse-grained mesoscopic simulations, when the computational samples include tens of thousands of individual CNTs. In the mesoscopic model, each CNT is represented by a chain of stretchable cylindrical segments. The mesoscopic force field accounts for stretching and bending of individual CNTs, van der Waals interaction between them, and load transfer through covalent cross-links. All components of this mesoscopic force filed are parameterized based on results atomistic simulations or calculated using the molecular mechanics methods. The inter-tube interaction potential, in particular, is based on the tubular potential method, which eliminates artificial friction between CNTs and is capable of describing the self-assembly of nanotubes into a network of bundles, where the bundle cross sectional size can span a few orders of magnitude. The model is used to generate single-walled CNT thin films and bundles with continuous networks of entangled bundles as a result of dynamic self-assembly driven by van der Waals interaction and to characterize the structural properties of the network in the broad range of material density. The process parameters, e.g., temperature and self-assembly time, allow one to obtain steady-state quasi-equilibrium CNT networks with variable by demand structural properties. The *in silico* generated films and fibers composed of raw and cross-linked CNTs are then used to predict their mechanical properties in quasi-static in-plane stretching and compression. The simulations showed that the bundle size distribution strongly affects the mechanical properties of CNT films. The stretching of CNT films with small average bundle sizes is characterized by strong irreversible reorganization of the network structure during the deformation process. An increase in the bundle size results in the decrease of the film modulus and strength but strongly increases the ultimate strain. The compression of the CNT films results in nearly reversible coordinated folding and wrinkling of the films. The effects of other structural parameters become strong only for networks composed of thick bundles. The same conclusions remain valid for CNT fibers as well. This shows that, qualitatively, the effects of the structural parameters of the CNT network do not depend on the degree of structural anisotropy of CNT materials. This work is supported by U.S. National Science Foundation through the award CMMI-1554589.

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*Speaker

†Corresponding author: avolkov1@ua.edu