Elastic Properties of Carbon Nanotubes and their Heterojunctions

N.A. Sakharova*, J.M. Antunes*†, A.F.G. Pereira*, B.M. Chaparro† and J.V. Fernandes*

* CEMMPRE – Department of Mechanical Engineering, University of Coimbra,
Rua Luís Reis Santos, Pinhal de Marrocos, 3030-788 Coimbra, Portugal
e-mail: {nataliya.sakharova, andre.pereira, valdemar.fernandes}@dem.uc.pt,
web page: http://www.uc.pt/en/iii/research_centers/CEMUC

† Escola Superior de Tecnologia de Abrantes, Instituto Politécnico de Tomar
Rua 17 de Agosto de 1808, 2200 Abrantes, Portugal
email: jorge.antunes@ipt.pt, bruno.chaparro@sapo.pt, web page: http://www.esta.ipt.pt

ABSTRACT

In the past decade, systematic research has been conducted for developing nano-materials such as carbon nanotubes (CNTs) that are optimal nanostructures to reinforce composites, building blocks for optical and electronic nanodevices [1]. From the point of view of construction of nanodevices, the carbon nanotubes heterojunctions (CNT HJs) are necessary constituents for the circuits, amplifiers, switches and nanodiodes [2]. The single-walled (SWCNT) and multi-walled (MWCNT) carbon nanotubes have been studied experimentally, but a big inconsistency in experimental results has been observed, owing to the experimental difficulties in the characterization of nanomaterials at the atomic scale. For this reason, modelling and computer simulation for predicting the mechanical properties of CNTs and their heterojunctions have received much attention. The systematic characterization of the mechanical properties of SWCNTs, which are fundamental structural units for more complex structures, allows further studies towards understanding mechanical behaviour of MWCNTs and CNT heterojunctions.

This research work is focused on the characterisation of mechanical properties of SWCNTs and MWCNTs in a wide range of chiral indices, diameters and number of layers (for the case of MWCNTs), as well as SWCNT HJs of different configurations by modelling their structure and mechanical behaviour, using nanoscale continuum approach [3].

The systematic methodology for characterization of the mechanical behaviour of SWCNTs proposed, allows developing of the adequate numerical model of MWCNTs with and without taking into account the van der Waals interactions between adjacent layers, and carrying out a comprehensive numerical simulation study in order to understand the mechanical behaviour of SWCNT HJs of three different configurations (cone-heterojunctions with straight and bent connection, and radii-preserving heterojunctions).

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