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CHT-15: Investigation of Phonon Transport and Thermal Boundary Conductance at Interface of SWCNT and Poly (Ether-Ketone)

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The thermal and electrical applications of many polymers commonly used in commercial and defense applications are very scarce due to their low conductivities. The addition of carbon nano-structures such as carbon nanotubes (CNTs) in the polymer matrix can lead to significant improvement in the thermal and electrical properties of the resulting nano-composite. If CNTs are controllably functionalized in a covalent manner to polymeric entities, these entities can act as bridge or interconnects for efficient thermal transport in a CNT network dispersed in a polymer leading to high effective conductivity of the CNT-polymer assembly. An exceptional improvement in the electrical and thermal conductivity of fibers made by poly(ether ketone) (PEK) grafted few walled carbon nanotube has been observed in the experiments. However, the thermal interaction of CNT and PEK molecules has not been understood yet.

In this investigation, non-nequilibrium molecular dynamics (NEMD) is used to determine the thermal boundary conductance (TBC) and elucidate phonon transport at the interface of CNTs and PEK. Phonon life times of isolated CNT and CNT embedded in PEK nano-composite is estimated using normal mode decomposition technique. The phonon life times of isolated CNTs and CNTs embedded in PEK are very different which will significantly affect the thermal properties of CNTs and also the CNT-PEK assemblies. Thermal boundary conductance at the CNT-PEK interfaces is essentially influenced by the nature of bonding. This is studied by estimating TBC for CNT-PEK assemblies with various degrees of bonded interfaces. This study will provide insights into tuning interfacial structure to improve phonon transport at CNT-polymer interfaces.