Journal of Sound and Vibration 421 (2018) 319–333

Contents lists available at ScienceDirect

Journal of Sound and Vibration

journal homepage: www.elsevier.com/locate/jsvi

Molecular dynamics simulations of classical sound absorption in a monatomic gas

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ARTICLE INFO

Article history:
Received 3 August 2017
Revised 29 January 2018
Accepted 3 February 2018
Available online XXX

Keywords:
Molecular dynamics
Classical sound absorption
Viscous and thermal losses
Sound attenuation
And themoacoustic exergy concepts

ABSTRACT

Sound wave propagation in argon gas is simulated using molecular dynamics (MD) in order to determine the attenuation of acoustic energy due to classical (viscous and thermal) losses at high frequencies. In addition, a method is described to estimate attenuation of acoustic energy using the thermodynamic concept of exergy. The results are compared against standing wave theory and the predictions of the theory of continuum mechanics. Acoustic energy losses are studied by evaluating various attenuation parameters and by comparing the changes in behavior at three different frequencies. This study demonstrates acoustic absorption effects in a gas simulated in a thermostatted molecular simulation and quantifies the classical losses in terms of the sound attenuation constant. The approach can be extended to further understanding of acoustic loss mechanisms in the presence of nanoscale porous materials in the simulation domain.

1. Introduction

Nanomaterials show promise as sound-absorbing materials for noise control in applications such as engines, buildings, vehicles, aircraft, spacecraft and watercraft [1–7]. However, the absorption mechanisms of nanoscopic fibers are not fully understood and the application of numerical and analytical modeling methods to this problem is still at an early stage. Although the mechanisms of sound absorption are currently well understood for conventional porous acoustic materials having particle diameters or pores at the microscale (down to 1μm), the relative influence of the various mechanisms is expected to change for materials with pores or fibers at the smaller nanoscale (down to 1 nm) where other mechanisms and non-linear effects may also have a significant influence. Therefore, modeling acoustic mechanisms at the nanoscale requires molecular simulations that can model the flow behavior in the transition regime [8,9], because the characteristic length scale of the nanoscale structures is comparable to the molecular mean free path, and hence the commonly used acoustic assumptions, such as continuity, are invalid [10]. Molecular simulations such as molecular dynamics (MD) can play an important role in shedding light on the detailed mechanisms by which nanomaterials absorb sound [10–12]. However, conventional molecular dynamics simulation techniques assume some conserved quantity and thus it is not straightforward to measure dissipation of acoustic energy. Thus, a need exists for a method to quantify attenuation of acoustic energy during sound wave propagation in a medium (gas) that allows absorption to be modeled in a thermostatted molecular dynamics simulation. Attenuation of sound occurs in a monatomic gas due to viscous and thermal losses (also known as classical losses) of acoustic energy. Viscous losses occur due to the differences in relative motions between adjacent portions of the medium such as during the compression and expansion of the medium that

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https://doi.org/10.1016/j.jsv.2018.02.003
0022-460X/

accompany the transmission of an acoustic wave [13]. Thermal losses result from heat conduction between adjacent portions of the medium generated by higher temperature condensations and lower temperature rarefactions. A detailed description of such loss mechanisms can be found in the literature [13,14]. In many situations, especially at low frequency, acoustic dissipation is insignificant and can be ignored for the length and time scales of interest [13]. However, with high-frequency sound wave propagation, the losses are significant for distances on the order of a wavelength. Hence, estimation of losses in a medium for high-frequency sound waves is very important to distinguish between the losses that occur in the fluid and the losses that occur due to the interaction between the fluid and any other components (for example, absorptive media). Here, a simulation framework for molecular dynamics was developed to study the sound field characteristics of high-frequency wave propagation in a simple gas with the long term aim of extending the study to investigate the absorption behavior of nanomaterials. As such, in this study, MD simulations were performed for an acoustic system consisting of a monatomic gas that accounts for the effects of classical absorption in high-frequency sound propagation, in which losses occur due to the conversion of the coherent acoustic energy into random thermal energy as the wave propagates. A noble contribution of this paper is the use of the thermoacoustic concept of exergy to identify acoustic damping in MD simulations. Exergy is a form of energy that accounts for the ability to do useful work in a system in the presence of a freely accessible thermal reservoir at a particular temperature [15]. A method using the thermoacoustic concept of exergy is demonstrated to distinguish between the coherent acoustic energy and random thermal energy, in which the losses/dissipation of acoustic energy are defined in terms of entropy generation. Estimates of the losses were compared with those of the classical mechanics and standing wave theory for three different frequencies.

In conventional computer simulations of acoustic wave propagation (such as Computational Fluid Dynamics), classical losses are defined using continuum theory and the losses are quantified as a function of sound attenuation based on continuum fluid assumptions [16,17]. As mentioned earlier, the classical sources of attenuation in a sound wave are internal viscous friction and heat conduction. The losses of energy caused by internal friction are determined by the transmitted energy (which is proportional to ρv^2, where v is the particle velocity) and the kinematic viscosity μ/ρ (where μ and ρ are the dynamic viscosity and density of the gas, respectively) [18]. The thermal losses caused by heat conduction are determined by the thermal conductivity κ of the propagation medium and the generated temperature gradient ∇T (where T is the gas temperature) between the hotter (condensed) and cooler (rarefied) regions of the waves [13,14]. The equation for the rate of energy loss in a volume element can be derived from the classical theory of Navier-Stokes and its extension to the Burnett and super-Burnett limits for an acoustic field in terms of an attenuation constant, which is proportional to the square of the frequency [8,13,14,18,19]. However, the theoretical approximations of attenuation for an acoustic system based on a fluid continuum are only applicable at low frequencies, where the relaxation time for absorption (viscous and thermal) is similar to the mean time between collisions [10,13]. Thus, for frequencies approaching the relaxation frequency, where the wavelength is about the same size as the mean free path, the assumption of fluid continuum is inaccurate [10,13]. Hence, the classical theory is not applicable for high-frequency wave propagation or nanoscale systems for which the characteristic length scale is comparable to the molecular mean free path. As such, classical losses estimated based on the theory of continuum mechanics may not be applicable for evaluating attenuation in molecular dynamics simulations of acoustic wave propagation in a gas at the nanoscale. Hadjiconstantinou and Garcia [8] conducted DSMC (Direct Simulation Monte Carlo) simulations of sound wave propagation in the gigahertz (GHz) range. They derived the sound speed and attenuation coefficient by non-linear fitting the simulation results of velocity amplitude, assuming plane-wave theory. It was observed that the predictions were significantly affected by the free molecular flow near the sound source in a high-frequency sound wave propagation, where the wavelength was comparable to the mean free path. Thus, the curve fits of the waveforms indicated the sensitivity of the results to the choice of the distance for data fits from the sound source [8]. Therefore, it is important to have a method that can accurately measure losses due to classical acoustic-absorption mechanisms in a nanoscale domain for high-frequencies, without relying on factors such as free molecular flow or continuum approximations [10,12]. Hence a comprehensive method is developed here based on entropy generation.

This paper is organized as follows. First, Section 2 describes the simulation domain and simulation parameters required to model the sound wave propagation. Second, Section 3 presents the development of the relevant theories and modified calculation methods that were used to obtain sound attenuation parameters of the simulated wave. Finally, the simulation results are discussed in Section 4. The deviations from classical mechanics are also discussed in this section. Overall, this paper demonstrates the utility of the MD simulation method to study classical acoustic absorption in a simple gas at the nanoscale.

2. Simulation details

A rectangular domain of length $L_z = 150$ nm in the wave propagation direction shown in Fig. 1 was used to simulate plane sound wave propagating in a monatomic gas (argon). The simulation domain had dimensions of $L_x = L_y = 70$ nm transverse to the wave propagation direction. The simulation domain was chosen for high-frequency sound-wave propagation at a frequency of $f \approx 1.5$ GHz, with a domain length equivalent to approximately half the wavelength of the acoustic wave to reduce computational cost without sacrificing the accuracy of the simulation results. Molecular dynamics simulations were performed at frequencies of $f \approx 1.5$, 2 and 2.5 GHz to enable observations of the changes in the sound field as the excitation frequency changed. It should be clarified that the flow regimes of the simulated waves were in the transition regime ($0.1 < Kn < 10$) [8,9], as the Knudsen number measuring the ratio of the molecular mean free path ($\lambda_{\mathrm{mfp}} = 7.28 \times 10^{-8}$ m) to the characteristic length scale (H, in this case the acoustic wave length, λ) was $Kn = \frac{\lambda_{\mathrm{mfp}}}{H} \approx 0.25$, 0.34, and 0.42 for the simulated frequencies of $f \approx 1.5$, 2 and 2.5 GHz, respectively.