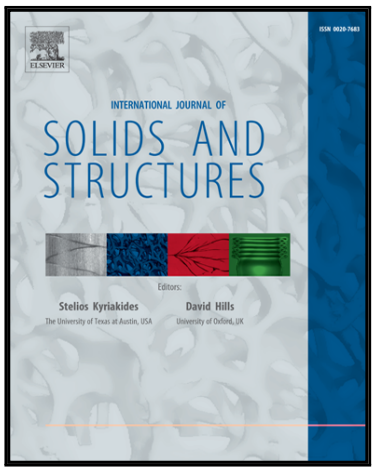

Effects of mechanical deformation on electronic transport through multiwall carbon nanotubes

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Effects of mechanical deformation on electronic transport through multiwall carbon nanotubes

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Abstract

The effects of mechanical deformation on the electron transport behavior of carbon nanotubes (CNTs) are of primary interest due to the enormous potential of nanotubes in making electronic devices and nanoelectromechanical systems (NEMS). Moreover it could help to evaluate the presence of defects or to assess the type of CNTs that were produced. Conventional atomistic simulations have a high computational expense that limits the size of the CNTs that can be studied with this technique and a direct analysis of CNTs of the dimension used in nano-electronic devices seems prohibitive at the present. Here a novel approach was designed to realize orders-of-magnitude savings in computational time in calculating the deformation-induced changes in the electrical transport properties of the nanotubes. The computational method has been validated with respect to fully atomistic simulations and in a simulation of laboratory experiments. In this work is used to investigate the electromechanical behavior of a 0.24 μm long multi wall CNT, a system with more than a million atoms.

Keywords: Carbon nanotubes, Electromechanical behavior, Numerical Methods.