Thermomechanical Properties of Single-Wall Carbon Nanotubes

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Abstract

The morphology variations of carbon nanotubes (CNT) at temperature are studied by using molecular dynamics simulations. It is found that thermally induced morphology changes arise from a combined effect of internal energy and entropy. Firstly, with increasing temperature, the anharmonic interatomic potential will cause both atomic bond length and bond angle to change, leading to thermally induced expansion. In addition, as the temperature increases, the higher configuration and vibration entropy of the system cause the carbon nanotube to vibrate. These vibration modes are similar to the natural mechanical vibration modes of shells (for short CNT) and beams (for long CNT) obtained from continuum mechanics. The total energy of the system increases with rising temperature, which excites various vibration modes/frequencies and/or different vibration amplitudes. Consequently, the vibrations of the nanotubes lead to the apparent thermal induced contraction of carbon nanotubes. Therefore, the overall thermal-mechanical behaviors of carbon nanotubes are exhibited through the competition between two distinct mechanisms: the thermal expansion due to the increase of bond length and bond angle, and the apparent thermal contraction due to the CNT vibration. In the temperature range from 0K to 800K we have explored, the effect of thermal vibration is more dominant, so the net effect of thermally induced CNT morphology change is contraction. The findings can be readily expanded to other similar types of nanotubes and nanowires, and the study will have important applications in nanoelectronics devices made by nanotubes and nanowires.