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Quantized long-wavelength optical phonon modes in graphene nanoribbon in the elastic continuum model

Jun Qian [a], Matthew J. Allen [b], Yang Yang [c], Mitra Dutta [a,d], Michael A. Stroscio [a,d,e,*]

[a] Department of Electrical and Computer Engineering, University of Illinois at Chicago, Chicago, IL 60607, USA
[b] Department of Chemistry, University of California, Los Angeles, CA 90095, USA
[c] Department of Materials Science and Engineering and California NanoSystems Institute, University of California, Los Angeles, CA 90095, USA
[d] Department of Physics, University of Illinois at Chicago, Chicago, IL 60607, USA
[e] Department of Bioengineering, University of Illinois at Chicago, Chicago, IL 60607, USA

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ABSTRACT

This paper presents an analytical displacements and dispersion relations for optical phonons of a graphene sheet. These results are used to derive the optical deformation potential interactions for graphene as well as to obtain descriptions of the confined optical phonons for graphene.

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1. Introduction

Graphene has attracted a great deal of attention since it was first successfully made by Geim [1,2] for its unique electronic, magnetic and thermal properties [3–8]. Carrier-phonon scattering will affect the electrical properties of graphene, such as resistivity and Fermi level shift [9–13]. It is important to study both the acoustic and optical phonons in graphene. Phonon dispersion has been studied by Raman and neutron scattering in graphite [14–16] and

* Corresponding author at: Department of Electrical and Computer Engineering, University of Illinois at Chicago, Chicago, IL 60607, USA.
E-mail address: stroscio@uic.edu (M.A. Stroscio).

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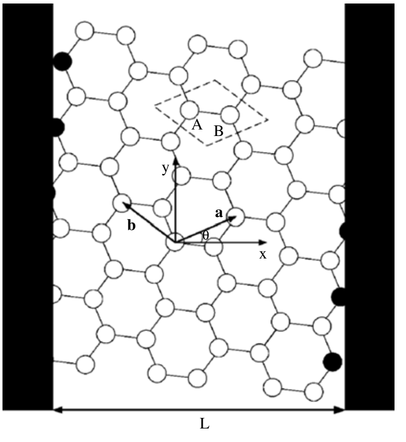

Fig. 1. The clamped graphene nanoribbon lattice structure. The dashed lines illustrate a construction of the unit cell containing two carbon atoms A and B, while two primitive vectors are denoted as **a** and **b**. The coordinate system (x, y) is chosen respecting to the deposited electrodes with the x axis perpendicular and y axis parallel to the clamping electrodes. An angle analogous to the chiral angle θ is defined identical to the carbon nanotube with a chiral angle between the vector **a** and the x axis.

graphene [17–20]. Theoretical works have been undertaken to simulate the dispersion curves [15,21]. Graphene nanoribbon (GNR) can be seen as unwrapped carbon nanotube and is suitable for future device applications [22–25]. Herein we concentrate on the optical phonon modes, since one-center acoustic modes can only cause intraband carrier transitions but not interband carrier transitions [13]. It is important to study confined phonon modes in clamped graphene nanoribbons (GNRs), since boundaries occur in many device applications; for example, metal electrodes may be deposited on electric devices [24,25]. The continuum model is widely used to study phonon modes in semiconductor nanostructure [26] and provide a high accuracy for long wavelength phonons in the carbon based materials, such as C_{60} [27], carbon nanotubes [28–32] and graphene [10].

In this paper, we used the elastic continuum model to study the optical phonon in GNRs subject to a long wavelength limit. First, we employed Goupalov's generalized equation [30] for LO phonons to derive detailed expressions for the relative displacement. Then, using a frequently assumed form of the boundary condition, it is assumed that the GNR is clamped at the boundaries, we apply quantized phonon modes and have dispersion curves for both armchair-end and zigzag-end GNRs. These results are limited to the few lowest order modes, i.e. lowest quantum numbers, since the elastic continuum model applies most accurately to these lower modes which have long wavelengths. The quantum normalized amplitude is calculated and used to obtain the optical deformation potential.

2. Model: Optical phonon in graphene sheet

As shown in Fig. 1 of the configuration of clamped GNR, x and y axes are in-plane perpendicular and parallel to the "clamping" boundaries or electrodes, respectively; the z axis is out-of-plane and perpendicular to the graphene surface. The width of the GNR is L, the length is infinite, and the thickness is neglected. We can treat the GNR as a 2D elastic sheet in a long wavelength limit and use the elastic continuum model to describe the optical vibration modes. The unit length along the x axis is $a\cos\theta$, where $a = \sqrt{3}a_{c-c} = 2.46$ Å is the length of the unit vector and θ is the 'chiral' angle from the unit vector $\boldsymbol{a}$ with respect to the x axis. In a purely formal analogy with carbon nanotubes, we define two kinds of specific GNRs depending on the carbon atoms arrangement on the free-standing sides, which is identical to the definition of the carbon nanotubes [33]. The armchair-end and zigzag-end GNRs correspond to $\theta = 30°$ and $0°$, respectively. Thus, the unit lengths along the x axis of armchair-end and zigzag-end graphene nanoribbons are $\sqrt{3}a/2$ and a.

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