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Special Finite Element Modeling for Predicting the Mechanical Properties of CarbonNanotubes at the Atomic Scale

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ABSTRACT

Due to the difficulties of experimental methods, computational methods are considered to be powerful tools to predict the mechanical properties of carbon nanotubes. In this paper a special finite element model based on harmonic inter-atomic potential is carried out in order to predict the elastic properties of nanotubes at atomic scale. The importance of contribution of the bond dihedral element in the modeling is studied, its results have shown that it stabilize the calculation. Moreover, the effect of length, diameter and chirality onthe mechanical properties are also studied and discussed. The obtained results show good agreement with otherresults in the literature and they have proved the importance of this method in the rapid prediction of theelastic behavior of the CNT compared to the moleculardynamic method (MD).

Keywords—Atomic scale, Carbon nanotube, Finiteelement method, Harmonic inter atomic potential, Mechanical properties.

DOI: 10.21467/abstracts.122 ISBN: 978-81-954993-3-5