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Experimental and Numerical Investigation of a Carbon Nanotube Acoustic Absorber

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Summary

The interest in applications of nanomaterials for acoustic absorption purposes is growing rapidly with advances in nanotechnology. A need also exists for a simulation framework that is applicable for modelling acoustic absorption in nanomaterials in order to develop an understanding of nanoscopic acoustic absorption mechanisms. The current study investigates the acoustic absorption characteristics of a carbon nanotube (CNT) acoustic absorber to develop an understanding of the absorption behaviour and mechanisms of the CNTs. This task involves undertaking an exploratory study of the absorption characteristics of a CNT forest and modelling the absorption effects of the CNT at the nanoscale. The absorption characteristics of the CNTs were explored by studying the normal incidence absorption coefficient of 3 mm- and 6 mm-long vertically aligned CNT arrays measured experimentally using the two-microphone impedance tube method, while the modelling of the absorption effects was performed using a non-continuum particle-based method. The experimental investigation showed promising results for the acoustic absorption capability of CNT acoustic absorbers and suggests that the absorption performance could be enhanced with longer CNTs and a lower spatial density of the nanotube arrays. The study of absorption using a theoretical model based on classical absorption mechanisms indicated that the absorption behaviour of nanomaterials is likely to deviate from continuum behaviour emphasising the necessity of acoustic modelling at the nanoscale using non-continuum methods. An examination of the physical phenomena that are likely to be relevant for simulating acoustic wave propagation in the presence of CNTs revealed that the modelling of such a system would be a multi-physics problem involving heat transfer and dynamic interaction of particle vibrations. A study of various particle approaches of non-continuum methods indicated that molecular dynamics (MD) is the method best suited to simulate and study the acoustic absorption of CNTs at the nanoscale. A survey of previous molecular simulations demonstrated that the MD simulations carried out thus far have not simultaneously accounted for all relevant

aspects of the multi-physics problem required for modelling the acoustic absorption effects of CNTs. Hence, three independent validation studies were performed using MD simulations for modelling a subset of the relevant phenomena, namely fluid/structure interactions, bi-directional heat transfer, and acoustic wave propagation. Each of these MD simulations were performed for a model incorporating Lennard-Jones (LJ) potentials for the non-bonded interactions of gas and CNT atoms and the REBO potential for the CNT, and the results validated against the reference case studies.

A molecular system was then designed to study acoustic wave propagation in a simple monatomic gas in a domain containing a 50 nm-long CNT opposite to the sound source and parallel to the direction of the acoustic wave propagation. The simulation domain was modelled using argon gas as the wave propagation medium, a piston made of solid argon layers as a sound source, and a specular wall as the termination wall. MD simulations were also performed without the CNT present for comparison. The characteristics of the acoustic field were studied by evaluating the behaviour of various acoustic parameters and comparing the change in behaviour with frequency. The attenuation of the acoustic wave was estimated using thermodynamic exergy concepts and compared against standing wave theory and predictions from continuum mechanics. Similarly, the acoustic field characteristics and attenuation due to the CNT were studied using MD simulations incorporating the CNT. A standing wave model, developed for the domain with the CNT present, was used to predict the attenuation by the CNT and verified against estimates from exergy concepts. Comparison of the simulation results for acoustic wave propagation with and without the CNT present demonstrated that acoustic absorption effects in the presence of CNTs can be simulated using the developed MD simulation setup although the degree of absorption was not sufficient for the CNTs simulated to investigate absorption mechanisms. The modelled MD system can also be used to study deviations from continuum theory in the characteristics of high frequency sound. The study suggests that the investigation of absorption mechanisms in nanomaterials can be conducted using the developed platform for MD simulations, however further investigations are required to capture the loss mechanisms involved in the molecular interactions between the acoustic wave and the CNT. Additionally, to permit simulations in the audible frequency range, it is necessary to speed up the computational process by modifying the system model such as by employing a hybrid model with molecular dynamics coupled to a continuum domain.

Declarations

Originality

This work contains no material which has been accepted for the award of any other degree of diploma in any university or other tertiary institution. To the best of my knowledge and belief, this work contains no material previously published or written by another person, except where due reference has been made in the text.

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- AG: Air Gap
- ASTM: American Society for Testing and Materials
- CNT: Carbon Nanotube
- CVD: Chemical Vapour Deposition
- BGK: Bhatnagar-Gross-Krook
- BNT: Boron Nitride Nanotube
- CFD: Computational Fluid Dynamics
- DCV-GCMD: Dual control volume-grand canonical MD
- DPD: Dissipative Particle Dynamics
- DSMC: Direct Simulation Monte Carlo
- DWCNT: Double walled carbon nanotube
- EMD: Equilibrium Molecular Dynamics
- GCMC: Grand Canonical Monte Carlo
- LAMMPS: Large-scale Atomic/Molecular Massively Parallel Simulator
- LBM: Lattice Boltzmann Method
- MD: Molecular Dynamics
- MWCNT: Multiple walled carbon nanotube.
- NEMD: Non-Equilibrium Molecular Dynamics
- PBC: Periodic Boundary Condition

- PCA: Principal Component Analysis
- PU: Polyurethane
- REBO: Reactive Empirical Bond Order
- RW: Rigid Wall
- SCCM: Standard Cubic Centimetres per Minute
- SEM: Scanning Electronic Microscopy
- SPC: Simple Point Charge
- SRD: Stochastic Rotational Dynamics
- ST: Substrate
- SWCNT: Single walled carbon nanotube
- TBC: Thermal Boundary Conductance
- TBR: Thermal Boundary Resistance
- TEM: Transmission Electron Microscopy
- TNA: Titania Nanotube
- VMD: Visual Molecular Dynamics
- WCA: Weeks-Chandler-Andersen