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Pressurized CNTs under Tension: a Finite-Deformation Lattice Model

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Abstract

We propose a finite-deformation lattice model for carbon nanotubes (CNTs), in which an energetic cost is assigned to changes in bond lengths, bond angles, and dihedral angles, while atomic interactions are governed by a Reactive Empirical Bond-Order potential. For the first time, we consider the effect of severe traction and pressure applied simultaneously, with the ultimate goal of understanding how material properties are affected by such loads. In particular, the radial stiffness and the axial stiffness have been investigated: on making use of the second generation Brenner potential, we have found that peculiar transitions softening-hardening-softening occur in both the radial and axial stiffness, a behavior that could be compared with the ones observed in experiments or predicted by *ab initio* methods. The constitutive response described here can be exploited in the design of CNT-based hydrogen storage systems, and it opens a new possibility for tuning material properties, in order to make CNTs softer or harder in a controlled way.

Keywords: Nano-structures, smart materials, mechanical properties, analytical modelling, lattice model

Keywords

Contents

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