Molecular Dynamics Simulations of Heat Conduction of Peapods

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We have been studying the heat conduction along a single-walled carbon nanotubes (SWNTs) by the molecular dynamics method with the Tersoff-Brenner bond order potential [1-3]. 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. According to the recent experiment, it has been suggested that the thermal conductivity of Peapods is higher than empty tubes [4]. Here, we have studied the thermal conductivity of Peapods and change in the phonon dispersion relations and DOS of phonons.

In the previous research, we used the Brenner-Tersoff potential function between each carbon molecules [5]. In order to simulate the structure of Peapod as showed in Fig. 1, in addition to the Brenner potential, van der Waals force was assumed as the Lennerd-Jones potential between two carbon atoms that were not part of a molecule. A SWNT model with chirality of (10,10) was filled with C_{60} molecules along the axis. By applying the phantom heat bath model to each end of a SWNT, the temperature difference was applied. Here, no periodic boundary condition was applied to minimize the "boundary scattering of phonons." With our configuration, thermal conductivity was calculated from temperature gradient and heat flux which was obtained by the integration of the additional force by the phantom molecules. The preliminary results showed that the thermal conductivity of Peapods was slightly higher than empty (10,10) tubes.

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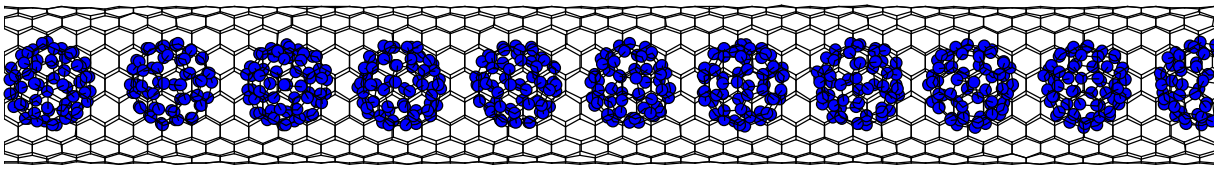

Fig. 1 A peapod structure with C_{60} molecules in a (10,10) SWNT.