Normal Modes in Graphene for Different Geometries

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Normal Modes in Graphene for Different Geometries

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Abstract. Using classical molecular dynamics, we study the time evolution of out-of-plane standing waves on a square and circular single-layer graphene membrane. We explore the first six normal modes, obtaining the oscillation frequencies from the atomic motion. The modes show long-time stability in the harmonic regime, with no decoupling on multiple frequencies. Using the frequencies of oscillation, we calculated the transverse speed of sound in graphene and the tension on the membrane.

1. Introduction

The high flexibility, remarkable electronic properties and exceptional mechanical strength of graphene make it a useful material in technological applications [1–3]. Another fascinating property of this material is its high Q-factor [4] which makes graphene an interesting material to study the oscillation of normal modes, as the rate of energy loss is very low relative to the stored energy. Recent advances in nanotechnology allow for the production of nanoscale mechanical resonators [3,5], a field where graphene is considered promising for many applications. Therefore, a further characterization of different vibration modes of graphene for different geometries is needed, both experimental and theoretical [6].

In this work, we use classical molecular dynamics simulations with interactions modelled by the an empirical potential to study the flexural normal modes, also called lowest frequency acoustic branch ZA in phonon analysis, of single-layer graphene membranes of square and circular shapes. The primary aim is to compare the simulation with the theoretical results, obtaining a criteria for harmonic oscillation in the membrane. In addition, we estimate the speed of transverse waves in graphene.

2. Theory

The wave equation with Dirichlet boundary conditions governs the dynamics of a membrane of any shape, whose borders are fixed. That is, if $z(x, y, t)$ is the out-of-plane deviation of the membrane at time t in the position (x, y), then its evolution is controlled by the equation

$$\nabla^2 z(x, y, t) = \frac{\rho}{T} \frac{\partial^2 z(x, y, t)}{\partial t^2} \tag{1}$$

with the boundary condition

$$z(x, y, t)|_{\partial\Omega} = 0 \ , \tag{2}$$

where $\partial\Omega$ is the surface boundary, ρ the mass per area unit, and T is the tension per length unit. The ratio of the last two quantities corresponds to the square of the speed of sound in the media, given by

$$c = \sqrt{\frac{T}{\rho}} \,. \tag{3}$$

For a rectangular membrane, the solution is given by

$$z_{n_x,n_y}(x,y;t) = z_0 \sin\left(n_x \frac{x\pi}{L_x}\right) \sin\left(n_y \frac{y\pi}{L_y}\right) \sin\left(\phi + \omega_{n_x,n_y} t\right) \,, \tag{4}$$

where L_x and L_y are the dimensions of the rectangle, n_x and n_y integers numbers, and

$$\omega_{n_x,n_y} = \pi c \sqrt{\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}} \tag{5}$$

is the oscillation frequency. The phase ϕ and the height z_0 in Eq. 4 are determined by the initial conditions. If the membrane is square-shaped, then $L_x = L_y = L$, and

$$\omega_{n_x,n_y} = \pi \frac{c}{L} \sqrt{n_x^2 + n_y^2} \,. \tag{6}$$

For a circular membrane of radius a, the solution takes the form

$$z_{m,n}(r,\theta;t) = z_0 \, J_m\left(\frac{r}{a}\alpha_{m,n}\right) \sin(m\theta + \psi) \sin(\omega_{m,n} t + \phi) \,, \tag{7}$$

with $m = 0, 1, 2, \ldots$, $n = 1, 2, 3, \ldots$, where J_m is m-th Bessel function of the first kind, $\alpha_{m,n}$ the n-th positive root of J_m, and ϕ, ψ and z_0 are constants to be determined by the initial conditions. In this case the oscillation frequencies are given by

$$\omega_{m,n} = \frac{\alpha_{m,n} c}{a} \,, \tag{8}$$

where c is the speed of transverse wave in the media.

3. Methodology

The classical molecular dynamics simulations were performed using the Tersoff potential [7,8] for the interatomic interactions. The lattice constant a for this potential was found by minimizing the energy respect to the area. We found the energy is minimized for $a = 2.46$ Å, in agreement with the value accepted in the literature [6, 9]. Then, the graphene monolayer is strained uniformly in every direction and fixed at its edges to generate tension in the membrane, such that carbon atoms are separated 1.56 Å from each other. We considered a nearly square membrane of side 224 Å, fixing the position of all the atoms that were 10 Å from the border of the membrane, so that nearly 14500 atoms are allowed to move. For the circular membrane, we use the same strained atom lattice, but we only allow the movement of atoms that are at a distance $d = 107.47$ Å from the center. The atoms outside this region are interacting with the moving atoms, but they are not allowed to move. In this case, the dynamic region is composed by nearly 11500 atoms. For the initial conditions, we chose an initial height $z_0 = 0$ at time $t = 0$ for all atoms, and a velocity profile corresponding to the shape of a given eigenfunction, that is,

$$v_{n_x,n_y}(x,y;t=0) = v_0 \sin\left(n_x \frac{x\pi}{L}\right) \sin\left(n_y \frac{y\pi}{L}\right) \tag{9}$$

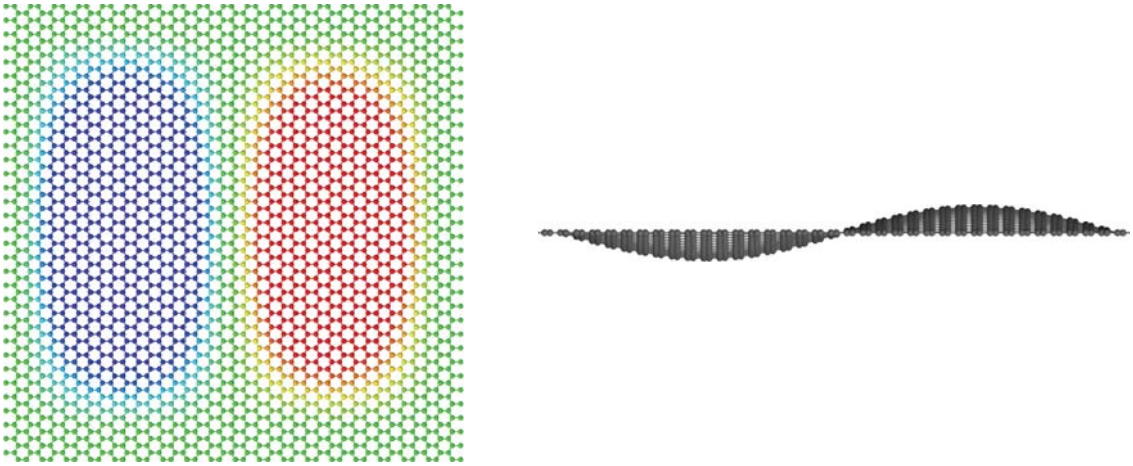

Figure 1. Oscillation of the second normal mode in the square-shaped graphene membrane. Left panel: top view; right panel: lateral view.

for the square-shaped membrane, and

$$v_{m,n}(r,\theta;t=0) = v_0\, J_m\left(\frac{r}{a}\alpha_{m,n}\right)\sin(m\theta) \tag{10}$$

for the circular membrane. The amplitude of these velocity profiles determines the amplitude of the oscillation in the out-of-plane direction, and also controls harmonicity of the motion. An initial velocity that is too high induces large vibration amplitudes that can introduce anharmonic contributions that decouple the normal mode in a combination of normal modes. To ensure harmonicity, we tried different values for the amplitude of the velocity profile in Eqs. (9) and (10). For each value, we took the Fourier transform of the kinetic energy of the membrane, which is periodic in the harmonic regime, to guarantee that no other modes appear in the simulation. The simulations were performed in the microcanonical ensemble (NVE), using the LAMMPS [10] software package, with a timestep of 1 fs, and at least 100 ps were used to monitor stability of the modes.

4. Results

Following the described protocol, we performed molecular dynamics simulation for several normal modes. For instance, in Figure 1 it can be seen the form of the actual oscillation corresponding to the second normal mode for the square-shaped graphene sheet. The frecuency of each mode is obtained from the atomic motion. The Fourier analysis performed over each simulation showed that there was only a single frequency in each mode generated. The modes show long-term stability, and the dependence of the frequency on the oscillation amplitude, which is controlled by the initial velocity v_0, has not been observed on our simulations.

In Figures 2 and 3 we show the measured frequencies in both membranes. From a linear fit to the data in Figure 2, we can obtain a slope of 0.156 ± 0.002 ps^{-1} that, according to Eq. (6), corresponds to the speed of sound of $c = 1.060 \pm 0.010$ km/s. The linear fit to the frequencies of the circular membrane in Figure 3 gives a slope 0.102 ± 0.001 ps^{-1}. Using Eq (8), we deduce a speed of transverse waves of $c = 1.096 \pm 0.007$ km/s. These two independent measures give an average value of $c = 1.078 \pm 0.006$ km/s which, according to Eq. 3, corresponds to a tension of $T = c^2\rho = 0.756$ N/m.

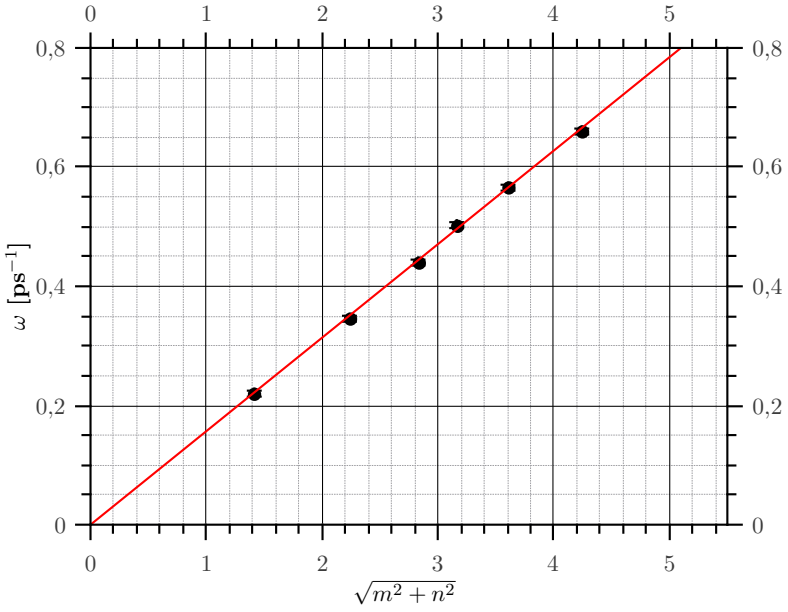

Figure 2. Frequencies of the square-shaped graphene membrane as a function of m and n, the integers that characterize the mode in Eq. (4). A linear fit (solid, red line) gives a slope of 0.156 ± 0.002 ps^{-1}.

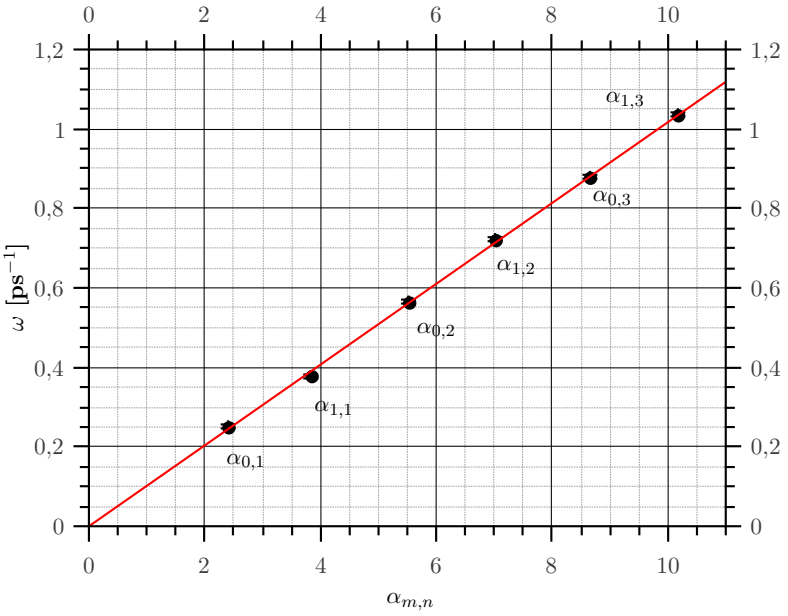

Figure 3. Frequencies of the circular-shaped graphene membrane as a function of α_{mn}, the n-th zero of the Bessel function J_m. A linear fit, in red, gives a slope of 0.102 ± 0.001 ps^{-1}.

5. Conclusion

We have measured the transverse speed of sound of strained graphene, associated with the lowest frequency acoustic branch ZA, using the classical molecular dynamics simulations. The normal modes generated in both shapes, square and circular, show a long-time stability that gives a speed of the transverse waves of $c = 1.078 \pm 0.006$ km/s for a graphene membrane that has been strained 10% from the original lattice constant. This velocity is lower than in-plane sound velocities associated with the TA and LA phonon branches of unstrained graphene [11]. We conclude that a ten percent of strain in graphene corresponds to a tension of $T = 0.756$ N/m. The velocities inferred from both geometries only differs by 3%, which means that this result is independent of the size or shape of the membrane.

The stability of the modes shows that it is indeed possible to generate single-layer graphene membranes that can be used as nanoresonators. Although other factors, such as temperature and impurities, have not been included in this work, they would be valuable in future works, as well as the study of isospectral membranes.

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