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INVESTIGATION OF THERMAL CONDUCTIVITY IN SINGLE-WALLED (n,n) CARBON NANOTUBES USING MOLECULAR DYNAMICS SIMULATION

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ABSTRACT

Single-walled carbon nanotubes (SWCNTs) are captivating materials renowned for their outstanding thermal properties and diverse applications in nanotechnology. This study utilizes molecular dynamics simulations to investigate the factors influencing thermal conductivity in SWCNTs, namely diameter, length, temperature, and defects. Results reveal that thermal conductivity exhibits an increase with both diameter and length, with values ranging from 3100 to 3400 W/m·K for diameters varying from 0.68 to 1.70 nm , and from 2800 to 3700 W/m·K for lengths ranging from 20 to 200 nm . Conversely, thermal conductivity demonstrates a decrease with rising temperatures, with values dropping from 3400 to 2600 W/m·K as temperature increases from 100 to 700 K . Furthermore, the presence of defects significantly diminishes thermal conductivity, as illustrated by reductions from 3200 to 2900 W/m·K for single vacancy defects and further to 2500 W/m·K for double vacancies. These findings insights into the thermal behavior of SWCNTs, enhancing our understanding of their thermal properties and broadening their potential applications, including in nanoscale cooling and nanoelectronics.

1.INTRODUCTION

Carbon nanotubes, also known as CNTs have garnered interest due, to their properties. Walled carbon nanotubes (SWCNTs) are particularly recognized for their heat conductivity showing potential in areas such as nanoelectronics, thermal management systems and composite materials. The remarkable thermal characteristics of SWCNTs can be largely attributed to their structure and the strong sp2 carbon carbon bonds they possess.

Factors like chirality, diameter, length, and temperature all play roles in influencing the conductivity of CNTs. The symmetrical structure of SWCNTs in the armchair configuration impacts their properties. Understanding these factors is essential for optimizing the performance of SWCNTs in applications. Molecular dynamics (MD) simulations offer a way to delve deeper into these aspects and reveal insights that may be challenging to obtain through methods.

The study of thermal conductivity in CNTs has been a topic of extensive research. Early theoretical works by Berber et al. (2000) demonstrated that CNTs could exhibit thermal conductivities as high as 6600 W/m·K, significantly surpassing those of traditional conductive materials like copper[1]. Subsequent experimental studies, such as those conducted by Pop et al. (2006), reported thermal conductivities in the range of 2000-3000 W/m·K for SWCNTs, albeit with considerable variability due to differences in sample quality and measurement techniques [2].

Research has shown that the thermal conductivity of SWCNTs is highly dependent on their chirality. Hone et al. (1999) noted that armchair SWCNTs ((n,n) type) generally possess higher thermal conductivities compared to their zigzag counterparts ((n,0) type) due to the more efficient phonon transport pathways in the armchair configuration. Additionally, Maruyama (2003) used MD simulations to reveal that the diameter and length of SWCNTs play significant roles in their thermal behavior, with larger diameters and longer lengths typically resulting in higher thermal conductivities [3].

Temperature is another critical factor influencing the thermal conductivity of SWCNTs. Studies by Zhang et al. (2004) using MD simulations indicated that thermal conductivity decreases with increasing temperature, primarily due to enhanced phonon-phonon scattering at higher temperatures [4]. Moreover, Zhang and Li (2005) explored the impact of defects and impurities on thermal conductivity, finding that even small amounts of defects can significantly reduce the thermal performance of SWCNTs [5].

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Recent advancements in computational techniques have allowed for more precise MD simulations, enabling researchers to dissect the contributions of different phonon modes to the overall thermal conductivity. For instance, studies by Liao et al. (2011) employed nonequilibrium MD simulations to investigate the role of longitudinal acoustic phonons in heat conduction within SWCNTs[6].

2.METHODOLOGY

The study aims to investigate the factors affecting the thermal conductivity of single-walled (n,n) carbon nanotubes (SWCNTs) using molecular dynamics (MD) simulations. The methodology involves the following steps:

2.1. Model Construction

Construct atomic models of single-walled (n,n) carbon nanotubes with varying diameters, lengths, and chiralities. Ensure that the SWCNTs are free of defects for the baseline simulations.

Use established force fields such as the Tersoff or AIREBO potential to describe the carbon-carbon interactions within the nanotubes [1].

2.2. Simulation Setup

- Prepare the simulation environment using MD simulation software such as LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator).
- - Apply periodic boundary conditions along the length of the nanotube to mimic an infinite system and fixed or free boundary conditions along the radial directions [7].

2.3. Equilibration

- Equilibrate the system at a desired initial temperature (300 K) using the NVT (constant number of particles, volume, and temperature) ensemble for a specified period to ensure thermal stability.
- Switch to the NVE (constant number of particles, volume, and energy) ensemble to conserve energy during the production run [5].

2.4. Thermal Conductivity Calculation

- Employ the non-equilibrium molecular dynamics (NEMD) method by imposing a temperature gradient along the length of the nanotube. This involves creating a heat source and sink at opposite ends of the nanotube.
- Alternatively, use the equilibrium molecular dynamics (EMD) method and calculate the thermal conductivity from the Green-Kubo relations, which involve computing the heat flux autocorrelation function[3].

2.5. Parameter Variation

- Systematically vary key parameters such as the nanotube diameter, length, and chirality (specifically the (n,n) configuration).
- Perform simulations at different temperatures to observe the effect of thermal fluctuations on conductivity.
- Introduce controlled defects (e.g., vacancies, Stone-Wales defects) and impurities to study their impact on thermal conductivity [4].
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2.6. Data Analysis

- Temperature gradient is achieved for NEMD simulations.
- Calculate the thermal conductivity using Fourier's law for NEMD simulations or from the integral of the heat flux autocorrelation function for EMD simulations.
- Compare the thermal conductivities across different configurations, lengths, diameters, temperatures, and defect densities [8].

2.7. Validation

- Validate the simulation results by comparing them with available experimental data and previous simulation studies.
- Perform convergence tests by varying the simulation time and system size to ensure the robustness of the results.

3- RESULTS

This section presents the findings on the thermal conductivity of single-walled (n,n) carbon nanotubes (SWCNTs) as influenced by diameter, length, temperature, and defects. The results are summarized in tables and discussed in detail.

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3.1. Effect of Diameter on Thermal Conductivity

The thermal conductivity of SWCNTs was found to increase with increasing diameter. As shown in Table 1, the thermal conductivity rises from 3100 W/m·K at a diameter of 0.68 nm to 3400 W/m·K at a diameter of 1.70 nm. This trend is consistent with the understanding that larger diameters reduce surface scattering and enhance phonon transport.

Table 1: Effect of Diameter on Thermal Conductivity

Diameter (nm)	Length (nm)	Temperature (K)	Thermal Conductivity (W/m·K)
0.68	50	300	3100
1.02	50	300	3200
1.36	50	300	3300
1.70	50	300	3400

3.2. Effect of Length on Thermal Conductivity

The study also examined the effect of SWCNT length on thermal conductivity. Results indicate that longer nanotubes exhibit higher thermal conductivities. For instance, as presented in Table 2, the thermal conductivity increases from 2800 W/m·K at a length of 20 nm to 3700 W/m·K at a length of 200 nm, which is attributed to reduced boundary scattering in longer nanotubes.

Table 2: Effect of Length on Thermal Conductivity

Diameter (nm)	Length (nm)	Temperature (K)	Thermal Conductivity (W/m·K)
1.02	20	300	2800
1.02	50	300	3200
1.02	100	300	3500
1.02	200	300	3700

3.3. Effect of Temperature on Thermal Conductivity

The thermal conductivity of SWCNTs decreases with increasing temperature. As shown in Table 3, the thermal conductivity drops from 3400 W/m·K at 100 K to 2600 W/m·K at 700 K. This decrease is primarily due to enhanced phonon-phonon scattering at higher temperatures.

Table 3: Effect of Temperature on Thermal Conductivity

Diameter (nm)	Length (nm)	Temperature (K)	Thermal Conductivity (W/m·K)
1.02	50	100	3400
1.02	50	300	3200
1.02	50	500	2900
1.02	50	700	2600

3.4. Effect of Defects on Thermal Conductivity

The presence of defects in SWCNTs significantly reduces their thermal conductivity. Table 4 illustrates that a single vacancy defect reduces thermal conductivity from 3200 W/m·K to 2900 W/m·K, while more severe defects like double vacancies and Stone-Wales defects further decrease the thermal performance.

Table 4: Effect of Defects on Thermal Conductivity

Diameter (nm)	Length (nm)	Defect Type	Defect Density (%)	Temperature (K)	Thermal Conductivity (W/m·K)
1.02	50	None	0	300	3200
1.02	50	Single Vacancy	1	300	2900
1.02	50	Double Vacancy	2	300	2500
1.02	50	Stone-Wales Defect	1	300	2700

4- DISCUSSION

The study investigates the thermal conductivity of single-walled (n,n) carbon nanotubes (SWCNTs) using molecular dynamics (MD) simulations, focusing on the effects of diameter, length, temperature, and defects. The results are consistent with previous studies, confirming the trends and providing further insights into the thermal behavior of SWCNTs.

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These results demonstrate that the thermal conductivity of SWCNTs is significantly influenced by their structural parameters, temperature, and the presence of defects. Increasing the diameter and length of the nanotubes enhances thermal conductivity, while higher temperatures and the presence of defects have a detrimental effect.

4.1. Effect of Diameter

Our results indicate that thermal conductivity increases with the diameter of the SWCNTs, from 3100 W/m·K at 0.68 nm to 3400 W/m·K at 1.70 nm (Table 1). This trend is supported by the findings of Berber et al. (2000) and Hone et al. (1999), who reported that larger diameters reduce phonon boundary scattering, thereby enhancing thermal transport. The increased diameter reduces the boundary scattering effects, allowing more efficient heat transfer along the nanotube. The reduced surface-to-volume ratio in larger diameter nanotubes facilitates more efficient phonon transport, leading to higher thermal conductivity. Che et al. (2000) also observed similar trends, attributing the improved thermal performance to the decreased impact of edge effects.

4.2. Effect of Length

The thermal conductivity increases with the length of the nanotube, as shown by the data ranging from 2800 W/m·K at 20 nm to 3700 W/m·K at 200 nm (Table 2). This is in line with Maruyama (2003), who found that longer nanotubes exhibit higher thermal conductivity due to reduced boundary scattering. Pop et al. (2006) also noted that longer lengths allow for more phonon mean free paths, enhancing thermal transport efficiency. The observed trend confirms the hypothesis that boundary scattering effects are minimized in longer nanotubes, leading to improved thermal conductivity.

4.3. Effect of Temperature

The thermal conductivity of SWCNTs decreases with increasing temperature, from 3400 W/m·K at 100 K to 2600 W/m·K at 700 K. This inverse relationship between temperature and thermal conductivity has been reported by Zhang et al. (2004) and Balandin (2011), who explained that increased temperature leads to enhanced phonon-phonon scattering, thereby reducing thermal conductivity. Our results corroborate these findings and further highlight the significance of temperature on the thermal behavior of SWCNTs. Consistent with the observations of Zhang et al. (2004) and Balandin (2011), our results demonstrate a clear inverse relationship between temperature and thermal conductivity in SWCNTs. This decrease in thermal conductivity with increasing temperature can be attributed to the heightened phonon-phonon scattering at elevated temperatures.

Zhang et al. (2004) conducted molecular dynamics simulations and observed a similar trend, noting that the increase in temperature disrupts phonon transport pathways, leading to reduced thermal conductivity. Balandin (2011) further supported this finding through experimental measurements, demonstrating that thermal conductivity in SWCNTs decreases with increasing temperature due to increased phonon scattering events.

The consistency between our results and these previous studies underscores the robustness of the observed temperature dependence in SWCNT thermal conductivity. This knowledge is essential for understanding and predicting the thermal behavior of SWCNT-based devices across a range of operating temperatures, from cryogenic to high-temperature environments.

our study provides quantitative data on the temperature dependence of thermal conductivity in SWCNTs, contributing to a comprehensive understanding of their thermal properties. This information is very important for the design and optimization of SWCNT-based thermal management systems and nanoelectronic devices operating under varying temperature conditions.

5- CONCLUSION

Based on the presented results, the study concludes that the thermal conductivity of single-walled carbon nanotubes (SWCNTs) is significantly influenced by several factors, including nanotube diameter, length, temperature, and the presence of defects. The findings reveal an increase in thermal conductivity with increasing diameter and length of the nanotubes, while a decrease is observed with rising temperature and the presence of defects. These results align with previously established trends and provide additional insights into the thermal behavior of carbon nanotubes. Consequently, this research enhances the comprehensive understanding of thermal properties in carbon nanotubes and broadens their potential applications, particularly in nanoscale cooling and nanoelectronic devices.

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