# Phonon transport in finite length SWNTs using molecular dynamics simulations

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Single-walled carbon nanotubes (SWNTs) are expected to possess high thermal conductivity due to their quasi-one-dimensional structure and strong carbon bonds [1]. While experimental attempts to characterize heat conduction of SWNT encounter technical difficulties, the classical molecular dynamics (MD) simulations hold advantage as the heat conduction is phonon-dominated. MD simulations give us access to detail properties such as length dependence of thermal conductivity. Furthermore, by analyzing temporal evolution of spatio-temporal spectra by performing the wavelet transform or the short time Fourier transform, one can probe dynamics of individual phonon modes and their contribution to the overall heat conduction.

Our early MD studies showed the power-law length dependence of SWNT thermal conductivity up to sub-micrometers length [2]. This has been discussed in relation with the one-dimensional heat conduction where theoretical models exhibit divergence of the thermal conductivity with respect to the tube length [3]. Here, we report our recent results of the simulation covering larger range of nanotube length and with longer sampling time. Results indicate that thermal conductivity is likely to converge where the length dependence falls off from the power law at the nanotube length of the order of a micrometer. The results, together with the observation of detailed phonon dynamics, will be compared with available studies of phonon transport equations. The detail pictures of the phonon transport can be probed by exciting heat pulse or wave packet and tracing their propagation. For finite length SWNTs, phonon dependent contributions to the heat conduction are investigated in terms of transport properties of phonon modes in the key branches.

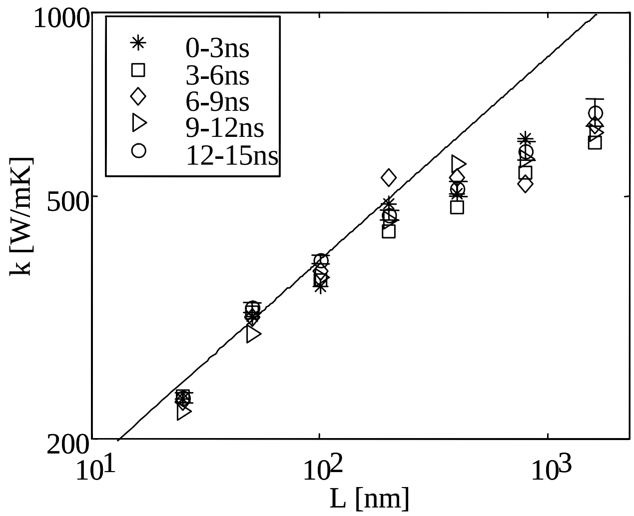


Fig. 1 The length dependence of thermal conductivity of finite length (5,5)-SWNTs. Different marks denotes the sampling intervals. The solid line indicates the power-law relation, $k \propto L^{1/3}$.

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

[2]. S. Maruyama, et.al., *Micro. Therm*. Eng. **7**, (2003) 41

[3]. R. Livi and S. Lepri, *Nature* **421**, (2003) 327

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