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Calculation of Phonon Dispersion and Thermal Conductivity in Carbon Nanotubes MAYANK VARSHNEY, VLADIMIR A. FONOBEROV, ALEXANDER A. BALANDIN, Nano-Device Laboratory (<http://ndl.ee.ucr.edu/>), Department of Electrical Engineering, University of California, Riverside, CA 92521 — Many potential applications of carbon nanotubes in nanoelectronic circuits rely on effective removing of excess heat from the device active area. Heat in carbon nanotubes is mostly carried by acoustic phonons. In this work we have calculated phonon dispersion in carbon nanotubes using atomistic approach. The phonon dispersion was then used to calculate phonon density of states, heat capacitance and thermal conductivity. The thermal conductivity has been determined using the modified Callaway – Klemens approach, which accounts for the low-dimensional size effects [1]. The results of our calculations are compared with the experimental Raman spectroscopic study of carbon nanotubes and reported values of the thermal conductivity. The authors acknowledge the support of MARCO and its Functional Engineered Nano Architectonics (FENA) Focus Center. [1] A.A. Balandin, Thermal Conductivity of Semiconductor Nanostructures, in Encyclopedia of Nanoscience and Nanotechnology (ASP, Los Angeles, 2004) p. 425.

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