Thermal Properties of Fullerene and Fullerene Derivatives

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In this work, we perform molecular dynamics (MD) simulations to study the effects of alkyl chains on the thermal properties of fullerene (C_{60}) and fullerene derivatives, and compare the MD prediction with experimental results from Time Domain Thermoreflectance (TDTR). The thermal conductivities of fullerene and its derivative phenyl-C61-butyric acid methyl ester (PCBM) are obtained using non-equilibrium MD simulations for systems with different sizes at room temperature. The results show a length-dependent thermal conductivity for C_{60} but not for PCBM. Around the room temperature, the thermal conductivity of C_{60} obtained from linear extrapolation (up to 33 nm) is 0.2 W m^{-1} K^{-1}, while the thermal conductivity of PCBM saturates at ~0.075 W m^{-1} K^{-1} around 20 nm. The different length-dependent behavior of thermal conductivity indicates that the long-wavelength and low-frequency phonons have large contribution to thermal conduction in C_{60}, and the decrease in thermal conductivity of fullerene derivatives can be attributed to the strong scattering of those phonons with the alkyl chains. This fact is also indicated by the significant mismatch of vibrational density of states in low frequency regime between buckyballs and alkyl chains in PCBM. The spectra of density of states (DOS) suggest that those dominant phonon modes at ultra-low frequency regime (< 2 meV) are assigned to rotational and vibrational motions of buckyballs in C_{60}, which are suppressed by alkyl chains in PCBM.