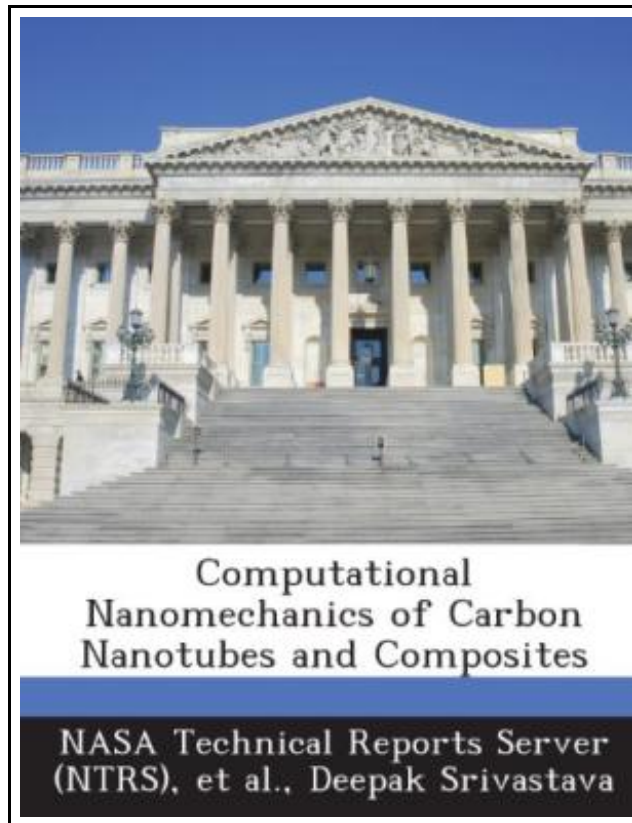


# Computational Nanomechanics of Carbon Nanotubes and Composites



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## COMPUTATIONAL NANOMECHANICS OF CARBON NANOTUBES AND COMPOSITES

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BiblioGov. Paperback. Book Condition: New. This item is printed on demand. Paperback. 24 pages. Dimensions: 9.7in. x 7.4in. x 0.1in. Nanomechanics of individual carbon and boron-nitride nanotubes and their application as reinforcing fibers in polymer composites has been reviewed with interplay of theoretical modeling, computer simulations and experimental observations. The emphasis in this work is on elucidating the multi-length scales of the problems involved, and of different simulation techniques that are needed to address specific characteristics of individual nanotubes and nanotube polymer-matrix interfaces. Classical molecular dynamics simulations are shown to be sufficient to describe the generic behavior such as strength and stiffness modulus but are inadequate to describe elastic limit and nature of plastic buckling at large strength. Quantum molecular dynamics simulations are shown to bring out explicit atomic nature dependent behavior of these nanoscale materials objects that are not accessible either via continuum mechanics based descriptions or through classical molecular dynamics based simulations. As examples, we discuss local plastic collapse of carbon nanotubes under axial compression and anisotropic plastic buckling of boron-nitride nanotubes. Dependence of the yield strain on the strain rate is addressed through temperature dependent simulations, a transition-state-theory based model of the strain as a function of strain rate and simulation temperature is presented, and in all cases extensive comparisons are made with experimental observations. Mechanical properties of nanotube-polymer composite materials are simulated with diverse nanotube-polymer interface structures (with van der Waals interaction). This item ships from La Vergne, TN. Paperback.



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