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Heat Transfer Dynamics at Carbon Nanotube Thermal Switch and Silicon Interface[1] TAEJIN KIM, MOHAMED OSMAN, Washington State University — Carbon nanotubes are very attractive for interconnect and thermal management due to their very high thermal and electrical conductivities. However, the properties of the interface between CNT and other materials influence the overall performance of the CNT interconnects and thermal materials. For example, a thermal switch based vertical carbon nanotube exhibited higher thermal resistance compared to one using mercury drops even though mercury's thermal conductivity is lower than that of carbon nanotubes. In this contribution, we describe a molecular dynamics model for examining heat transfer between a carbon nanotube thermal switch and silicon. The MD model takes into account the 2x2 reconstruction at the silicon surface and use the optimum sites for bonding between silicon and carbon atoms. In the MD simulations, both silicon and nanotubes are first heated to 300K followed by applying a 10 picoseconds heat pulse to the CNT only. As a result of heat diffusion to silicon, the temperature difference between the CNT and silicon exhibits an exponential decay with a time constant $\tau = 38$ps (when a single time constant is assumed) which is used to estimate the interface thermal resistance. We will report on the results of our simulations, details of the MD model, role of the phonon coupling at silicon-CNT interface, and compare the results to those obtained from nonequilibrium MD approach.

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