Molecular simulation of sound for development of nanoacoustics

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Large scale molecular dynamics simulations have been performed to clarify the nonlinear and non-equilibrium processes of high-frequency sound waves in a gas. Since the number density of molecules in a gas is considerably small compared with those in liquids, the evaluation of macroscopic quantities requires a number of samples. Furthermore, since the wavelengths of sound is very large compared with molecular scales even for high-frequency (gigahertz) sound, we put more than 0.3 million molecules in a simulation box with the length of several micrometers in the direction of wave propagation. The one-dimensional sound wave is generated by a harmonic oscillation of sound source with the Lennard-Jones intermolecular potential, which is the same as that of gas molecules. As a result, we find that the large amplitude and high-frequency sound propagates with strong attenuation, in some cases, exhibiting a stream-like profile accompanied with mass, momentum, and energy transports. This leads to a completely different picture and a different dispersion relation from a classical theory of high-frequency sound based on the linear standing wave analysis.

1 Introduction

Large-amplitude and very-high-frequency sound is a promising candidate for the mass, momentum, and energy transfer in nano- and micro-scale devices. However, nonlinear and non-equilibrium processes of high-frequency sound in fluids (liquid and gas) have been unknown, and they form a serious obstacle in engineering applications of nano- and micro-scale acoustics. The development of a new research field of nanoacoustics may be long-awaited.

If the characteristic length scale of the system concerned (e.g., wavelength) is sufficiently large compared with the mean free path of molecules, the nonlinear process can be studied in the theory of nonlinear acoustics based on continuum mechanics for not only fluids but also solids. This is because a sufficient large number of molecular interactions occurs in the characteristic length scale larger than the mean free path, and this establishes the local equilibrium state required in continuum mechanics. On the other hand, the wavelengths of very-high-frequency sound ($\sim$ 1 GHz) in gases are comparable with the mean free path of gas molecules, and hence continuum mechanics cannot be applied to resolve the nonlinear phenomena. In the present paper, we take up the fundamental problem of propagation of plane waves to tackle the abovementioned difficulty with molecular dynamics simulations.

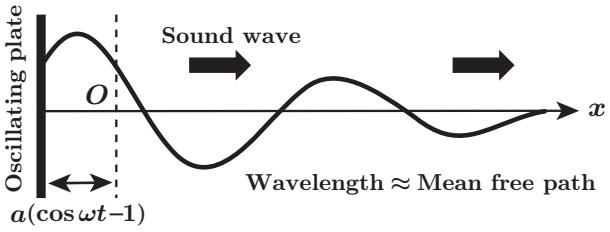

Figure 1: Schematic of model.

2 Problem and model

We consider the sound waves radiated into a gas by a sound source (plate), as shown in Figure 1. The gas is composed of monatomic molecules and its intermolecular potential U is assumed as Lennard-Jones 12-6 type potential

$$U = 4\epsilon\left[\left(\frac{r}{\sigma}\right)^{12} - \left(\frac{r}{\sigma}\right)^{6}\right], \tag{1}$$

where r is the intermolecular distance and (ϵ, σ) are the Lennard-Jones parameters. The dynamics of each molecule is determined by solving Newton's equation of motion with the intermolecular force by the Lennard-Jones potential.

On the sound source, we assume that the Lennard-Jones potential with the same (ϵ, σ) as those of gas molecules exists, and the location of the potential $X(t)$ oscillates in the x-direction as

$$X(t) = a(\cos\omega t - 1), \tag{2}$$

where t is the time, a is the amplitude and ω is the angular frequency of oscillation of the sound source. The amplitude of oscillation speed is then given by $a\omega$, which corresponds to the maximum gas velocity. In classical linear acoustics, this boundary condition yields a progressive plane sound wave,

$$v = -a\omega\sin(\omega t - kx), \quad p = p_0(1 + \gamma v/c_0), \tag{3}$$

where v is the x-component of gas velocity, p is the gas pressure, c_0 is the speed of sound, k $(= \omega/c_0)$ is the wavenumber, and γ is the ratio of specific heats ($\gamma = 5/3$ for monatomic molecules).

3 Molecular dynamics simulation

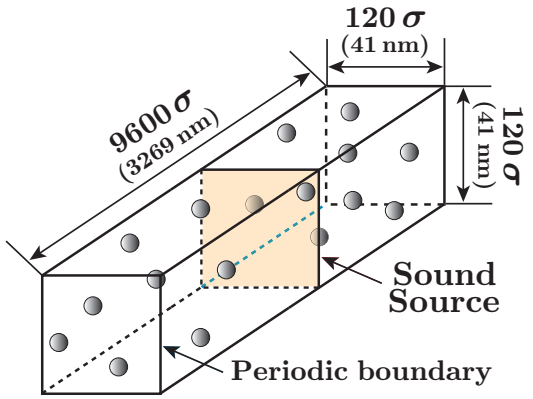

Figure 2: Simulation box and sound source.

Newton's equations of motion are numerically solved with the leap-frog scheme for the molecules in the rectangular simulation box (see Figure 2). The periodic boundary condition is assumed and the length of the box is sufficiently large so that the wave front may not affect the other side of the gas. The time step of numerical integration of Newton's equation of motion is 0.0005 $\sigma\sqrt{m/\epsilon}$ (m is the mass of a molecule), which corresponds to 1 fs for the case of argon. Thanks to the periodic boundary condition, the total number of molecules (N=327680) are conserved,

although total Hamiltonian and total momentum are not conserved because the sound source does the work.

4 Numerical results

In Figures 3 and 4, we present typical profiles of gas pressure and gas velocity, which corresponds to the progressive sound wave with frequency 1 GHz for the case of argon. The simulations are repeated 5 times and their sample averages are shown in Figures 3 and 4. The very important feature is that the wave front behaves not a wave-like but a stream-like, which means the direct transports of mass, momentum, and energy. The wave font moves with a speed larger than the sound speed of ideal gas $\sqrt{\gamma RT}$, where $R = k_B/m$ is the gas constant (k_B is the Boltzmann constant) and T is the gas temperature. The results shown in Figures 3 and 4 are the case of large amplitude oscillation of sound source, $a\omega \approx 0.8\sqrt{\gamma RT}$. We therefore conclude that the nonlinear and non-equilibrium effects cause a completely different picture and a different dispersion relation from a classical theory of high-frequency sound based on the linear standing wave analysis [1,2].

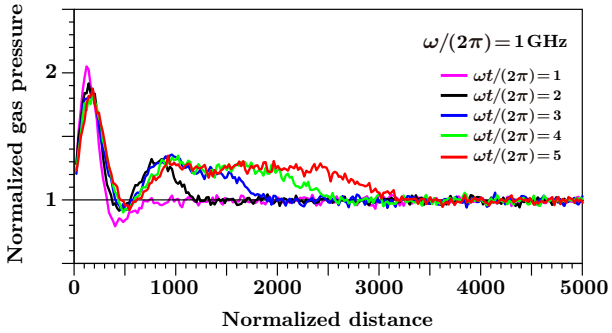

Figure 3: Profile of gas pressure in a large-amplitude progressive sound wave with frequency 1 GHz.

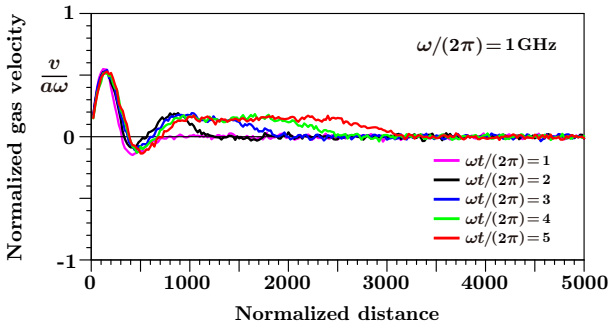

Figure 4: Profile of gas velocity in a large-amplitude progressive sound wave with frequency 1 GHz.

A similar stream-like profile has been reported in the case of propagation of nonlinear plane waves [3,4], where the wave motions are analyzed on the basis of the system of Euler equations. In this case, as a result of streaming, we have found the density reduction and temperature elevation near the sound source. The result of the present molecular simulation also shows the temperature elevation in the gas (Figure 5).

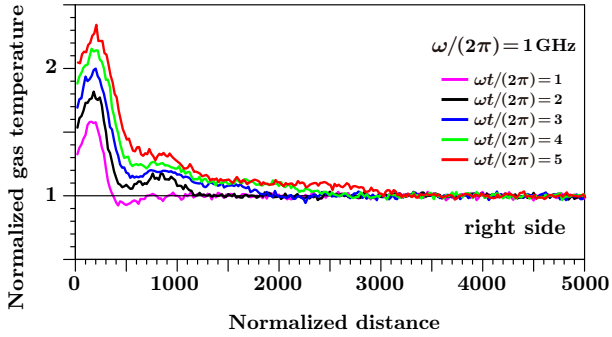

Figure 5: Temperature elevation in the gas.

5 Conclusions

By the molecular dynamics simulations, we have demonstrated that the nonlinear and non-equilibrium process of high-frequency sound exhibits quite different features from those known in the linear theory. Further quantitative study focusing on nonlinear and non-equilibrium effects is underway.

References

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