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Roberto Alessi, Antonino Favata, Andrea Micheletti

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Pressurized CNTs under Tension: a Finite-Deformation Lattice Model

Roberto Alessi^a, Antonino Favata^a, Andrea Micheletti^b

^a*Dipartimento di Ingegneria Strutturale e Geotecnica
Sapienza University of Rome, Italy*

^b*Dipartimento di Ingegneria Civile e Ingegneria Informatica
University of Rome Tor Vergata, Italy*

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

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Email addresses: roberto.alessi@uniroma1.it (Roberto Alessi), antonino.favata@uniroma1.it (Antonino Favata), micheletti@ing.uniroma2.it (Andrea Micheletti)

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