OPTIMIZING LOAD TRANSFER IN MULTIWALL NANOTUBES THROUGH INTERWALL COUPLING: THEORY AND SIMULATION

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Keywords: Multi-wall carbon nanotube, Nanocomposite, Interwall bonding, Load transfer.

Summary. An analytical model is developed to determine the length scales over which load is transferred from outer to inner walls of multiwall carbon nanotubes as a function of bonding between walls. Molecular dynamics simulations provide data against which the model is tested.

ABSTRACT

The development of high performance materials using carbon nanotubes (CNTs) as reinforcing constituents requires a fundamental understanding of the mechanics of nanoscale reinforcement. An important factor in strengthening and toughening of composite materials is the load-carrying ability of the strengthening fiber. Multi-wall CNTs (MWCNTs) present the possibility of increased load carrying ability per unit area over single-wall CNTs (SWCNTs), if all walls can be made to share the load.

Experiments have shown that controlled sputtering and irradiation of pristine MWCNTs can enhance interwall coupling and sliding resistance via the formation of interwall $sp^3$ bonds [1]. Peng et al. [2] indicated that failure loads of MWCNTs with interwall coupling were up to $\sim$11.6 times the load expected if only their outermost wall had been loaded. Previous work by the present authors has also confirmed the benefits of interwall coupling for fiber fracture strength in the presence of intrawall defects [3], as well as interwall sliding resistance and buckling energy [4]. Interwall coupling thus appears to be a promising route to producing lightweight MWCNT-reinforced materials with enhanced strength and toughness.

In this work [5], we expand on our previous observations of load transfer [3] by developing an analytical shear lag model to determine the length scales over which load is transferred
from outer to inner walls of MWCNTs as a function of the amount of bonding between walls. The model predicts that the characteristic length for load transfer scales as $l \sim t \sqrt{\frac{E}{\bar{K}}}$, where $t$ is the CNT wall spacing, $E$ is the effective wall Young’s modulus, and $\bar{K}$ is the average interwall shear modulus due to interwall coupling. Molecular Dynamics simulations provide data against which the model is evaluated. Results show excellent agreement between analytic and numerical models when interwall bonding is uniformly distributed in the axial direction, proving that continuum mechanics concepts apply down to the atomic scale in this problem. The simulation models also show, however, that load transfer is sensitive to natural statistical fluctuations in the spatial distribution of the interwall bonding between pairs of walls, and such fluctuations generally increase the net load transfer length needed to fully load a MWCNT. For more realistic scenarios of interwall bonding formation via irradiation, where the interwall bond density likely decreases from outer to inner walls, the deviations in load transfer length from the ideal case are relatively small if the interwall bond density variation is not too large.

Optimal load transfer is achieved when bonding is uniformly distributed axially, and all interwall regions have the same shear stiffness, implying a linear decrease in the number of interwall bonds with the distance from the outer wall. Optimal load transfer into an $n$-wall MWCNT is shown to occur over a length of $\sim 1.5n\ell$. The guidelines presented in this work can be used to assist in the design of engineered MWCNTs, where interwall coupling is introduced to enhance load transfer, energy dissipation, and thus composite strength and toughness in ceramic- and polymer-matrix composite materials.

REFERENCES


