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Thermal boundary resistance between carbon nanotube bundle and silicon MOHAMED OSMAN, School of Engineering and Applied Sciences, Washington State University Tri-Cities, TAEJIN KIM, Center for Cancer Research, National Cancer Institute (NCI) — Heat transfer between different materials is strongly affected by the discontinuity in the atom arrangement at the interface which influences the propagation of phonons responsible for heat flow across the interface. Molecular dynamics simulations has been used to investigate the thermal boundary resistance (TBR) between a bundle of (5,5) nanotubes and surrounding silicon. The thermal boundary resistances from MD simulations at 100K and 300K, were 7.1x10^{-9} m^2K/W and 4x10^{-9} m^2K/W respectively. The decrease in TBR at 300K compared to 100K is due to increased phonon population. However, the TBR value at 300K is four times larger than the results reported in [1]. The difference can attributed to the fact that in our simulated structure, heat flow is in the radial direction and the bonding between Si and C atoms at the interface changes the carbon nanotube sp^2 bonding to sp^3 bonding, where as in [1] heat flow is axial and the bonding at the CNT open end does not affect the sp^2 bonding significantly.

[1] Y. Feng, J. Zhu, and D. Tang, **AIP Advances**, **4**, 127118 (2014).

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