Abstract

Since their discovery in 1991, carbon nanotubes have attracted great interest from the scientific and research community over the world. This is due in great measure to their exceptional mechanical, electrical and termical properties. Their outstanding features provide them promising applications in the framework of biomechanics, aircraft industry and engineering. Anyway, the broad use of these new materials in a near future requires necessarily some improvements at the grown procedures, up to the obtention of nanotubes in a economical way.

An important part of previous research works related to these singular molecules has been aimed to the prediction of their stress-strain response under external loading or excitations. In some cases, existing models have been applied to the strength behavior of nanotubes. Otherwise, new models with particular features have been defined. As a midpoint between the time-consuming methods from molecular dynamics and the classical models derived from the continuum mechanics, appear Molecular structural mechanics models (among them, the *stick-spiral* model) which allow to describe the atomistic structure of nanotubes at a reasonable computational cost.

This Ph. Thesis is focused on the general formulation of the *stick-spiral* model and its application to single-walled carbon nanotubes. Such formulation and their results have been explored as much in the framework of the geometrical linear analysis as in the nonlinear one. Moreover, the possible differences in the structural response of nanotubes regarding two interatomic potentials (AMBER and Morse) have been compared.

In the first part of the work, the static and kinematic indetermination of the model have been studied by using and adaptation of the Single value decomposition from Pellegrino and Calladine for space trusses, with the target of finding out the existence of statically admisible solutions. This study allows to establish the kinematic and static equations for each constituent element in the linear range and to approach the assembling rules of the kinematic and equilibrium matrices for the whole structural model. This first analysis has underlined that contragradience relation is verified in our model, and let us to state the kinematic determination of the system in function of the existing boundary conditions. As well as the high internal static indetermination that ensures the existence of solutions from a given external loading configuration.

In the second part of the work, the geometrically linear analysis of the model is tackled through a fully general (independent of the loading configuration) stiffness formulation derived by means of the systematic application of the virtual work equation to the structural members and the complete system. Symbolic expressions of the stiffness matrices for each element are provided, as well as the verification of the boolean assembling is shown for the model. In addition, the initial curvature of nanotubes has been drawn especial attention, including a system of initial internal forces (*preenergy* of prestressing) which tend to stabilize the cross-section and to shorten the nanotube. As representative variables, the mechanical parameters of the nanotube subjected to the usual loading schemes used in beams or rods (tension, compression, bending and torsion) are estimated. Their numerical values have been used to validate our formulation compared to other authors, as Natsuki and Endo, regarding two different interatomic potentials in order to find out the effect of the constitutive nonlinearity in the final response. Nevertheless, the validity of such mechanical parameters is criticized due to their

dependency on some geometrical parameters, as the controversial equivalent wall-thickness. Furthermore, the advantages of the presented model are described in contrast with the doubtful applicability of continuum models and the computationally expensive molecular dynamics methods.

Later on, buckling analysis of nanotubes is carried out from a geometrically nonlinear point of view. The development of symbolic expressions for the tangent stiffness matrix and the proof that the boolean assembling extends to the nonlinear case highlight the power of this formulation for the obtention of critical strains at a reasonable computational effort. From a numerical point of view, incremental-iterative procedures have been implemented for each interatomic potentials taken into account, in such a way they let us to verify that geometrical nonlinearity is triggered before the constitutive one, according to Falvo et al. and Iijima et al. As output results of our developed codes, nonlinear equilibrium paths, critical strains and final deformed shapes under the usual loading schemes in beam or rod structures are provided.

Finally, the suitability of the initial geometry provided from the conformal mapping on an ideal cylindrical surface is studied. Specifically, the initial diameter of the cylinder was determined by using the minimization of the total energy of the system under the three chiralities, assuming the bond lengthening vanish compared to the length of reference in the planar graphene sheet. The obtained diameter values and internal forces were compared with the results from the linear analysis of our model, finding a close agreement between the output values from both procedures. The consideration of this new initial geometry represents an alternative way to introduce the nanotube curvature into its mechanical behavior.