

The Structural Stability and Energetics of Single Walled Carbon Nanotubes Under Uniaxial Strain with $O(N)$ Parallel Tight Binding Molecular Dynamics Simulation

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Abstract

A sequential $O(N^3)$ TBMD simulation program is converted into an $O(N)$ parallel code. The code is tested in a distributed memory system consisting of a cluster with 8 PC's that run under Linux. Our results on the speed up, efficiency and system size are given. The accuracy of the $O(N)$ description is found to be enhanced by the use of basis functions of neighboring atoms (buffer). The importance of buffer size in evaluating the simulation time, total energy and force values together with electronic temperature has been shown. The metallic and semiconducting behavior of (10×10) armchair and (17×0) zig zag SWNT's, respectively, has been demonstrated through the local density of state results. (10×10) SWNT consisting of 400 atoms with 20 layers is simulated under tensile loading. It is observed that the simulated carbon nanotube is able to carry the strain up to 122% of relaxed tube length in elongation and up to 93% for compression. The Young's modulus, tensile strength and Poisson ratio are calculated and the values found are 0.311 TPa, 4.92 GPa and 0.287, respectively. The elastic limit is observed at the strain rate of 0.09 while the breaking point is at 0.23. The frequency of vibration for the pristine (10×10) carbon nanotube in radial direction is 4.71×10^3 GHz and it is sensitive to the strain rate.