Congress on Numerical Methods in Engineering
Lisboa, June 29 to July 02, 2015

RESUMO N° 370

NON-LINEAR BEHAVIOUR OF NANOTUBES UNDER COUPLED BENDING-TWISTING

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Keywords: Carbon Nanotubes, Nanomechanics, Molecular Dynamics

The main objective of this paper is to investigate the strength and stiffness of CNTs under combinations of bending and twisting. In order to assess the collapse behaviour of CNTs, MD simulations of bended and twisted CNTs are performed. The LAMMPS code is used, the AIREBO potential is considered for C-C bonds, the temperature is kept in 300 K and the incremental bending rotations (theta) and twisting rotations (phi) are imposed at the CNT ends. Three types of CNT are analysed, including zig-zag (8,0), armchair (5,5) and chiral (6,3) CNTs. All CNTs are analysed for pure bending and pure twisting and the main results are shown in the form of diagrams of energy and force against curvature and imposed rotations. After that, several rates of bending-twisting are applied to the CNT. The main results are also shown in the form of diagrams of energy and energy-derivative curvature and imposed rotations. The kinematics of C-C bonds are studied using some geometric parameters of the hexagonal lattice, such as the bond length, the dihedral angle and the CNT diameter. It is shown that the variation of these parameters plays a key role in the behaviour, stiffness, strength and collapse of CNTs. Finally, the different failure modes of CNTs are shown. Some relevant conclusions are drawn concerning the influence of loading (bending and twisting) on the collapse of CNTs.

Silvestre N., Faria B., Canongia Lopes J.N. (2015) – Non-linear behaviour of carbon nanotubes under coupled bending-twisting, Computational Materials Science.