Isotope Effects on Heat Conduction of Carbon Nanotubes

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We have been studying the heat conduction along a single-walled carbon nanotube (SWNT) by the molecular dynamics method with the Tersoff-Brenner bond order potential [1, 2]. It is well known that the inclusion of only 1 % of ^{13}C natural isotope dramatically reduces the thermal conductivity of diamond. However, isotope effects on heat conduction of SWNTs have not been elucidated. We estimated isotope effects by molecular dynamics simulation with regarding two different configuration of the isotopes: Two SWNTs made up of different isotopes was connected in one configuration (separated configuration), whereas two kind of isotopes are randomly mixed in a SWNTs in the other (random configuration).

In the separated configuration, the temperature jump explained by the thermal boundary resistance was observed at the connection of tubes with different carbon mass. This thermal boundary resistance between tubes increased with the artificially increase of the atomic mass of heavier isotope. In the random configuration, the thermal conductivity of a SWNT was reduced by an inclusion of isotopes depending on the ratio of introduced isotope. We have explained the effect of isotope ratio on the degree of SWNT conductivity deterioration using a simple equation derived with several assumptions on phonon dispersion (Fig. 1). In the alcohol CCVD experiment [3], we have synthesized several types of SWNTs made up from ^{13}C-isotopically modified ethanol in the different atomic positions, whose Raman spectra are shown in Fig. 2. The difference observed in these spectra is explained based on our molecular dynamics simulations and will be presented at the symposium.

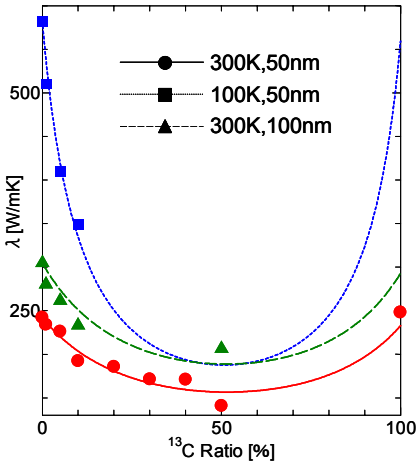

Fig.1 The change of the thermal conductivity by isotope effects

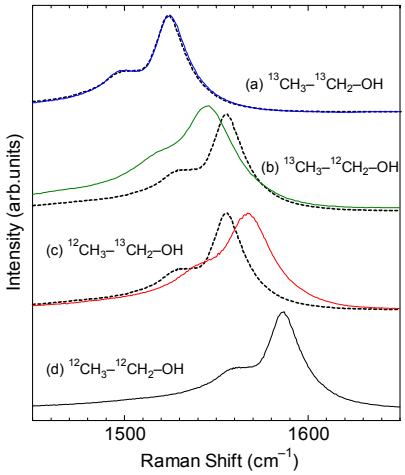

Fig.2 Raman spectrum of SWNTs made from isotopically modified ethanol

[1] S. Maruyama, *Physica B,* **323**, 1-4, 272-274 (2002).

[2] S. Maruyama, *Micro. Thermophys. Eng.*, **7**-1, 41-50 (2003).

[3] S. Maruyama et al., *Chem. Phys. Lett.*, **360**, 229-234 (2002).

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