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Investigation of the Effects of Geometric and Structural Parameters of Carbon Nanotubes on Sound Absorption in an Argon Gas Environment Using a Molecular Dynamics Simulation Approach

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Abstract

Noise pollution is one of the major environmental challenges affecting human health and ecosystem stability. Carbon nanotubes (CNTs), due to their exceptional mechanical strength, high surface area, and unique nanoscale geometry, offer promising potential for sound absorption at the nanometer scale. In this study, molecular dynamics simulations were performed to investigate acoustic wave propagation and absorption in argon gas in the presence of single-walled carbon nanotubes. The simulation model was first validated against reference data in the absence of nano-absorbers. Subsequently, the effects of geometric and structural parameters including CNT diameter, tube count, spatial arrangement, and excitation frequency were examined. Results showed that increasing CNT diameter enhances effective gas–solid interactions and improves attenuation, whereas increasing the number of nanotubes reduces molecular free paths and increases the absorption coefficient. Among the examined configurations, the triangular arrangement exhibited the highest absorption due to stronger confinement and intensified gas–wall interactions. Frequency-dependent analysis was in good agreement with previous studies, confirming the accuracy of the model. Overall, the findings underscore the crucial role of geometry and structural optimization in designing efficient high-frequency nano-acoustic absorbers.

Keywords: Sound Absorption, Carbon Nanotubes, Molecular Dynamics Simulation, Acoustic Attenuation, Argon Gas, Nano-Absorber, Frequency Effects.

1. Introduction

Noise pollution has been recognized as one of the major global environmental challenges due to its harmful physiological and psychological impacts on human health as well as its disruptive effects on ecological stability [1–3]. These concerns have motivated extensive research efforts toward developing efficient sound absorbing materials applicable in industrial, environmental, and advanced engineering systems. Traditional porous absorbers, despite their widespread utilization, often exhibit limited performance in high-frequency regimes. Consequently, recent studies have increasingly focused on nano-engineered structures with superior mechanical, morphological, and acoustic characteristics [4, 5].

Among these nano-engineered systems, carbon nanotubes (CNTs) have attracted significant attention due to their exceptional stiffness-to-weight ratio, hollow cylindrical geometry, and ability to interact with gas molecules at sub-continuum length scales. These features make CNTs promising candidates for next-generation acoustic absorbers, particularly in rarefied regimes where the Knudsen number becomes significant and classical continuum models fail to capture molecular-scale interactions. Molecular dynamics (MD) simulations offer a powerful framework for accurately resolving sound propagation, attenuation, and gas–wall interactions under such nanoscale conditions [6–8].

The objective of the present study is to examine the influence of geometric and structural parameters of single-walled carbon nanotubes including diameter, number of nanotubes, and spatial arrangement—on sound absorption behavior in an argon gas environment. The simulation framework is first validated using reference acoustic characteristics from the literature. Subsequently, the model is subjected to harmonic excitation to extract key acoustic parameters such as attenuation coefficient, wave number, and absorption coefficient. The findings provide insights into nanoscale acoustic dissipation mechanisms and offer design guidelines for optimizing CNT-based nano-absorbers for high-frequency noise-control applications.

2. Methodology

Molecular dynamics (MD) simulations were performed using the LAMMPS package to model acoustic wave propagation in an argon gas environment containing single-walled carbon nanotubes (SWCNTs). The simulation domain was a rectangular box with dimensions of 15 nm × 15 nm × 150 nm, selected based on convergence analyses to ensure negligible lateral boundary effects. Periodic boundary conditions were applied along the x and y directions, while fixed boundaries were imposed along the z direction to generate a standing acoustic wave. The overall configuration of the simulation environment is illustrated in Figure 1.

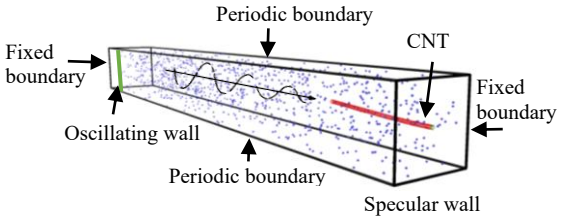

Figure 1. Schematic view of the simulation domain and CNT–argon configuration.

Acoustic excitation was introduced by applying sinusoidal oscillations to the left boundary using at a base frequency of 1.5 GHz. The right boundary acted as a fully reflective wall, generating a standing-wave pattern. Velocity components along the z-direction were sampled in 40 spatial bins to extract the harmonic functions $A(z)$ and $B(z)$. Nonlinear curve-fitting techniques were applied to determine the attenuation coefficient and wave number, enabling the calculation of the absorption coefficient.

A parametric study was carried out to analyze the influence of (i) CNT diameter, (ii) number of nanotubes, (iii) spatial arrangement (linear and triangular), and (iv) excitation frequency on acoustic damping behavior. All simulations were conducted for 100 acoustic cycles using a time step of 1 fs.

2.1. Acoustic Standing-Wave Model

The velocity field in the presence of a standing acoustic wave can be expressed using the harmonic decomposition:

$$v(z,t) = A(z)\sin wt + B(z)\cos wt \quad (1)$$

Where $A(z)$ and $B(z)$ are spatial envelope functions. Based on the analytical standing-wave solution, these envelopes are obtained from:

$$A(z) = v_0\,[e^{-mz}\cos(kz) - e^{-m(2l_z-z)}\cos(k(2l_z-z))] \quad (2)$$

$$B(z) = -v_0\,[e^{-mz}\sin(kz) - e^{-m(2l_z-z)}\sin(k(2l_z-z))] \quad (3)$$

These two relations were simultaneously fitted to MD-extracted velocity data to determine the attenuation coefficient m and the wave number k.

3. Results and Discussion

3.1. Model Validation

To ensure the reliability of the molecular dynamics framework, sound wave propagation was first simulated in pure argon gas in the absence of carbon nanotubes. Acoustic velocities were extracted for two excitation frequencies of 1.5 GHz and 3.0 GHz, and the corresponding wave numbers (k) and attenuation coefficients (m) were obtained through nonlinear fitting of the standing-wave envelopes $A(z)$ and $B(z)$.

The predicted sound speeds were c= 407.1 m/s at 1.5 GHz and c= 407.1 m/s at 3.0 GHz, which show excellent agreement with published reference data (307–435 m/s range), confirming the physical accuracy of the employed MD setup. A similar increasing trend in attenuation with frequency was also observed, consistent with previous studies on monatomic gases. Table 1 summarizes the extracted acoustic parameters.

Table 1. Validation of MD model: attenuation coefficient, wave number, and sound speed in argon gas.

f(GHz)	m(10^7m^{-1})	k(10^7m^{-1})	c(m/s)
1.5	0.820	2.31	407.1
3.0	0.902	4.41	426.8

These results verify that the MD model accurately reproduces the frequency-dependent acoustic behavior of rarefied argon gas and provides a reliable foundation for analyzing CNT-based nano-absorbers.

3.2. Effect of CNT Diameter

Three different diameters of single-walled CNTs (0.68, 1.22, and 2.2 nm) with a fixed length of 25 nm were examined to evaluate the influence of nanotube geometry on acoustic attenuation. To comply with the journal's limitation on the number of figures, only one representative spatial velocity profile—corresponding to the CNT with D=1.22 nm is presented in Figure 2, while the complete numerical results for all diameters are summarized in Table 2.

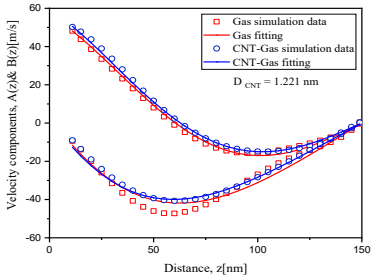

Figure 2. Representative spatial envelopes $A(z)$ and $B(z)$ for the CNT with diameter D= 1.22 nm at f= 1.5 GHz.

The spatial envelopes of the velocity components extracted from the MD simulations were fitted simultaneously to the analytical relations given by Equations (2) and (3), allowing accurate determination of the attenuation coefficient *m* and the wave number *k*. As reported in Table 2, both *m* and the resulting absorption coefficient α increase with CNT diameter (e.g., α increases from 0.097 for D= 0.68 nm to 0.156 for D= 2.2nm). This enhancement is attributed to the larger effective contact area and the intensified gas–wall interactions within wider nanotubes, which promote additional kinetic energy dissipation of the gas molecules.

Table 2. Effect of CNT diameter on acoustic parameters in argon gas (f = 1.5 GHz).

Diameter(nm)	$m(10^7 m^{-1})$	$k(10^7 m^{-1})$	α
0.68	0.922	2.34	0.097
1.22	0.926	2.29	0.100
2.2	0.989	2.40	0.156

3.3. Effect of CNT Number and Spatial Arrangement

To investigate the influence of structural configuration on acoustic dissipation, different quantities and spatial arrangements of CNTs were examined, including single, double, and triple nanotube systems. For the case of three CNTs, both linear and triangular configurations were considered. The MD results demonstrate that increasing the number of nanotubes enhances the dissipation of acoustic energy by reducing the effective molecular free path and increasing the frequency of gas–wall interactions. Among all tested configurations, the triangular three-CNT system exhibited the highest attenuation level due to the presence of confined regions between the tubes, which significantly increase residence time and collision probability of argon molecules. These findings highlight the importance of nanoscale geometric tailoring in optimizing absorber performance, even when the overall material volume remains constant.

3.4. Effect of Excitation Frequency

The influence of excitation frequency on acoustic attenuation was examined by applying harmonic waves at 1.5, 2.57 and 11 GHz. The MD results show that the general trend of attenuation enhancement with CNT presence is preserved across all frequencies. As the frequency increases, the wavelength becomes shorter, leading to a greater sensitivity of the acoustic field to nanoscale features. Consequently, both the attenuation coefficient *m* and the absorption coefficient α exhibit a modest increase at higher excitation frequencies. This behavior is consistent with previous MD-based studies, confirming that nanoscale scatterers such as CNTs remain effective even in the transitional flow regime where continuum assumptions break down. Overall, the frequency-dependent analysis validates the robustness of the model and demonstrates that CNT-based nano-absorbers can maintain high performance over a wide range of high-frequency acoustic excitations.

4. Conclusions

In this study, molecular dynamics simulations were conducted to investigate high-frequency sound absorption by single-walled carbon nanotubes in an argon gas environment. The results demonstrated that the MD framework reliably reproduces the acoustic behavior of rarefied gases, confirming its suitability for nanoscale acoustic analysis. Increasing the CNT diameter enhanced the attenuation and absorption coefficients due to the larger effective contact area and stronger gas–wall momentum exchange. Similarly, increasing the number of nanotubes substantially intensified acoustic dissipation, with the triangular three-CNT configuration exhibiting the highest absorption level as a result of increased molecular confinement in the interstitial region. Frequency analysis further showed that higher excitation frequencies produce greater attenuation and absorption, consistent with the reduced acoustic wavelength and increased collision rates near the nanotube surface.

Overall, the findings highlight the critical role of nanoscale geometry and spatial arrangement in optimizing CNT-based acoustic absorbers for high-frequency noise-control applications.

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