Low Temperature Thermal Behaviour of Armchair Single Walled Carbon Nanotubes

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Since their discovery in 1991, Carbon Nanotubes (CNTs) have attracted much attention from various branches of science. Carbon bonds make them strong and stiff in the axial direction and flexible in the radial direction. Due to their unique properties they have wide variety of applications such as reinforcing materials in nanocomposites and nanotube transistors in nanoelectronics. On the other hand, temperature is an important parameter that effects the physical, mechanical and electronic properties of CNTs [1-2]. Therefore, the investigation of thermal behaviour of CNTs is a key study for the nanotube based nanodevice performances.

In this work, we investigated thermal behaviour of Single Walled Carbon Nanotubes (SWCNTs) at low temperatures. Low temperature studies can provide the most valuable information about the dynamics of nanotubes. We studied the structural stability, physical properties and the radial thermal expansion coefficients of SWCNTs in 0.1-200K temperature region. We examined various armchair SWCNTs having diameter up to 2 nm. We used a parallel O(N) Tight-Binding Molecular Dynamics (TBMD) Simulation code designed by G.Dereli et al. [3-5]. According to the results, we showed the structural stability, physical properties such as bond-angle, bond-length and radial distribution functions of the tubes. We also examined the diameter enlargement of SWCNTs in low temperature region and calculated the radial thermal expansion coefficients of them. We reported the variation of radial thermal expansion coefficients of SWCNTs as a function of temperature and the effects of diameter on the radial thermal expansion coefficients of the tubes in the low temperature region.

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