

# Molecular Dynamics Simulations of Heat Conduction of Carbon Nanotubes

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We have been studying the heat conduction along a single-walled carbon nanotubes (SWNTs) by the molecular dynamics method [1,2] with the Tersoff-Brenner bond order potential [3]. One of the purposes of this study is to clarify the thermal conductivity of carbon nanotubes, which is speculated to be higher than any other material along the cylindrical axis. Our preliminary results showed that thermal conductivity was strongly dependent on the tube length for realistic length scale for device applications [1,2]. Some realistic heat conduction simulations with direct temperature difference for a capped nanotube is being performed. We also have studied the difference of the heat conduction among SWNT, peapod and a double-walled carbon nanotubes (DWNTs).

We estimated the difference of the thermal conductivity, the phonon dispersion relation and DOS of phonons among SWNTs, peapods and DWNTs by using the Brenner-Tersoff potential function for carbon bonding and the Lennard-Jones potential function for van der Waals force. The difference was so small to observe the effect of peapods and DWNTs. In order to emphasize the minute difference of the phonon dispersion relation, we have calculated the system with artificially large van der Waals force. One of the preliminary results is showed as Fig. 1 interaction with the 10 times larger energy parameters of Lennard Jones potential. Slight modification of the phonon DOS was observed in the low frequency region. The reason of these changes will be discussed.

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[2] S. Maruyama, *Micro. Thermophys. Eng.*, (2002), in press.

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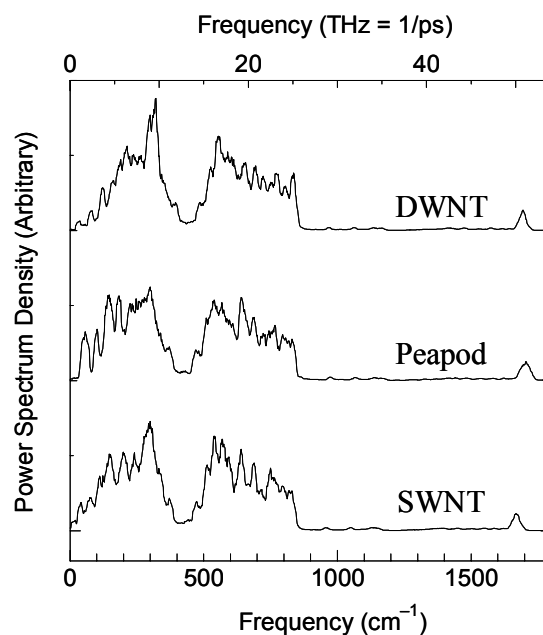


Fig.1 Phonon density of states calculated from radial velocity component.