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**Molecular dynamics simulation of Carbon Nanotube-to-SiO2 heat dissipation**[1] ZHUN-YONG ONG, ERIC POP, University of Illinois at Urbana-Champaign — Understanding the mechanism of heat dissipation from carbon nanotubes (CNTs) to their surrounding medium is essential for the operation of CNT-based electronic devices and heat sinks. At high current levels, significant Joule heating can occur in CNT devices, leading to hot phonons and energy dissipation bottlenecks which degrade electrical transport. We investigate thermal coupling between single-wall CNTs and SiO2 dielectrics by non-equilibrium classical molecular dynamics (MD) simulations. The thermal boundary conductance (TBC) is computed by setting up a temperature pulse in the CNT and monitoring its relaxation into the SiO2. The TBC is found to scale approximately linearly with CNT diameter (d $\sim$ 0.8 - 1.8 nm) and as a weak power law of temperature (T $\sim$ 200 - 600 K). We also find a linear dependence of the TBC on the strength of the CNT-SiO2 van der Waals coupling. Our simulation results are comparable to experimental data obtained from electrical breakdown thermometry of the CNT-substrate TBC. Using the power spectrum analysis technique, we also find that energy relaxation is most significant in the long wavelength, low frequency region of the phonon power spectrum.

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