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MODELLING OF SINGLE-WALL CARBON NANOTUBES MECHANICAL BEHAVIOUR

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Since their discovery by Iijima in 1991, carbon nanotubes (CNTs) have attracted the interest of most research in nanostructures, due to their extraordinary mechanical, optical, thermal and electrical properties [1]. From the point of view of structural applications, the high stiffness of CNTs together with their low density makes them promising as nanoscale fibers for reinforcing nanocomposite structures [2]. This perspective of using CNTs has required the investigation of their mechanical properties, along with the study of their deformation behaviour under different strain conditions. Although extensive experimental studies have been carried out to evaluate the mechanical properties of CNTs, there is a big inconsistency concerning the experimental results reported in literature, owing to the complexity in performing the characterization of nanomaterials at the atomic scale. As a result, research in this field has been mainly driven theoretically, by modelling and simulating the behaviour of CNTs.

In this work, modelling and numerical simulation by the finite element (FE) method of the mechanical behaviour of single-walled carbon nanotubes (SWCNTs) was performed based on the equivalent continuum mechanics modelling (ECM) approach [3]. This approach permits evaluating the elastic properties of nanotubes in tension and bending, as a function of their geometrical characteristics. Different SWCNTs structures, such as chiral (with chiral angle $0° < \theta < 30°$) and non-chiral (zigzag, $\theta = 0°$, and armchair, $\theta = 30°$) ones were assembled considering a wide range of chiral indexes, nanotube length and diameter. The selection of chiral indexes and chiral angles was made in order to cover a broad range of SWCNTs. The range selected for chiral and non-chiral structures represents the CNTs typically used in literature, either for FE analyses or experimental characterization. FE analysis was performed using commercial FEA code ABAQUS®.

Numerical simulations of conventional tension and bending tests were carried out in order to study the effect of the nanotube diameter, the length and the chirality of ideal SWCNT (without defects) on their mechanical properties.

The numerical simulation study allows concluding that the tensile and bending rigidities of SWCNTs can be directly related to chiral indexes. The tensile rigidity, $(EA)_{eq}$, as a function of chiral index, n, follows a *quasi* linear evolution; meanwhile the bending rigidity, $(EI)_{eq}$, as a

function of chiral index can be described by a third-degree polynomial, for all nanotube structures studied. Similar results were reported in literature for some cases of zigzag and armchair SWCNTs [3].
Moreover, the FE results concerning the evolution of tensile and bending rigidities with the sum of the chiral indexes *(n+m)*, within the range of diameters and chiral angles studied, can be fitted by the same trend, which is *quasi* linear for the case of tensile rigidity, and close to a cubic power for the case of bending rigidity.
The expressions for equivalent rigidities, $(EA)_{eq}$ and $(EI)_{eq}$ were obtained by fitting the numerical results, allowing an accurate evaluation of the Young´s modulus of SWCNTs.

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