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Thermal Transport in Nano Structured Carbon Nanotubes and Its Thermal Conductance

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ABSTRACT
We have studied thermal transport in nano-structured carbon nanotubes and have calculated its thermal conductance using the nonequilibrium Green's function method. The thermal conductance of carbon nanotubes linearly depended on the width of the unzipped part of the carbon nanotube but exponentially decayed and then converged to a finite value of the unzipped length increased. But characteristics are unusual to common bulk materials but are universal to nano materials of nanotube and graphene like structures. An exponentially decayed thermal conductance with the length was found at interfaces. Electronic conductance was found to show an exponential thermal transport in carbon nanotubes showed features distinctly different from those in common bulk materials. Carbon nanotubes have been found strong structural imperfections; their thermal conductance exhibited unexpectedly perfect linear scaling behavior as the width of the unzipped part changed. As the unzipped length increased, thermal conductance exponentially decreased by the one dimensional atomic chain model. The obtained results were found in good agreement with previous results.

KEYWORDS
Thermal Transport, Nano Structure, Carbon Nanotube, Thermal Conductance, Non-Equilibrium, Green Function, Interfacial, Unzipped, Imperfection.

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INTRODUCTION

The development of integrated circuits as well as other application of similar devices required study of interfacial thermal transport of the nanoscale. Thermal transport has attracted considerable research interest due to its crucial significance to fundamental science, such as the observation of quantized thermal conductance in suspended insulating nanostructures [1] and the breakdown of Fourier's law in nanotube conductors [2]. Thermal insulation [3] and thermo-electricity [4] critically relied on the thermal transport at the nanoscale. Carbon nanotubes and graphene have excellent electronic, magnetic, mechanical and thermal properties and for carbon based nanoelectronics [5-6]. Both materials possessed extremely high thermal conductivity [7], exceeding that of diamond. The behavior of thermal transport at interfaces between them [8], though it is crucial for carbon based nanoelectronics that required integration of both materials. The Junction between carbon nanotubes and graphene nanoribbons partially unzipped carbon nanotubes has been useful in electronics and spintonics. They exhibited high magneto resistance [9] and supported spin polarized transport [10-12]. They can be experimentally fabricated by solution based oxidation [13], argon, plasma etching [14] or exfoliation caused by intercalation [15]. Some investigators [16-20] studied symmetrically interfacial thermal transport in partially unzipped carbon nanotubes using the nonequilibrium Green's function method. Datta [21] studied and found that electronic conductance decayed exponentially to zero in contrast to the decay to a finite value. Cahill et al [22] showed that acoustic mismatched model was successfully applied to a lot of interfaces. Donadio and Galli [23] used classical method for nanoscale thermal transport study was largely, limited by its breakdown at low temperatures. The quantum effects were fully considered for study and calculations of results, which are significant for carbon systems at temperatures much lower than the Debye temperature [24].

METHOD

In this study we have used the nonequilibrium Green's function method, which provided a full quantum mechanics description of transport processes, offered a systematic way to deal with many body problems and gave accurate results for systems without many body interactions. Quantum effects were taken into account for calculations of results. We have performed structural relaxation then computed force constants using a second-generation reactive empirical bond order potential. Using the force constants the phonon Hamiltonian of the system was constructed and retarded Green's function of the central part and was calculated as

$$G_C^R[\omega] = \left[\left(\omega^2 + i\delta\right)I - D_{CC} - \Sigma_L - \Sigma_R\right]^{-1}$$

Where δ is a small positive member to avoid divergence, I is the identity matrix, D_{CC} is the force constant matrix of the central part and $\Sigma_{\frac{L}{R}}$ is the self energies of the thermal constants $\frac{L}{R}$. Phonon scattering caused by the nonuniformity of the system was included in the transmission function, which was obtained through

$$\Sigma_R(\omega) = Tr\left[G^R \Gamma_R G^A \Gamma_L\right]$$

Where $G^A = \left(G^R\right)^{\dagger}$

and $\Gamma_{\frac{L}{R}}(\omega) = i\left[\sum^R_{\frac{L}{R}}(\omega) - \sum^A_{\frac{L}{R}}(\omega)\right].$

The thermal conductance contributed by phonons have been achieved by the Landauer formula

$$\sigma = \frac{k_B T^2}{2\pi\hbar}\int_0^\infty dx \frac{x^2 e^x}{\left(e^x - 1\right)}\Sigma\left(\frac{k_B T}{\hbar} s\right)$$

Where $x = \frac{\hbar\omega}{k_B T}$, k_B is the Boltzmann constant, T is the absolute temperature, $\hbar$ Planck's constant. Anharmonic interaction is weak in carbon system at moderate temperatures; phonon-phonon interaction was ignored. Considering that thermal conduction was dominated by phonons in partially unzipped carbon nanotubes, only lattice thermal conductance was included for the study and calculation of results.

RESULTS AND DISCUSSION

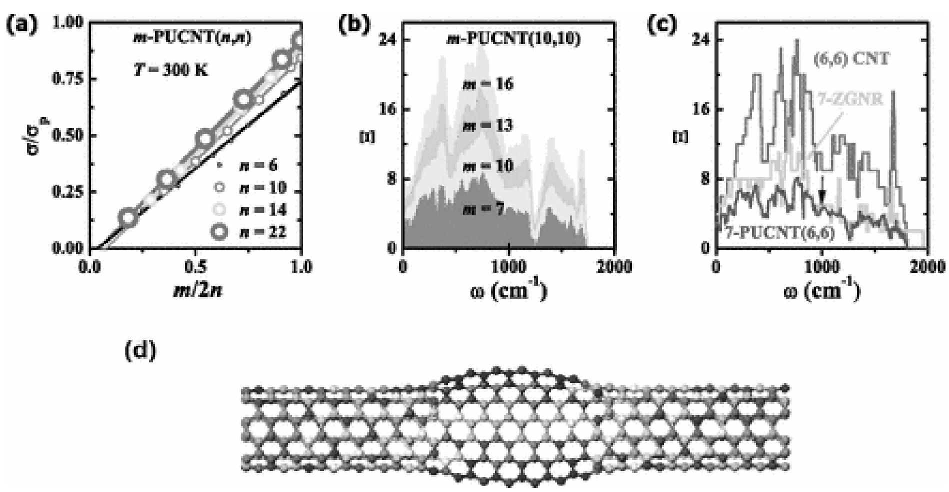
Graph (1) (a) shows the plot of room temperature versus thermal conductance contributed by phonons $\frac{\sigma}{\sigma_p}$ of m partially unzipped carbon nanotube (n,n) as a function of scaled width $\frac{m}{2n}$, where the unzipped length is fixed to be $L_u = 1.48\,nm$ without losing. $\frac{\sigma}{\sigma_p}$ of the partially unzipped carbon nanotubes gradually grown as increasing the scaled width.

At $\frac{m}{2n}=1$, which corresponded to the case of pure unzipping without any carbon atoms removed for 12- partially unzipped carbon nanotube (6,6), demonstrating a reduction of 26% in thermal conductance, while the reduction was only 8% for 44-partially unzipped carbon nanotube (22,22) indicating a larger influence of unzipping on $\frac{\sigma}{\sigma_p}$ in thinner carbon nanotubes. The thermal conductance of partially unzipped exhibited a linear dependence on the width of the unzipped part as shown in graph (1) (a).

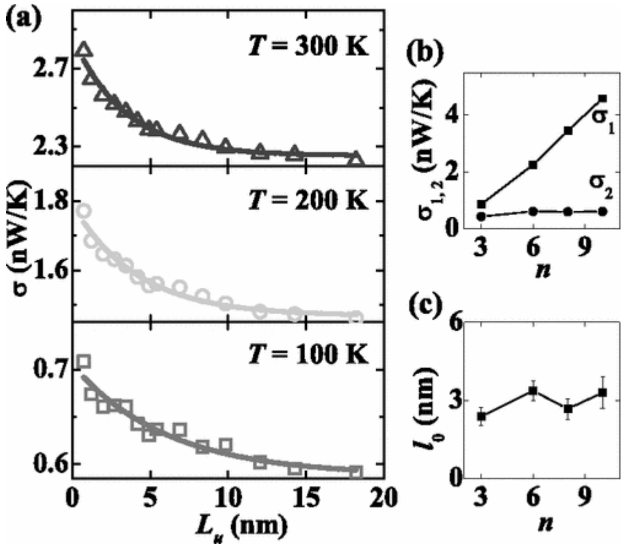
The linear scaling law manifested in the phonon transmission function as shown in graph (1) (b). The phonon transmission of m-partially unzipped carbon nanotube (10,10) grown with the unzipped width m over the entire frequency region because wider width supported phonon transport channels. This explains the increasingly higher thermal conductance for larger m. Graph (1) (c) shows phonon transmission of 7-partially unzipped carbon nanotube (6,6) at 1000 cm^{-1} is very close to that of corresponding zigzag graphene nanoribbon. Graph (2) (a) shows unzipping induced larger thermal conductance reduction at higher temperatures caused by significant phonon transmission reduction at the high frequency region as shown in graph (2) (c). The results showed a general trend, thermal transport of partially unzipped carbon nanotubes decreased rapidly at first and then gradually approached a finite value as L_u increased. The trend existed for all the partially unzipped carbon nanotubes at almost all temperatures. The observed fluctuation in thermal conductance existed at low temperature i.e. 100K, they actually diminished at higher temperatures. We have found that the L_u dependence of thermal conductance was described by the relation

$$\sigma\left(L_n\right)=\sigma_1+\sigma_2\exp\left(-\frac{L_u}{l_0}\right).$$

Where σ_1 is the converged thermal conductance of partially unzipped carbon nanotubes with infinite L_u, σ_2 is the amplitude of exponential decay and l_0 is the effective phonon mean free path. The obtained results were compared with previously obtained results and were found in good agreement.



Graph 1: Scaled thermal conductance $\frac{\sigma}{\sigma_p}$ at 300 K of m-partially unzipped carbon nanotube (*n*,*n*)



Graph 2: Thermal conductance σ of 12-partially unzipped carbon nanotube (6,6) as a function of the unzipped length L_u at temperatures of 100, 200 and 300K.

CONCLUSION

The study of thermal transport and thermal conductance was made in nanostructured carbon nanotubes. Systematic nonequilibrium Green's functions on thermal transport in carbon based nanostructures partially unzipped carbon nanotubes were made. The unusual interfacial thermal transport behaviors were revealed. We have found that thermal conductance of partially unzipped carbon nanotubes shown a perfect linear dependence on the width of the unzipped part and an exponential decay to a finite value with length of the unzipped part. The exponential length dependence was found at interfaces was a pure quantum phenomenon without classical counterpart. The characteristics were unusual to common on bulk materials but were universal to nanomaterials of nanotube or graphene like structures. The electronic conductance was found to show an exponential decay to zero value in contrast to the decay to a finite value. The results were found in good agreement with previously obtained results of theoretical and experimental works.

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