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Roles of Multi-Walled Structures in Thermal Transport Properties of Nanotubes TOMOYUKI HATA, HIROKI KAWAI, RYOTA JONO, KOICHI YAMASHITA, Department of Chemical System Engineering, Graduate School of Engineering, the University of Tokyo — The molecular structures of carbon nanotubes are thought to be deeply related with various physical properties. Understanding the relationship is one of the challenges in designing potential materials. In this research, we theoretically investigated the thermal transport properties of carbon nanotubes, focusing the multi-walled structures. We investigated the thermal conductance of the double-walled carbon nanotubes (DWCNTs) by using the nonequilibrium Green's function method. It is found that the inter-layer interaction causes the suppression of thermal conductance at low temperature. The analysis of the transmission coefficients revealed that this suppression was attributed to the energy shifts of the normal modes from the synchronized vibrations. The mechanism of such energy shifts is examined by the coupled vibration model with the parameters extracted from our simulations, and we grasp the multi-wall effects on the thermal transport properties of the nanotube structures.

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