RESEARCH ARTICLE

Quantum Matter
Vol. 4, 305–307, 2015

Relaxed Shape of Graphene Sheet Due to Ripples

Sanjay Prabhakar[1], Roderick Melnik[1,*], Luis L. Bonilla[2], and Shyam Badu[1]

[1]*M²NeT Laboratory, Wilfrid Laurier University, Waterloo, ON, N2L 3C5, Canada*
[2]*Gregorio Millan Institute, Universidad Carlos III de Madrid, Leganes, 28911, Spain*

We study the relaxed shape of graphene due to ripple waves induced by externally applied tensile edge stress along the armchair direction. We show that the oscillations in the strain tensor in graphene sheets can be induced due to ripples. The in-plane ripple waves can be generated via externally applied tensile stress along the armchair or zigzag directions. We show that the distributions of strain tensor components are enhanced with increasing values of the amplitude of the ripple waves.

Keywords: Graphene, Ripples, Electromechanical Effects.

1. INTRODUCTION

Graphene is one of the most promising candidates to build the next generation electronic devices because of its unusual properties due to the Dirac-like spectrum of the charge carriers and its high mobility of charge.[1–12] It is known that the surface of the graphene sheet is covered by the ripple waves.[13–15] Also the surface of graphene sheet exhibits intrinsic microscopic roughening and the surface normal varies by several degrees, where the out-of-plane deformations reach to nanometer scale.[13–15] These days, such ripples are found in several nanometers long waves; They lie in the out-of-plane of the sheet without a preferred direction. Ripples in graphene sheets can be induced by several different mechanisms such as applied tensile stress or temperatures that have been investigated by a number of authors.[4, 11, 14, 16–18] Such ripples are the intrinsic properties of graphene that are expected to strongly affect the bandstructures by coupling through pshedomorphic strain of graphene.[7, 12, 19] In experiments on graphene suspended on substrate trenches, there appear much longer and taller waves (close to a micron scale) directed parallel to the applied stress. These long wrinkles are thermally induced and can be explained by continuum elasticity. In this paper we present a model which is based on the Navier equations and provide the relaxed shape of graphene sheets due to applied tensile stress along the armchair direction.

2. THEORETICAL MODEL

The total elastic energy density associated to the strain for the two-dimensional graphene can be written as:[11, 17, 20]

$$U_s = \frac{1}{2}[C_{11}\varepsilon_{xx}^2 + C_{22}\varepsilon_{yy}^2 + 2C_{12}\varepsilon_{xx}\varepsilon_{yy} + 2C_{66}\varepsilon_{xy}^2] \quad (1)$$

where C_{iklm} is an elastic modulus tensor of rank four, called the elastic modulus tensor and ε_{ik} (or ε_{lm}) is the strain tensor. In (1), the strain tensor components can be written as

$$\varepsilon_{ik} = \frac{1}{2}(\partial_{x_k} u_i + \partial_{x_i} u_k) \quad (2)$$

Hence the strain tensor components for graphene in 2D displacement vector $\mathbf{u}(x, y) = (u_x, u_y)$ can be written as

$$\varepsilon_{xx} = \partial_x u_x, \quad \varepsilon_{yy} = \partial_y u_y, \quad \varepsilon_{xy} = \frac{1}{2}(\partial_y u_x + \partial_x u_y) \quad (3)$$

The stress tensor components $\sigma_{ik} = \partial U_s/\partial \varepsilon_{ik}$ for graphene can be written as[18]

$$\sigma_{xx} = C_{11}\varepsilon_{xx} + C_{12}\varepsilon_{yy} \quad (4)$$

$$\sigma_{yy} = C_{12}\varepsilon_{xx} + C_{22}\varepsilon_{yy} \quad (5)$$

$$\sigma_{xy} = 2C_{66}\varepsilon_{xy} \quad (6)$$

In the continuum limit, elastic deformations of graphene sheets are described by the Navier equations $\partial_j \sigma_{ik} = 0$. Hence the coupled Navier equations for graphene can be written as

$$(C_{11}\partial_x^2 + C_{66}\partial_y^2)u_x + (C_{12} + C_{66})\partial_x\partial_y u_y = 0 \quad (7)$$

$$(C_{66}\partial_x^2 + C_{11}\partial_y^2)u_y + (C_{12} + C_{66})\partial_x\partial_y u_x = 0 \quad (8)$$

Ripple in graphene is described by an out-of-plane and in-plane sinusoidal function in the sheet of graphene.[12, 19, 21] We apply tensile edge stress along the armchair direction to induce the ripples in the graphene sheet (see Fig. 1). The displacement vector due to applied tensile edge stress can be written as

$$u(x, 0) = A\sin(kx) \quad (9)$$

*Author to whom correspondence should be addressed.

 2164-7615/2015/4/305/003 doi:10.1166/qm.2015.1196

Quantum Matter 4, 305–307, 2015

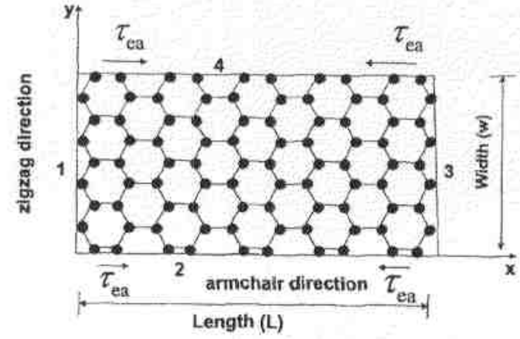

Fig. 1. Tensile stress is applied along the armchair directions that induce the ripples in graphene sheet.

where A is the amplitude of the ripple waves along the armchair direction and $k = 2\pi/\lambda$ with λ being the wavelength. Due to applied tensile edge stress along the armchair direction, the total edge energy per unit length is given by Refs. [4, 14]

$$U_e = \frac{1}{2}\tau_e\left(\frac{\partial u(x,0)}{\partial x}\right)^2 + \frac{1}{8}E_e\left(\frac{\partial u(x,0)}{\partial x}\right)^4 \qquad (10)$$

where τ_e and E_e denote the edge stress and the elastic modulus of the edge along the armchair direction of the graphene sheet. Thus, the total edge energy, $U_t = \int_0^L U_e\,dx$, of the graphene sheet is given by

$$U_t = \frac{\tau_e}{4}A^2k\left[kL + \frac{1}{2}\sin(2kL)\right] + \frac{E_e}{32}A^4k^3[12kL + 8\sin(2kL) + \sin(4kL)] \qquad (11)$$

In order to estimate reasonable values of the applied tensile edge stress, we need to find the optimum values of the amplitude of the ripple waves that mimic the experimentally reported values in Ref. [12]. Thus the optimum amplitude of the ripple waves can be found by utilizing the condition $\partial U_t/\partial A = 0$ as:

$$A = \sqrt{\frac{2\tau_e(2kL + \sin(2kL))}{E_e k^2[12kL + 8\sin(2kL) + \sin(4kL)]}} \qquad (12)$$

By considering $L = 1.5$ μm, $\tau_e = 4$ eV/nm, $E_e = 1000$ eV/nm and $\lambda = 0.1$ to 1.5 μm, the amplitude (A) of the ripple waves varies from 0.6 nm to 8.7 nm which is in agreement with the experimentally reported values in Ref. [12].

3. RESULTS AND DISCUSSION

The schematic diagram of the two dimensional graphene sheet in computational domain is shown in Figure 1. We have applied the tensile edge stress along the armchair direction to create the ripple waves in graphene sheet. We have used the multiscale multiphysics simulation and solved the Navier's Eqs. (7) and (8) via Finite Element Method to investigate the influence of electromechanical effects on the relaxed shape of graphene due to ripple waves. For the ripple waves along the armchair direction, we have used the Neumamn boundary conditions on sides 1, 3 and employed Eq. (9) at sides 2, 4. All reported results in Figures 2 and 3 have been obtained for a 1.5×0.5 μm^2 graphene sheet that mimics the geometry of experimentally studied structure in Ref. [12].

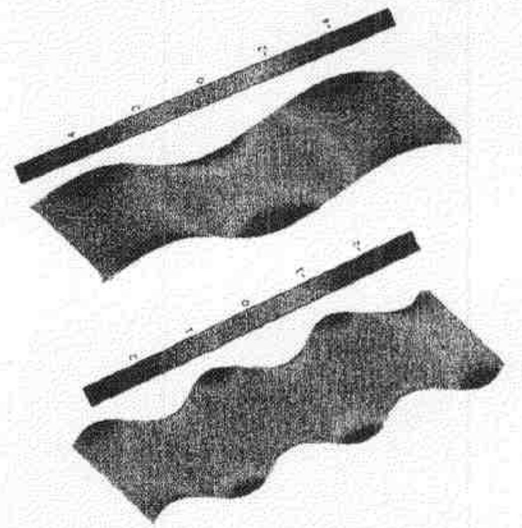

Fig. 2. Induced ripples in the relaxed shape of graphene due to applied tensile stress along the armchair direction for $\lambda = 1$ μm (upper panel) and $\lambda = 0.5$ μm (lower panel). Here we chose $\tau_e = 4$ eV/nm, $E_e = 1000$ eV/nm and the dimension of the graphene sheet is taken to be $L \times w = 1.5 \times 0.5$ μm^2. The material constants are chosen from Ref. [17] as: $C_{12} = 41$ [N/m] and $C_{66} = 159.2$ [N/m]. This relaxed shape of graphene due to applied tensile stress along the armchair direction mimics to the surface of the experimentally reported graphene sheet in Ref. [12]. Similar type of results are also presented in Refs. [4, 16].

Figure 2 shows the relaxed shape of graphene under applied tensile stress along the armchair direction. This relaxed shape

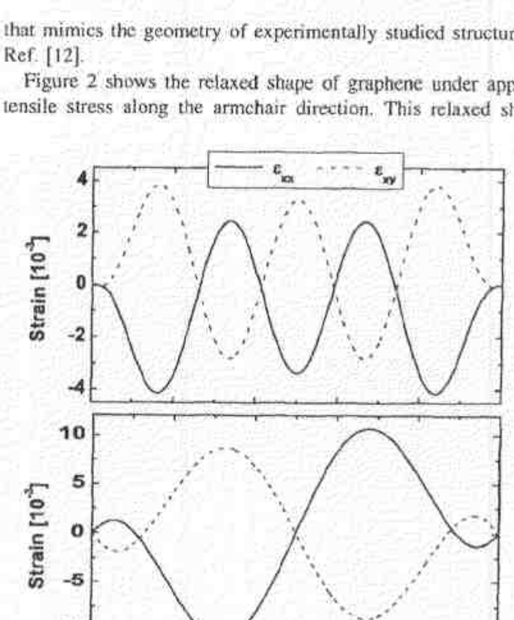

Fig. 3. Oscillations in strain tensor due to ripples in graphene sheet by applying tensile stress along the armchair direction at $y = w/2$ with $\lambda = 1$ μm (upper panel) and $\lambda = 0.5$ μm (lower panel). The parameters are chosen to be the same as in Figure 2.

of graphene due to induced ripples mimics the experimentally reported results in Ref. [12]. In Figure 3, we investigate the influence of ripples on the strain tensor under the applied tensile edge stress along the armchair direction. The oscillations in the strain tensor can be seen due to the fact that the applied tensile stress along the armchair direction induces the in-plane ripple waves. Also we note that increasing the wavelength of the ripple waves from $\lambda = 0.5\ \mu$m (lower panel) to $\lambda = 1\ \mu$m (upper panel) enhances the amplitude of the ripple waves which is in agreement with the experimentally observed results in Ref. [12].

4. CONCLUSION

We have developed a model, based on the Navier equations, which allows us to investigate the influence of ripple waves on the relaxed shape of graphene sheets. We have shown that ripple waves in graphene sheet induce oscillations in the strain tensor. Such oscillations can be enhanced with by increasing tensile stress either along the armchair or the zigzag directions. A natural extension of the presented model would be to account for the influence of temperature. Such an extended Navier-type model of thermoelasticity will be discussed elsewhere in the contest of the influence of the thermoelectromechanical effects on electronic properties of graphene.

Acknowledgments: This work has been supported by NSERC and CRC programs (Canada).

References and Notes

1. K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, *Science* 306, 666 **(2004)**.
2. K. S. Novoselov, D. Jiang, F. Schedin, T. J. Booth, V. V. Khotkevich, S. V. Morozov, and A. K. Geim, *Proceedings of the National Academy of Sciences of the United States of America* **(2005)**, Vol. 102, p. 10451.
3. A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *Rev. Mod. Phys.* 81, 109 **(2009)**.
4. V. B. Shenoy, C. D. Reddy, A. Ramasubramaniam, and Y. W. Zhang, *Phys. Rev. Lett.* 101, 245501 **(2008)**.
5. S.-M. Choi, S.-H. Jhi, and Y.-W. Son, *Phys. Rev. B* 81, 081407 **(2010)**.
6. P. A. Maksym and H. Aoki, *Phys. Rev. B* 88, 081406 **(2013)**.
7. W. Bao, K. Myhro, Z. Zhao, Z. Chen, W. Jang, L. Jing, F. Miao, H. Zhang, C. Dames, and C. N. Lau, *Nano Lett.* 12, 5470 **(2012)**.
8. A. A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao, and C. N. Lau, *Nano Lett.* 8, 902 **(2008)**.
9. Z. Yan, G. Liu, J. M. Khan, and A. A. Balandin, *Nature Communications* 3, 827 **(2012)**.
10. E. Cadelano, P. L. Palla, S. Giordano, and L. Colombo, *Phys. Rev. Lett.* 102, 235502 **(2009)**.
11. E. Cadelano and L. Colombo, *Phys. Rev. B* 85, 245434 **(2012)**.
12. W. Bao, F. Miao, Z. Chen, H. Zhang, W. Jang, C. Dames, and C. N. Lau, *Nat. Nano.* 4, 562 **(2009)**.
13. J. C. Meyer, A. K. Geim, M. I. Katsnelson, K. S. Novoselov, T. J. Booth, and S. Roth, *Nature* 446, 60 **(2007)**.
14. L. L. Bonilla and A. Carpio, *Phys. Rev. B* 86, 195402 **(2012)**.
15. F. Guinea, M. I. Katsnelson, and A. K. Geim, *Nat. Phys.* 6, 30 **(2010)**.
16. H. Wang and M. Upmanyu, *Phys. Rev. B* 86, 205411 **(2012)**.
17. A. Carpio and L. L. Bonilla, *Phys. Rev. B* 78, 085406 **(2008)**.
18. J. Zhou and R. Huang, *Journal of the Mechanics and Physics of Solids* 56, 1609 **(2008)**.
19. E. Cerda and L. Mahadevan, *Phys. Rev. Lett.* 90, 074302 **(2003)**.
20. L. D. Landau and E. M. Lifshitz, Theory of Elasticity, Pergamon Press Ltd. **(1970)**.
21. S. Prabhakar, R. Melnik, L. bonilla, and S. Badu, *Phys. Rev. B* 90, 205418 **(2014)**.

Received: 1 December 2013. Accepted: 1 March 2014.