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Thermal conductivity of single-walled carbon nanotubes with ^{13}C isotopes[1] JUNICHIRO SHIOMI, SHIGEO MARUYAMA, The University of Tokyo — Molecular dynamics simulations were performed to investigate the influence of impurities on thermal conductivity (k) of (5,5)-SWNTs. The impurities were represented by mixing ^{13}C isotopes to a ^{12}C-SWNT. Random mixing of ^{13}C isotopes to ^{12}C- SWNTs results in decrease of k. The results show not only that k decreases against the fraction of mixed ^{13}C, but also that k is dependent on the structure of ^{13}C clusters, seemingly on their sizes. In order to highlight the influence of axial scales of the impurities, we consider SWNTs which consist of ^{12}C and ^{13}C periodically connected with certain interval thickness. The result shows that there is a critical interval thickness which gives the minimum value of k. Spectral analyses reveal the role of phonon modes. Adopting the phantom heat bath model to each end of a SWNT, k can be computed through the Fourier's law. Non-Fourier aspects of the heat transfer in the non-equilibrium SWNTs are also examined by applying a local heat pulse with duration ranging from 40 fs to 4 ps. The results of the simulations exhibit the heat waves of selected phonons traveling from the heated end of the SWNT towards the other. The characteristic properties of the heat flow will be discussed.

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