

Linear Oscillations of Suspended Graphene

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Abstract Due to their excellent mechanical properties and extra high electroconductivity, suspended graphene sheets recently were proposed as perspective working elements of nanosystems. This work is devoted to derivation of natural frequencies of such sheets. Two different approaches are proposed. The first one is based on representation of the graphene sheet as a thin rectangular membrane. In this case the transversal oscillations are described with the classical one-dimensional wave equation. Evaluation of the tension force in the membrane is performed basing on the misfit between the graphene and silicon substrate crystal lattices. As a result, the natural frequencies are found as the functions of the membrane length. Another approach is to represent a graphene sheet as a thin plate. In this case a bending rigidity of graphene has to be taken into account. As a result, it is shown that the bending rigidity is more significant for the short resonators and leads to the higher frequencies in comparison the long resonators.

1 Introduction

This work is devoted to the suspended graphene oscillations. Graphen is a monoatomic thin film with unique elastic, electrical, optical and thermal properties [7]. Thin films are used in novel nanoelectromechanical systems (NEMS), e.g. nanoresonators [6, 8]. Recently, graphene sheet were proposed for using in such systems. Up to now, the existing graphene-based experimental set-ups [4, 5, 13] have not achieved as high oscillation properties as silicon-based resonators. However, the technical problems

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will be hopefully solved soon, and the advantages of graphene systems will be used for practical applications. First of all, they can be much easier miniaturized to the nanoscale. As single-atomic graphene layer is a thinnest material at all, it is much more sensitive to external effects than other films. It allows to use them as mass sensors for nanoparticles.

This paper shows that graphene-based resonators can be used as the sources of the high-frequency (up to several THz) oscillations. The transversal linear oscillations of graphene sheet stretched over the trench in silicon oxide substrate are considered. Two models are used to calculate the natural frequencies. First model represents graphene sheet as a membrane with a constant tension. The second one represents graphene as a thin plate. This model takes a bending rigidity of graphene into account in addition to the tensile stiffness.

There are several works devoted to calculation of the natural frequencies of graphene (see e.g. [1, 9, 10]). Most of them do not take the bending rigidity of graphene into account. Recently, some authors paid their attention to this property of monoatomic graphene sheets. As it will be shown later in this work, the bending rigidity plays a significant role in case of the short resonators.

2 Membrane Model

2.1 Basic Equations

Let us consider the graphene sheet suspending over the trench in SiO₂ substrate. Suppose that it can be approximately represented as a flexible membrane fixed at two supports. Let us consider the uniform deformations along the preferential direction in a plane orthogonal to the direction of oscillations. In this case we can write the equations of small oscillation of the membrane as

$$\frac{Hm}{S_0} \ddot{w} = T\varphi', \quad \varphi = w', \quad (1)$$

here T is a tension force, φ is an angle of membrane element rotation, w is a membrane bending deflection, H is a sheet width, ρ_0 is a linear density of graphene sheet (mass of a unit of area). A point and an accent correspond to the time (t) and longitudinal (x) derivatives respectively. For Eq.(1) is was used that $\rho_0 H dx dx$. Relations (1) give the equations of transversal oscillations of the membrane

$$\ddot{w} - c^2 w'' = 0, \quad c^2 = \sigma/\rho_0, \quad (2)$$

where $\sigma = T/H$ is a longitudinal distributed force in graphene sheet.

Let us note that the thickness of the membrane was not included into Eqs. (1) and (2). This fact has a simple explanation. The thickness of an single-atomic layer can

not be determined uniquely hence it is non-objective and can not be included into the equations of dynamics [12]. Moreover, the width of the graphene sheet H also is not used in Eq. (2).

The boundary equations are following: $w = 0$ at $x = 0$ and $x = l$. Here l is a length of the membrane. Let us suppose that

$$w(x, t) = W(x)e^{i\omega t},$$

then

$$W'' + \kappa^2 W = 0, \quad \kappa = \omega/c. \quad (3)$$

Its common solution may be written as

$$W = A_1 \cos \kappa x + A_2 \sin \kappa x. \quad (4)$$

A satisfaction to the boundary conditions let us find $\kappa = \pi n/l$, where $n = 1, 2, 3, \dots$. After κ is found, the natural frequencies can be determined by formulae

$$\omega = \kappa c = \frac{\pi n}{l} \sqrt{\frac{\sigma}{\rho_0}}. \quad (5)$$

2.2 Tension of the Sheet

Let us evaluate a tension in the graphene sheet. Let us believe that a tension is connected with a misfit of graphene and substrate (SiO_2) crystal lattices. It may give a maximum elongation of the graphene sheet on the order of $a/2$. Then a corresponding tension stress may be approximately found as

$$\sigma = \frac{a}{2l} E, \quad (6)$$

where E is a two-dimensional Young modulus of graphene measured in N/m.

A surface density of graphene sheet can be found as

$$\rho_0 = m/S_0, \quad S_0 = \frac{3\sqrt{3}}{4} a^2, \quad (7)$$

where S_0 is a area per atom in graphene sheet (a half of the elementary cell); a is a distance between the nearest atoms. The substitution of Eqs. (6) and (7) to Eq. (5) gives

$$\omega = k_E \left(\frac{a}{l}\right)^{3/2} \omega_E, \quad k_E = \frac{\pi n}{2} \sqrt{\frac{3}{2}} \sqrt{3}, \quad \omega_E = \sqrt{\frac{E}{m}}. \quad (8)$$

Here k_E is a dimensionless ratio, ω_E has the same unit of measure as a frequency. For the first natural frequency $k_E \approx 2.53$, (8) gives a following evaluation for the frequency of oscillations

$$\omega = 2.53 \left(\frac{a}{l} \right)^{3/2} \omega_E. \quad (9)$$

2.3 Frequencies Calculation

Let us evaluate a first frequency of the transversal graphene sheet oscillations on a base of previous results. According to [11], a graphene 2D Young modulus is $E = 350 \text{ N/m}$. A carbon atom mass $m = 1.99 \cdot 10^{-26} \text{ kg}$. Then, using calculations with formula (8) one can obtain for the frequency ω_E

$$\omega_E = 1.33 \cdot 10^{14}, \quad \nu_E = \frac{1}{2\pi} \omega_E = 21.1 \text{ THz}. \quad (10)$$

Then let us find the frequencies of the graphene sheets with different lengths taking into account that a nearest distance between atoms in graphene is $a = 0.142 \text{ nm}$ [11]. The results if the calculations are given in Table 1. An average distance between the rows of atoms in graphene differs dependently on the direction. It changes from $0.75 a$ to $\frac{\sqrt{3}}{2} a \approx 0.87 a$. Due to this, an average distance $0.8 a = 0.114 \text{ nm}$ was used to calculate an approximate number of the atomic rows along the graphene layer as $N = l/(0.8a)$. It is shown in a second column of the table.

3 Plate Model

3.1 Basic Equations

Let us consider a graphene sheet laying over a trench in a silicon oxide substrate as a plate on the two supports. Similar to the previous part, let us consider the uniform deformations along the preferential direction in a plane orthogonal to the direction of oscillations. In this case a problem of the plate small oscillations can be reduced to the problem of Bernoulli-Euler beam oscillations:

Table 1 Natural frequencies of the graphene sheets (membrane model)

l (nm)	N	ν
1	8,803	90 MHz
100	880	2.9 GHz
10	88	90 GHz
1	9	2.9 THz

$$H\rho_0\ddot{w} = N', \quad N = -M', \quad M = DH\varphi', \quad \varphi = w'. \quad (11)$$

Here N is a transversal force, M is a bending moment, φ is an angle of the plate element rotation, w is a plate deflection, H is a graphene sheet width, ρ_0 is a linear density of graphene sheet (mass of the unit of the square), D is a bending rigidity; a dot and a stroke correspond to the time and x coordinate respectively. When obtaining the Eq. (11) it was used that $\rho_0 H dx$ is a mass of the element with a width H and a length dx , and a bending stiffness D is a ratio between a distributed bending moment M/H and the angular deformation φ' . Equation (11) give the equation of the bending oscillations of the plate

$$\ddot{w} + b^4 w'''' = 0, \quad b^4 = D/\rho_0. \quad (12)$$

A thickness of the plate was not included into the Eqs. (11) and (12) as well as the thickness of the membrane was not included in the oscillations equation in the previous part. The explanation is the same: atomic sheet thickness can not be determined uniquely hence it is non-objective and can not be included into the equations of dynamics (11) and (12). The width of the layer H also was not included in Eq. (12).

The boundary conditions at $x = 0$ and $x = l$ where l is a plate length are the following:

$$w = 0, \quad w' = 0 \text{ (solid support)}, \quad w'' = 0 \text{ (joint)}, \quad (13)$$

relatively for the solid support or for the joint.

Let us allow $w(x, t) = W(x) e^{i\omega t}$. Then one can obtain

$$W'''' - \kappa^4 W = 0, \quad \kappa^2 = \omega/b^2. \quad (14)$$

Its general solution may be found as

$$W = A_1 \cos \kappa x + A_2 \sin \kappa x + A_3 \cosh \kappa x + A_4 \sinh \kappa x. \quad (15)$$

After the satisfaction to the boundary conditions one can find κ as $\kappa = \gamma/l$. Here a dimensionless ratio γ is a solution of the following equations

$$\sin \gamma \sinh \gamma = 0 \text{ (joint)}, \quad \cos \gamma \cosh \gamma = 1 \text{ (solid support)}. \quad (16)$$

From the solutions of these equations (exact solution for the joint bearing and an approximate one for the solid support) it follows

$$\sin \gamma = 0 \Rightarrow \gamma = \pi n \text{ (joint)} \quad (17)$$

or

$$\cos \gamma = 0 \Rightarrow \gamma = \frac{\pi}{2} + \pi n \text{ (solid support)}, \quad (18)$$

where $n = 1, 2, 3 \dots$. The maximum error 1.8% follows from the approximate solution for the first natural frequency. For the other frequencies the approximate solution is very close to the exact one. The exact solution of equations (16) give the following values for the first natural frequency

$$\gamma = 3.145193 \text{ (joint)}, \quad \gamma = 4.730041 \text{ (solid support)}. \quad (19)$$

After γ is found the natural frequencies are determined from (12) to (14)

$$\omega = \kappa^2 b^2 = \frac{\gamma^2}{l^2} \sqrt{\frac{D}{\rho_0}}. \quad (20)$$

There is an important conclusion following from the last formula. It can be noticed that the natural frequencies are inversely as the square of the plate length. It gives an opportunity to change a frequency of the graphene oscillator in a very wide range. For instance, if the length of the plate increases 10 times then the frequency increases 100 times.

3.2 Evaluation of the Bending Oscillations Frequency

The bending rigidity of the graphene layer is given by formula [3]

$$D = \frac{\sqrt{3}}{6} \frac{3c_T + c_B}{c_T + c_B} c_B, \quad (21)$$

where c_T and c_B are the torsional and binding stiffnesses respectively. We use this parameters basing on the concept of mechanical representation of the carbonic bond [2]. Unfortunately, so far there are no experiments to determine c_T and c_B . Hence, we will use the relations between these parameters and c_D , where c_D is a transversal stiffness of carbonic bond in graphene.

$$c_T = \frac{1}{12} \frac{c_D a^2}{1 + \nu}, \quad c_B = \frac{1}{12} c_D a^2, \quad (22)$$

where a is a bond length, ν is a dimensionless parameter of interaction. Let us substitute the (22) to formula (21). Then

$$D = \frac{\sqrt{3}}{36} k(\nu) c_D a^2, \quad k(\nu) = \frac{1}{2} \frac{4 + \nu}{2 + \nu}. \quad (23)$$

There is a limit $-1 \leq \nu \leq \frac{1}{2}$ for parameter ν which gives for $k(\nu)$

$$\frac{9}{10} \leq k(\nu) \leq \frac{3}{2}. \quad (24)$$

Hence, this parameter does not change significantly and can be taken approximately equal to 1.

A linear density of graphene can be found as

$$\rho_0 = m/S_0, \quad S_0 = \frac{3\sqrt{3}}{4} a^2; \quad (25)$$

where S_0 is a square per one atom in graphene list (half of elementary cell square); a is an interatomic distance.

Substitution of the formulae (23) and (25) into (6.22) allows to find the following expression for the bending oscillations frequencies of graphene list

$$\omega = k_D \frac{a^2}{l^2} \omega_D, \quad k_D = \frac{\gamma^2}{4} \sqrt{k(\nu)}, \quad \omega_D = \sqrt{\frac{c_D}{m}}. \quad (26)$$

Here k_D is a dimensionless parameter, ω_D is a frequency of the transversal oscillations of the atom held by the bond with a stiffness c_D . Taking the Eqs. (19) and (24) into account for the solid support boundary conditions one will obtain

$$4.66 \leq k_D \leq 8.39. \quad (27)$$

Let us take for simplicity $k_D = 6$. Then the following approximate estimation for the graphene layer

$$\omega = 6 \frac{a^2}{l^2} \omega_D. \quad (28)$$

3.3 Frequencies Calculation

Let us evaluate the first natural frequency of the bending oscillations of graphene layer using the results obtained above. Following [11], the transversal stiffness of the bond between the carbon atoms in graphene is $c_D = 402 \text{ N/m}$. Mass of the carbon atom is $m = 1.99 \cdot 10^{-26} \text{ kg}$. Then using (26) one could calculate a frequency of the transversal oscillations of the carbon atom

$$\omega_D = 1.42 \cdot 10^{14} \text{ s}^{-1}, \quad \nu_D = \frac{1}{2\pi} \omega_D = 22.6 \text{ THz}. \quad (29)$$

Here and after symbol ω denotes the cyclic frequency, ν is an ordinary frequency (inversely to the oscillations period) which is 2π times lower than the cyclic one.

Table 2 Natural frequencies of the graphene sheets (plate model)

l (nm)	N	ν (MHz)
1	8,803	2.7
100	880	273
10	88	27
1	9	2.7

Now let us use (28) to calculate a frequency of the graphene layer oscillations $\nu = \omega/(2\pi)$. Let us take a distance between the nearest carbon atoms in graphene as $a = 0.142$ nm [11]. The results of the oscillations are given in Table 2. A second column shows an approximate number of the rows of atoms along the sheet length. It can be found as $N = l/(0.8a)$ as it was done for Table 1.

Following (28), the frequency is inversely as a square of the graphene layer length. Hence, change of the length lead to the much more significant change of the frequency. According to this fact, one can variate the graphene frequency in a very large limit. For instance, as it follows from Table 2 decrease of the resonator length from 1 mkm to 1 nm lead to the increase of the frequency from 2.7 MHz to 2.7 THz. Thus, the short resonators (1 nm or less) can give the frequencies of terahertz range.

4 Conclusions

Figure 1 shows a comparison of the calculation results obtained with the plate and membrane models. The graphs show that for the lengths more than 1 nm the membrane model gives higher frequencies. If the lengths are less than 1 nm then a plate

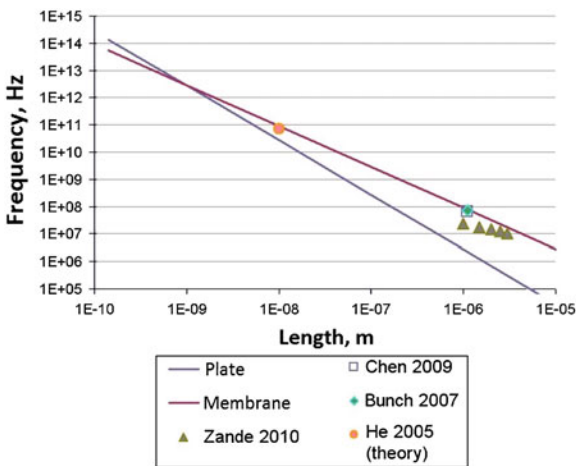


Fig. 1 Comparison of the frequencies of graphene oscillations obtained by different methods

model gives higher frequencies. This means that the plate type of the oscillations dominates for the shortest graphene sheets having up to 10 rows of atoms. Let us note that this result was obtained for the sufficiently high tension of graphene. If the tension is low, then plate type of the oscillations can be realized even for the graphene sheets longer than several nanometers.

A difference between results obtained with membrane and plate models is connected with a bending rigidity influence. The shorter is graphene layer, the more significant bending rigidity is. Thus, a plate model should work better for the shorter resonators but in the case of long resonators the bending rigidity of graphene can be neglected.

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