Thermal conductivity of SWNTs in practical systems

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It is theoretically predicted that single-walled carbon nanotubes (SWNTs) have extremely high thermal conductivity [1]. Furthermore, some experimental reports are supporting the prediction, though with certain uncertainty due to technical difficulties in probing the nanoscale material. Nevertheless, with the quasi-one dimensional structure constructed with the strong bonds, it should be fair to expect SWNTs to be a good heat conductor. However, in practical situations, there are potential causes for attenuation of the heat conduction. One is the intra-tube local thermal resistance due to defects and hetero-junctions. The macroscopic quantities such as thermal boundary resistance have been deduced from non-equilibrium molecular dynamics [2]. For further understanding of the phonon transmission, reflection and scattering at the junction, we performed non-stationary molecular dynamics simulations, where a local heat pulse is generated as coherent fluctuations and passed through the junction. Fig. 1 depicts the spatio-temporal isotherm contours of the heat pulse interfered by the junction of ^{12}C-SWNT and ^{13}C-SWNT. This allows us to visualize the dynamics at the junction including the unharmonic events.

SWNT heat conduction can also be altered by the interference with the surrounding materials. For example, as SWNTs form bundles in many cases, the influence of the inter-tube interaction to the lateral heat conduction should be of an interest. We perform series of simulation by varying the mean inter-tube distance. Furthermore, as a general case of interaction with surrounding materials, we investigate the SWNT in contact with the surrounding Lennard-Jones matrix. When in solid phase, the matrix exhibits modal interaction with transverse phonons of SWNT, hence should have nontrivial influence on the SWNT thermal conduction. Finally, heat conduction of the SWNT confining water is investigated. As water confined in an SWNT experiences an anomalous phase change to form an ice tube [3], the tube structure internally adsorbed to the SWNT is expected to influence the thermal conductivity at low temperature.

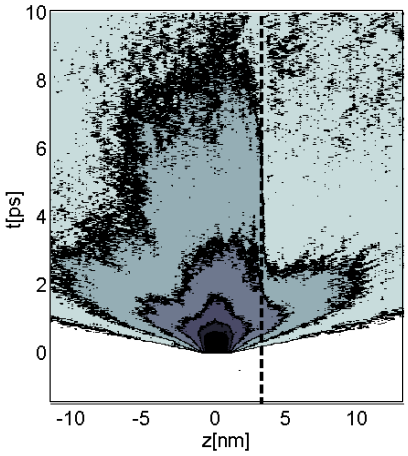

Fig. 1 Spatio-temporal contours of isotherms. Dotted line indicates the junction between ^{12}C-SWNT (left) and ^{13}C-SWNT (right).

[1]. S. Berber, *et.al.*, *Phys. Rev. Lett.* **84**, (2000) 4613.

[2]. Maruyama, et.al., to be submitted.

[3]K. Koga, *et.al.*, *Nature*, **412** (2001) 802.

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