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Localized Resonances and Modal Hybridization for Thermal Conductivities of Nano Materials

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ABSTRACT

The localized resonances and modal hybridization was used to present thermal conductivities of organic based nanomaterials. It was found that fullerene molecules were wielded onto single walled nanotubes were reduced. The hybridization between the modes of the fullerene and the carbon nanotubes formed resonant phonon band anticrossings by bonded fullerene molecules. When hybridization strength was increased due to increasing periodicity and surface coverage of fullerene generated a platform for the study of thermal transport in material systems. The nano materials termed as nanobuds structure produced extremely high current density were found optically transparent. The enhancement of physical properties fullerene functionalization prevented slippage of hybrid carbon nanotube materials made them immobile opposed to mobile character of fullerene and carbon nanotubes. The thermal transport in hybrid materials comprised chemically functionalized carbon nanotubes with fullerene molecules. We have made the study of influence of covalently bonded carbon molecules on the surface of carbon nanotubes on their thermal transport properties through a series of molecular dynamics simulations and lattice dynamics calculations. It was found that thermal conductivity of carbon nanotubes was reduced at room temperature with periodic inclusion of covalently bonded fullerene molecules on their sidewalls and produced large tenability in thermal transport of carbon nanotubes. The obtained results were found in good agreement with previously obtained results.

KEYWORDS

Localization, Resonance, Hybridization, Conductivity, Nanomaterial, Fullerene, Carbon Nanotube, Resonant Phonon, Thermal Transport, Slippage, Simulation.

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INTRODUCTION

Cahill e al. [1] presented that reduction of thermal transport in semiconducting solid was due to nano structuring and phonon scattering at interfaces defect sites. Kohn et al. [2] and Regner et al. [3] studied that nano structing lead to scattering of high frequency phonons with long mean free path. Garg et al. [4], Chen et al. [5] and Hua et al. [6]shown that heat conduction was mostly left unimpeded. Kim et al. [7], Cheaito et al. [8] and Liu et al. [9] presented that hierarchical approach was used for scattering of spectral bandwidth of vibrational energy carriers and it was found that it did not suppress the long wavelength phonon transport to realize the full potential for large reduction in thermal conductivities. Davis et al. [10], Honarvar et al. [11] and Xiong et al. [12] studied that photonic metamaterials based on silicon was used for effective scatter low frequency phonon by resonant effect. Wang et al. [13] showed that localized resonant method allowed for the manipulation of waves with characteristic wavelengths that are several times larger than the characteristic dimensions of the resonators. Avery et al. [14] and Panzer et al. [15] studied that carbon nanotubes have high thermal conductivities and were used in practical applications as energy storage and thermal management. Kharisov et al. [16] studied that carbon nanotube cannot be combined with other materials due to chemical neutrality. Nasibulin et al. [17] showed that chemically active carbon molecules had been valently attached on the side walls of single walled carbon nanotubes for increasing chemical reactivity and mechanical flexibility. Zhu and Su [18] presented that nanobud structures produced high current density were found optically transparent. Bhat et al. [19] studied that transport in hybrid materials were found chemically functionalized carbon nanotubes with fullerene molecules and it was used for fabrication of flexible microelectronic devices. Larkin and McGaughey [20] used equilibrium molecular dynamics for the study of size effects affecting the calculated thermal conductivities. Larkin et al. [21] presented the lower limit of thermal conductivity contribution from each mode utilizing Allen-Feldman theory. Kodama et al. [22] calculated the thermal conductivity by using cross sectional area of the carbon nanotube and Vander Wals thickness. Salawav et al. [23] obtained thermal conductivity depending on the choice of the interatomic potential. Xu et al. [24] and M.Ji et al. [25] presented that the attachment of fullerene on the carbon nanotube sidewalls leaded to the transformation of the in plane sp^2 carbon–carbon bonds into out of plan sp^3 carbon-carbon bonds.

METHOD

The Tersoff potential was used to obtain interatomic interactions. The non bonded interactions were taken through Lennard Jones potential. Fullerene molecules are covalently bonded by periodic form of carbon nanobuds. We have considered a single, double and four sided fullerene functionalization to assess the role of surface coverage on thermal transport. The axis of the single walled carbon nanotubes were oriented in the Z-direction and periodic boundary conditions were utilized in this direction. The simulations were used to calculate the results. The length of the simulation cell in the Z-direction depended on the periodicity of the fullerene. It produced converged values of thermal conductivities for all structures. We have used the Green-Kubo approach under the equilibrium molecular dynamics simulations framework. The lattice dynamics calculations were made to obtain the results. The carbon nanotube having (9,9) chirality and the addition of fullerene on the side walls of the carbon nanotubes were taken into account through cycloaddition. Bond formations of the hexagonal face of carbon and a hexagonal ring in the single walled carbon nanotube was connected to form six carbon-carbon covalent bonds. The density functional calculation were considered to form stable nanobud structures. Thermal conductivities of single walled carbon nanotube and nanobud structures were calculated by using the relation

$$K_\alpha = \frac{1}{k_B V T^2}\int_0^\infty \left\langle S_\alpha(t) S_\alpha(o)\right\rangle dt.$$

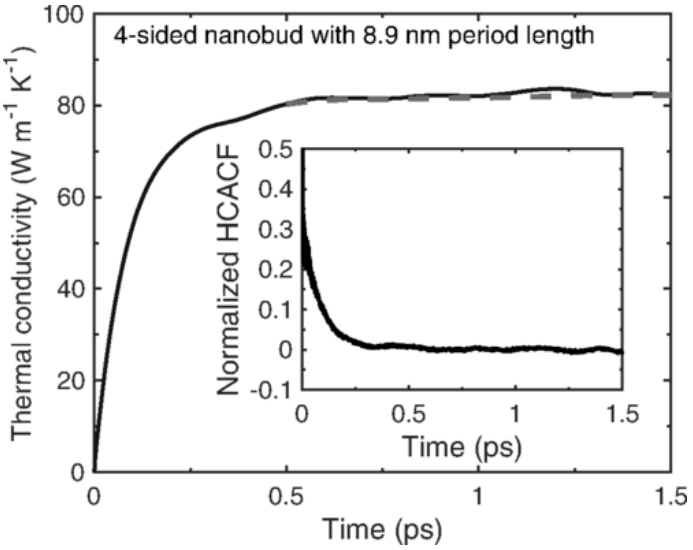
Where $\langle S_\alpha(t) S_\alpha(o) \rangle$ is the α th component of the heat current autocorrelation function, *T* is the temperature, *V* is the volume and *t* is the time. The localized resonant method allowed the wave with characteristic wavelengths several times larger than the characteristic dimensions of the resonators. This provided for the study of thermal transport properties in materials. The concept of localized resonances and modal hybridization to present thermal conductivities in organic based nanomaterial were used, which was termed as nanobuds in which fullerene molecules were wielded onto single walled carbon nanotubes were reduced. The effect of covalently bounded carbon molecules on the surface of carbon nanotubes on thermal transport properties were studied. Allen-Feldman theory was used to compute the contribution from diffusive and nonpropagating modes using this relation

$$K_{AF} = \sum_{diffusion} = \frac{k_B}{V} D_{AF,n}(\omega_n)$$

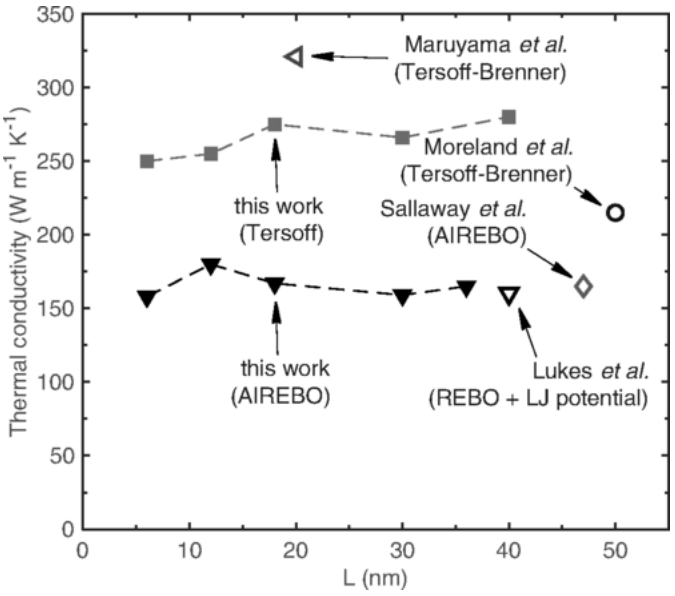
Where $D_{AF,n}$ is the harmonic approximation, ω_n is the frequency of *n*th and $D_{AF,n}$. The Lorentzian broadening of delt function was studied with comparison with mode spacing. The obtained results were compared with previously obtained results.

RESULTS AND DISCUSSION

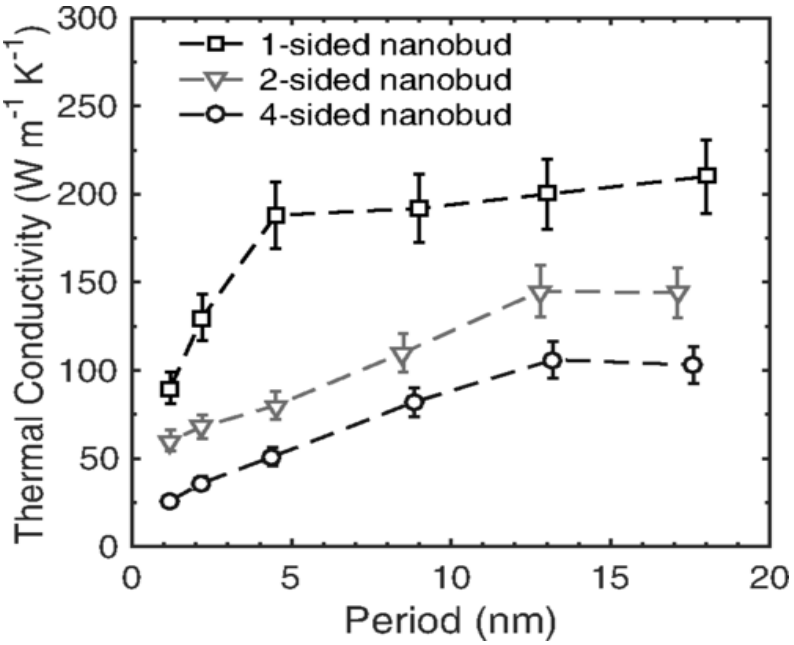
We have studied the influence of covalently bonded carbon molecules on the surface of carbon nanotubes on thermal transport properties by a series of molecular dynamics simulations and lattice dynamics calculations. Equilibrium molecular dynamics simulations were used for the calculations thermal conductivities of functionalized carbon nanotubes having fullerene at different periodicities. Graph (1) shows the converged value of thermal conductivity for a four-sided nanobud with 8.9 nm period length. Graph (2) shows the thermal conductivity of (9, 9) single walled carbon nanotube as a function of domain length L. The calculations of thermal conductivity represent the cross sectional area of the carbon nanotube having diameter of (9, 9) carbon nanotube and thickness of walls, which differed from previous values. It also indicated the effect of cross sectional area, potential and simulated method used. Graph (3) shows the plot of thermal conductivity of the one, two and four sided nanobuds as function of period length. The thermal conductivity of nanobuds with short period lengths were found lower in comparison to pristine carbon nanotube. When the period length monotonically decreased the thermal conductivity of all nanobud type decreased which is shown in Graph (3). Graph (3) also shows that thermal conductivity began to level off as increased periodically. In the case of large number of fullerene molecules were periodical the thermal conductivity decreased further. Increased reduction in group velocities due to increase of hybridization of energy states were more than an order of magnitude lower than the calculated values of thermal conductivity of pristine carbon nanotube at 300K. Graph (4) shows the temperature dependence of thermal conductivities for two and four-sided nanobuds. Graph (4) (c) the temperature dependence of thermal conductivity of pristine carbon nanotube. The reduction in thermal conductivity from room temperature to 100 K for a pristine carbon nanotube, the reductions in nanobuds the thermal conductivities were much less. Long period nanobuds in comparison to short period nanobuds showed larger reductions in thermal conductivity for high temperature. The finding at moderate temperatures from prior theroretical work in the case of three phonon scattering processes, the temperature dependence of thermal conductivity of pristine carbon nanotube were driven by anharmonic umklap scattering processes. Graph (4) (a) and (4) (b) does not explain the obtained results of nanobuds. The fullerene molecules efficiently blocked the low frequency phonons and partially scattered the high frequency modes. An harmonicity greatly affected the high frequency phonon at high temperatures scattered high frequency phonons more efficiently. The results found were compared with previously obtained results and were found in good agreement.



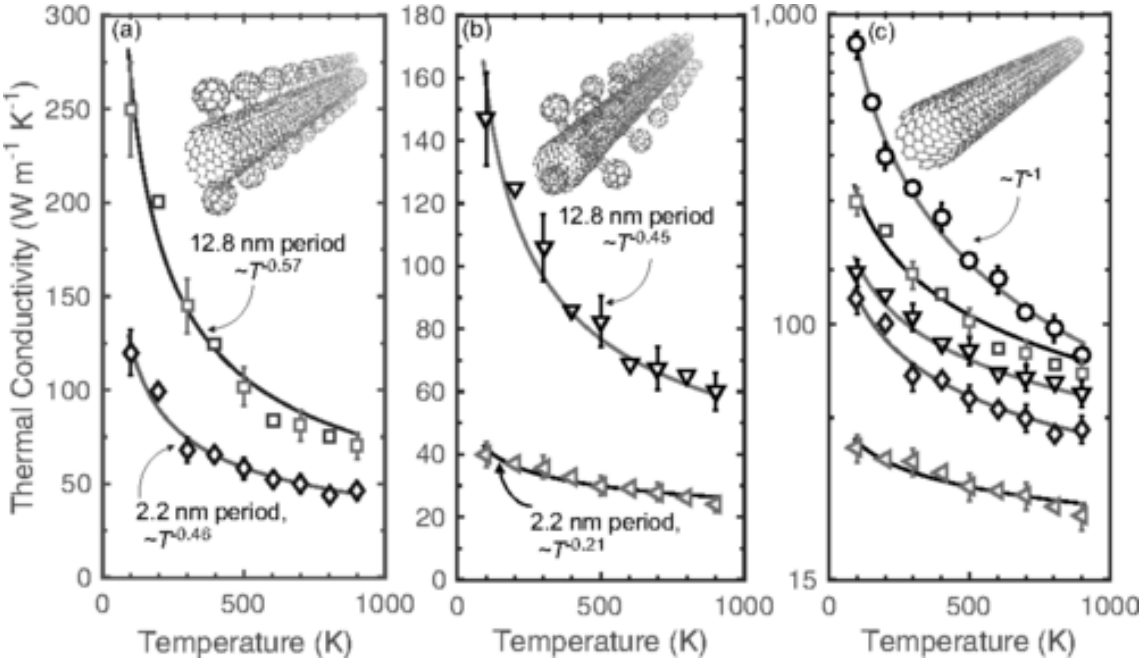
Graph 1: Plot of converged thermal conductivity for a four sided nanobud vs period length of the integral heat current.



Graph 2: Plot of thermal conductivity of single walled carbon nanotube vs function of length.



Graph 3: Plot of thermal conductivity of the one-, two- and four- sided nanobuds as a function of period length.



Graph 4: Temperature dependent thermal conductivities.

CONCLUSION

We have studied he localized resonances and modal hybridization for thermal conductivities of nano materials. The fullerene molecules were wielded onto single walled carbon nanotubes were found reduced. The effect of phonon transport of high and low frequency modes was due to creating defects which acted as both high frequency phonon scattering sites and coherently manipulated low frequency waves through resonance having long wavelength phonons. We have used simulations for fullerene functionalization on the side walls of carbon nanotubes as efficient phonon blocked the localized resonances which appeared through hybridization between the modes of the fullerene and carbon nanotubes. We have found large surface coverage and high periodicity for covalently bonded fullerene. The obtained results were found in good agreement with previously obtained results.

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