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Ripples in Graphene Sheets and Nanoribbons

Sanjay Prabhakar[1] and Roderick Melnik[1,2]

[1]The MS2Discovery Interdisciplinary Research Institute, M [2]NeT Laboratory, Wilfrid Laurier University, Waterloo, ON, N2L 3C5 Canada

[2]BCAM-Basque Center for Applied Mathematics, E48009 Bilbao, Spain

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Abstract. We study the influence of ripple waves on graphene sheets and graphene nanoribbons. Such waves are originating from the electromechanical effects, among other possible mechanisms. By considering variations in the in-plane and out-of-plane displacement vector, we show that the spontaneous generation of ripple waves has no preferred orientation. Intrinsic properties of ripple waves induce a large pseudopotential that in its turn is to induce large pseudomagentic fields that can be implemented into the band engineering of graphene structures.

I. Introduction

Graphene has attracted potential interest for the design of optoelectronic devices because it possesses unique electronic and physical properties due to the presence of Dirac-like energy spectrum of the charge carriers. [1-5] In graphene, one finds an opportunity to control electronic properties of graphene-based structures using several different techniques such as gate controlled electric fields and magnetic fields. Further one can engineer the straintronic devices by controlling the electromechanical properties via the pseudomorphic gauge fields. [6-10] Two dimensional images of graphene sheets taken from high resolution transmission electron microscopes or scanning tunneling microscopes show that its surface normal varies by several degrees and the out-of-plane deformations reach to the nanometer scale that is considered to be due to the presence of ripple waves in such graphene sheet. [11-13] Ripples in graphene are induced by several different mechanisms that have been widely investigated. [6, 7, 9, 12, 14-23] Such ripples are part of the intrinsic properties of graphene that are expected to strongly affect the band structures due to their coupling through pseudomorphic vector potential. [8, 10, 24] In this paper we present a model that solves the Navier equations, accounting for electromechanical effects, and investigate the intrinsic properties of ripple waves in graphene.

II. Theoretical Model

The total elastic energy density associated with the strain for the two dimensional graphene sheet can be written as [26, 19, 21] $2U_s = C_{iklm}\varepsilon_{ik}\varepsilon_{lm}$. Here C_{iklm} is a tensor of rank four (the elastic modulus tensor) and ε_{ik} (or ε_{lm}) is the strain tensor. In the above, the strain tensor components can be written as

$$\varepsilon_{ik} = \frac{1}{2}\left(\partial_{x_k}u_i + \partial_{x_i}u_k + \partial_{x_k}h\partial_{x_i}h\right), \tag{1}$$

where u_i and h are in-plane and out-of-plane displacements, respectively. [27, 19] [10, 6, 24] Hence, the strain tensor components for graphene in the 2D displacement vector $\mathbf{u}(x, y) = (u_x, u_y)$ can be written as

$$\varepsilon_{xx} = \partial_x u_x + \frac{1}{2}\left(\partial_x h\right)^2, \tag{2}$$

$$\varepsilon_{yy} = \partial_y u_y + \frac{1}{2}\left(\partial_y h\right)^2, \tag{3}$$

$$\varepsilon_{xy} = \frac{1}{2}\left(\partial_y u_x + \partial_x u_y\right) + \frac{1}{2}\left(\partial_x h\right)\left(\partial_y h\right). \tag{4}$$

The stress tensor components $\sigma_{ik} = \partial U_s / \partial \varepsilon_{ik}$ for graphene can be written as [20]

$$\sigma_{xx} = C_{11}\varepsilon_{xx} + C_{12}\varepsilon_{yy}, \tag{5}$$

$$\sigma_{yy} = C_{12}\varepsilon_{xx} + C_{22}\varepsilon_{yy}, \tag{6}$$

$$\sigma_{xy} = 2C_{66}\varepsilon_{xy}. \tag{7}$$

In the continuum limit, elastic deformations of graphene sheets are described by the Navier equations $\partial_j \sigma_{ik} = 0$. Hence, the coupled Navier-type equations of electroelasticity in the presence of external body force [26] for graphene can be written as

$$2\left(C_{11}\partial_x^2 + C_{66}\partial_y^2\right)u_x + 2\left(C_{12}+C_{66}\right)\partial_x\partial_y u_y + \partial_x\left[C_{11}\left(\partial_x h\right)^2 + C_{12}\left(\partial_y h\right)^2\right] + 2C_{66}\partial_y\left(\partial_x h\right)\left(\partial_y h\right) + \frac{F_x}{t} = 0, \tag{8}$$

$$2\left(C_{66}\partial_x^2 + C_{11}\partial_y^2\right)u_y + 2\left(C_{12}+C_{66}\right)\partial_x\partial_y u_x + \partial_y\left[C_{12}\left(\partial_x h\right)^2 + C_{22}\left(\partial_y h\right)^2\right] + 2C_{66}\partial_x\left(\partial_x h\right)\left(\partial_y h\right) + \frac{F_y}{t} = 0, \tag{9}$$

where t is the thickness of the single layer graphene, $F_x = \partial_x U_x$ and $F_y = \partial_y U_y$. We assume that $U_x = \tau_e \sin(qx)$ and $U_y = \tau_e \sin(qy)$, where τ_e is the externally applied tensile edge stress. Here $q = 2\pi/\iota$ with ι being the period length of the in-plane ripple waves. We assume symmetric out-of-plane ripple waves ($\partial_x h = kh_0 \cos kx, \partial_y h = kh_0 \cos ky$, where $k = 2\pi/\ell$, ℓ is the period and h_0 is the height of out-of-plane ripple waves) travel along x and y direction in the plane of two dimensional graphene sheet.[28, 29, 10] Thus we write Eqs. 8 and 9 as:

$$\left(C_{11}\partial_x^2 + C_{66}\partial_y^2\right)u_x + \left(C_{12}+C_{66}\right)\partial_x\partial_y u_y = \frac{1}{2}C_{11}k^3h_0^2\sin(2kx) + C_{66}k^3h_0^2\cos(kx)\sin(ky) - \frac{\tau_e q}{t}\cos(qx), \tag{10}$$

$$\left(C_{66}\partial_x^2 + C_{11}\partial_y^2\right)u_y + \left(C_{12}+C_{66}\right)\partial_x\partial_y u_x = \frac{1}{2}C_{22}k^3h_0^2\sin(2ky) + C_{66}k^3h_0^2\sin(kx)\cos(ky) - \frac{\tau_e q}{t}\cos(qx). \tag{11}$$

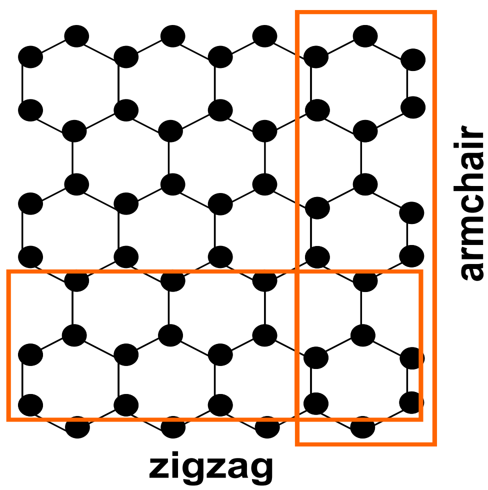

Fig. 1: The lattice structure of hexagon graphene sheet with the armchair and zigzag edges. The vertical and horizontal rectangles correspond to the armchair and zigzag graphene nanoribbons.

III. Computational Method

The schematic diagram of the two-dimensional graphene sheet and graphene nanoribbons (GNRs) in a computational domain is shown in Fig. 1. For strained graphene, we assume the vanishing displacement vector at the boundary and solve the Navier equations by utilizing the finite element method [30] to investigate the intrinsic properties of ripple waves. For GNRs considered here, typical numbers of elements depend on grid refinements and exceed 6500.

IV. Results and Discussions

Initially there is no variation in the in-plane and out-of-plane ripple waves, and the graphene sample is considered to be flat (no ripple waves). By applying tensile edge stress through the boundaries and considering the variations in the out-of-plane ripple waves, we find that the two dimensional graphene sheet are covered with ripple waves that is shown in Fig.3. Thus variation in in-plane and out-of-plane displacement vector generate spontaneous ripples that has no preferred orientation. Also their size is comparable with that of observed experiments. Our shown results of ripple waves in two dimensional graphene sheet is consistent to the Ref. [12]

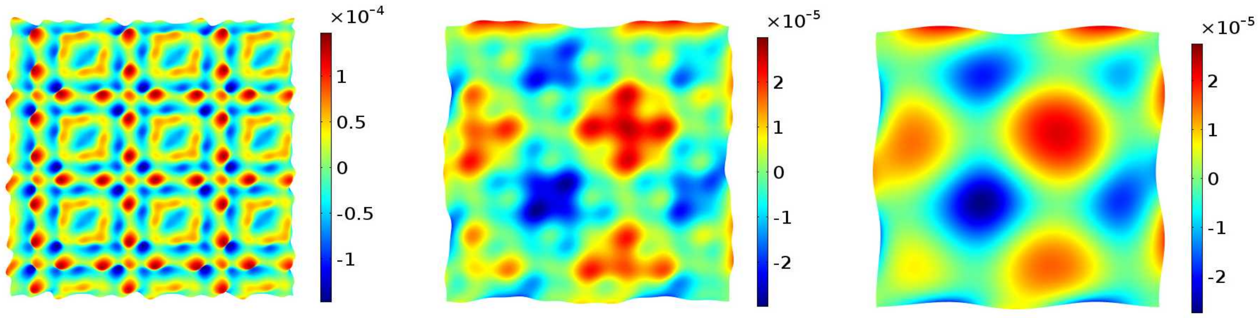

Fig. 2: Ripples formed in a suspended $1000 \times 1000\text{nm}^2$ honey comb graphene sheet. (left) Density plot of the off plane displacement $(\partial_y u_x + \partial_x u_y)$ as a function of in-plane co-ordinates at $\ell = 150/\text{nm}$ and $\lambda = 100/\text{nm}$. (middle) The same at $\ell = 250/\text{nm}$, $\lambda = 500/\text{nm}$. (right) The same at $\ell = 500/\text{nm}$, $\lambda = 500/\text{nm}$. Here we use normalization condition $\int\int (|u_x|^2 + |u_y|^2)\, dxdy = 1$. Also see Ref. [12]

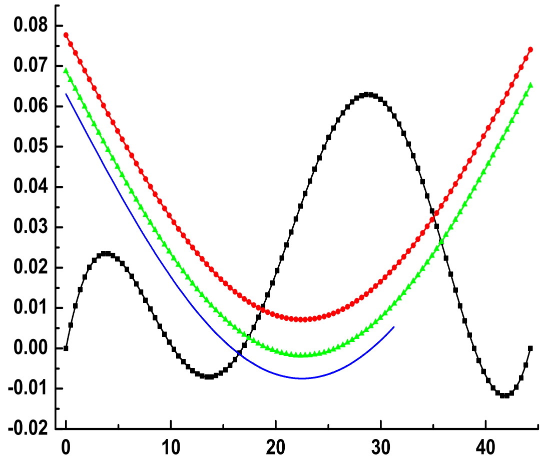

Fig. 3: Variation of displacement vector and strain tensor ($\ell = 88$nm(circle), 98nm(triangle pointing up), 108nm(triangle pointing down)) vs x in GNRs with armchair edge. The variation of strain in GNRs resembles the experimentally reported behavior in Ref.8 with some deviations to be explained (see the texts for details). The strain tensor can be treated as a pseudomorphic vector potential to get spin splitting of the band structures of GNRs for application in straintronic devices. We chose the parameters as follows: $\tau_e = 45\text{eV}/\text{nm}$, $c_{11} = 2246.3\text{eV}/\text{nm}^2$, $\iota = 90$nm, $t = 0.142$nm (see Ref. 25), $h_0 = 5$nm and $L = 44.3$nm.

For GNRs elongated along armchair direction, applying tensile edge stress along x-direction only, we assume that ε_{xx} is a non-vanishing strain tensor component. Thus, considering vanishing boundary conditions for the displacement vector at $x = \pm L/2$, Eq. (10) can be simplified as:

$$\begin{aligned} u_x &= \frac{\tau_e}{tC_{11}q}\left\{\cos(qx) - \cos\left(\frac{qL}{2}\right)\right\} \\ &\quad -\frac{1}{8}kh_0^2\sin(2kx) + \frac{kh_0^2}{4L}x\sin(kL)\,. \end{aligned} \tag{12}$$

From Eq. (2), we write the strain tensor as:

$$\varepsilon_{xx} = \frac{kh_0^2}{4}\left\{k + \frac{1}{L}\sin(kL)\right\} - \frac{\tau_e}{c_{11}t}\sin(qx). \tag{13}$$

Finally, we have plotted the variation of displacement vector and strain tensor vs x in GNRs with armchair edge in Fig. 3. This result is similar to Ref. 8 with only a slight deviation due to the fact that we apply vanishing boundary conditions for the displacements at the boundary of the GNRs. It is well known that the strain tensor induce large intrinsic magnetic fields that can be implemented in the Dirac Hamiltonian to see the application of ripple waves in designing graphene based optoelectronic devices. [23] We leave this coupling work for our future proposed work. For GNRs elongated along the zigzag direction and applying tensile edge stress along y-direction only, we assume ε_{yy} is non-vanishing strain tensor component. Thus, from Eq. (9), we write the strain tensor as: [28]

$$\varepsilon_{yy} = \frac{kh_0^2}{4}\left\{k + \frac{1}{L}\sin(kL)\right\} - \frac{\tau_e}{c_{11}t}\sin(qy). \tag{14}$$

Above equation induce similar form of ripple waves which is shown in Fig. 3.

V. Conclusion

Based on finite element numerical results, we have shown that the fluctuations in the in-plane and out-of-plane displacement vectors induce spontaneous ripple waves in two dimensional graphene sheets and graphene nanoribbons. These ripple waves in graphene are the intrinsic properties and have applications in designing optoelectronic devices.

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