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Mechanical properties of aligned carbon nanotube architectures: origin from 3D morphology ITAI Y. STEIN, BRIAN L. WARDLE, MIT — The scale-dependent properties of carbon nanotubes (CNTs) continue to motivate their study for next-generation material architectures. While recent work has shown that aligned CNT arrays can be made on the cm-scale, such systems exhibit properties that are orders of magnitude below those predicted by existing theories. This deviation mainly stems from the rudimentary assumptions made about the CNT morphology: CNTs are either devoid of local curvature (i.e. waviness) or have waviness that is easy to model, e.g. using helices and sine waves. Here, we use a simulation framework comprised of 10^5 CNTs with realistic 3D stochastic morphologies to elucidate the role morphology plays in the orders of magnitude over-prediction of the effective stiffness of aligned CNT structures. Application to aligned CNT polymer and carbon matrix nanocomposites reveals that the elimination of the torsion deformation mechanism, which dominates the effective compliance of CNT arrays, through CNT interactions with the matrix is responsible for the stiffness enhancement in CNT nanocomposites. This works paves the way to more accurate property prediction of CNT nanocomposites, and further work to predict the transport properties of aligned CNT architectures is planned.

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