

Abstract Submitted
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Mesosopic Distinct Element Method Simulations of the Mechanical Properties of Hybrid Nanoparticle-Carbon Nanotube Films¹
YUEZHOU WANG, TRAIAN DUMITRICA, University of Minnesota — The recently proposed mesoscopic distinct element method (mDEM) for carbon nanotubes (CNT) is extended to account for a second nanoparticle (NP) phase and used to investigate the impact NP fillers on the mechanical properties of the CNT networks. High throughput mDEM simulations explore the large parameter space (size, type, and concentration of the filling NPS, CNT network topology, degree of bundling, CNT length) with the goal of developing a fundamental understanding and informing experiments with parameters that optimize the system-scale properties of interest: stability, flexibility, fatigue, yield and failure resistance. Our simulations suggest that NP filling of the CNT network could represent a new solution to the currently open problem of carbon nanotube film stability based on an "excluded volume" approach.

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