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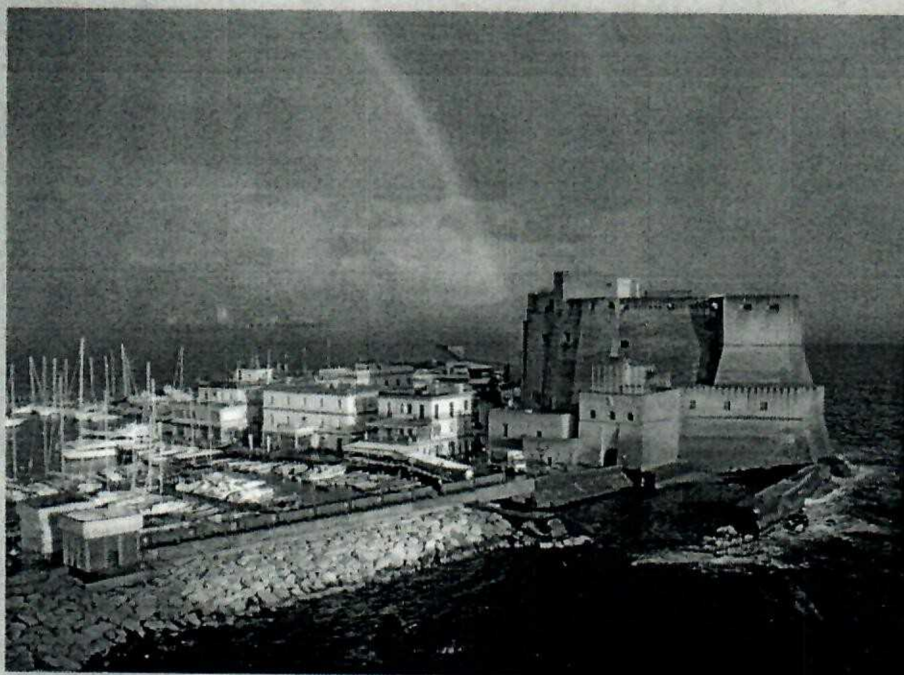

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Paper 66

The Influence of Thermo-Mechanical Effects on the Relaxed Shape Graphene

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Abstract

In this paper, we consider a two dimensional graphene sheet with armchair and zigzag edges. We investigate the influence of temperature on the in-plane oscillations of the strain tensor in this graphene. We show that the in-plane oscillations of the strain tensor are enhanced with temperature.

Keywords: armchair and zigzag graphene, electromechanical effects, finite element method.

1 Introduction

Graphene is a material of great interest for making next generation electronic devices because it possesses unique properties due to the Dirac-like spectrum of charge carriers [1, 2, 3, 4, 5]. Moreover, optoelectronic devices made from graphene possess several observed unique properties such as those based on the half integer quantum Hall effect, non-zero Berry phase, as well as the measurement of non-zero conductivity of electrons even when the density of the charge carriers vanishes [3, 4, 6]. By now, it is well known that just one atom thick graphene sheet demonstrates the properties of a two dimensional system that does not contain any bandgap at Dirac points [7]. However, it is possible to induce a bandgap by utilizing the intrinsic and Rashba spin-orbit couplings for the application of graphene in semiconductor and optoelectronic devices in areas including spintronics and photonics [8].

Under careful scrutiny, it is clear that the surface of graphene sheets is not perfectly flat. In experiments on graphene suspended on substrate trenches, there appear much longer and taller waves (often close to a micron scale) directed parallel to the applied stress [12, 13]. These long wrinkles are thermally induced and can be explained by continuum thermoelasticity. The influence of electromechanical effects on

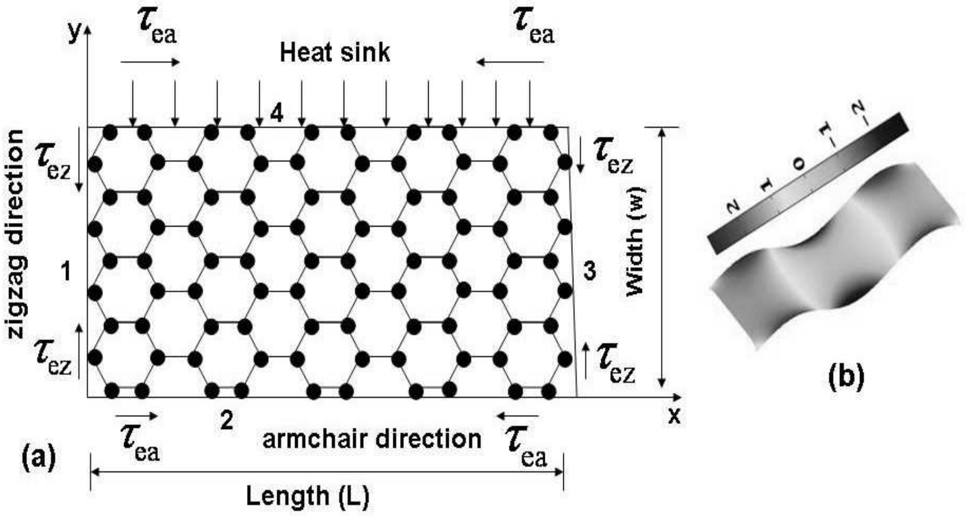

Figure 1: (a) Tensile stress is applied along armchair and zigzag directions, inducing the oscillations in the strain tensor of the graphene sheet. The boundary 4 is connected to the heat bath in order to investigate the influence of temperature on the strain tensor of graphene. (b) Relaxed shape of graphene due to applied tensile stress along armchair direction for wavelength $\lambda = 1\ \mu\mathrm{m}$ and the amplitude of the waves $A = 5.8\ \mathrm{nm}$. Here we chose temperature $T(x) = T_0 = 75$ K and the dimension of the graphene sheet was taken to be $L \times w = 1.5 \times 0.5\ \mu\mathrm{m}^2$.

the graphene sheet can be understood by applying suitable edge stress along the armchair and zigzag directions. The tensile forces, that can be applied on the graphene sheet with a compressed elastic string, are schematically shown in Fig. 1.

2 Theoretical Model

The total thermoelastic energy density associated to the strain for the two dimensional graphene sheet can be written as [9, 10]

$$U_s = \frac{1}{2} C_{iklm} \varepsilon_{ik} \varepsilon_{lm} - \beta_{ik} \Theta(x, y) \varepsilon_{ik} \delta_{ik}, \tag{1}$$

where C_{iklm} is a tensor of rank four (the elastic modulus tensor), ε_{ik} (or ε_{lm}) is the strain tensor and β_{ik} are the stress temperature coefficients. Also, $\Theta(x, y)$ is the distribution of temperature in the graphene sheet that can be found by solving Laplace equation $\partial_i q_i = 0$, where $q_i = -\alpha_{ii} \partial_i \Theta$ with α_{ii} being the heat induction coefficients of graphene. Thus, we write the equation for temperature as

$$\alpha_{11} \partial_x^2 \Theta + \alpha_{22} \partial_y^2 \Theta = 0. \tag{2}$$

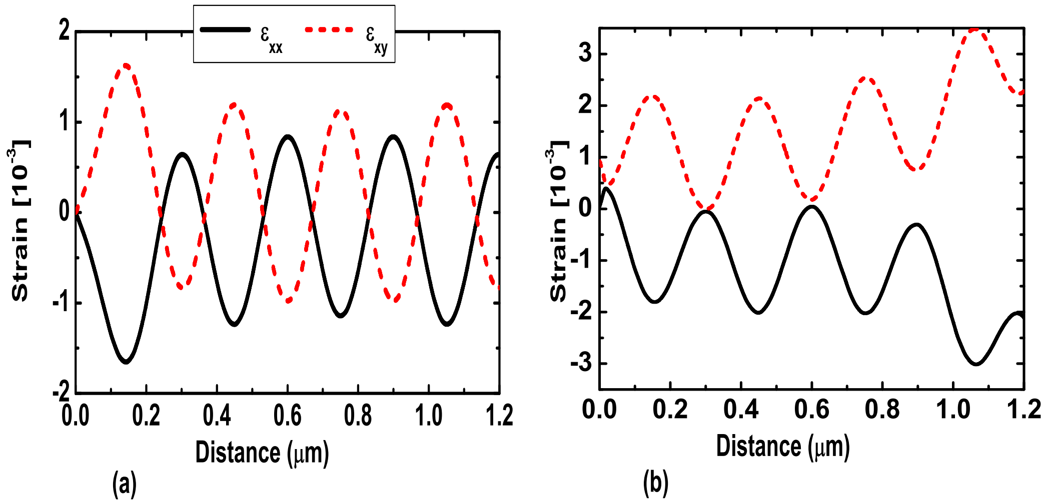

Figure 2: Oscillations in the strain tensor due to applied tensile stress along the armchair direction at $y = w/2$ and temperature $T_0 = 0$ K (Fig.2(a)) and $T_0 = 300$ K (Fig.2(b)). The parameters are chosen to be the same as in Fig. 1 but $\lambda = 300$ nm.

We suppose that the graphene sheet at the boundary 4 (see Fig. 1) is connected to the heat bath of temperature $T(x)$ and all other three boundaries 1,2,3 are fixed at zero temperature. Thus, the exact solution of Laplace Eq. (2) can be written as

$$\Theta\left(x,y\right)=\sum_{m=1}^{\infty}B_m\sinh\left(\frac{m\pi y}{L\sqrt{k_e}}\right)\sin\left(\frac{m\pi}{L}x\right), \tag{3}$$

where constants B_m relate to the temperature of thermal bath $T(x)$ as:

$$T(x)=\sum_{m=1}^{\infty}B_m\sinh\left(\frac{m\pi w}{L\sqrt{k_e}}\right)\sin\left(\frac{m\pi}{L}x\right). \tag{4}$$

Here $k_e = \alpha_{22}/\alpha_{11}$, m is an integer, L is the length and w is the width of the graphene sheet. The constants B_m can be found by performing Fourier's transform of (4):

$$B_m=\frac{2}{L\sinh\left(m\pi w/L\sqrt{(}k_e)\right)}\int_0^L T(x)\sin\left(\frac{m\pi x}{L}\right)dx. \tag{5}$$

In (1), the strain tensor components can be written as $\varepsilon_{ik} = \frac{1}{2}\left(\partial_{x_k}u_i + \partial_{x_i}u_k\right)$, where u_i are the in-plane displacements [10]. Throughout the paper, we assume that the wrinkles are generated by applying tensile edge stress along the armchair and zigzag directions [11, 12, 13]. Hence, the strain tensor components for graphene in 2D displacement vector $\mathbf{u}(x, y) = (u_x, u_y)$ can be written as

$$\varepsilon_{xx} = \partial_x u_x,\ \varepsilon_{yy} = \partial_y u_y,\ \varepsilon_{xy} = \frac{1}{2}\left(\partial_y u_x + \partial_x u_y\right). \tag{6}$$

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

$$\left(C_{11}\partial_x^2 + C_{66}\partial_y^2\right) u_x + \left(C_{12} + C_{66}\right) \partial_x \partial_y u_y - \beta_{11}\partial_x \Theta = 0, \tag{7}$$

$$\left(C_{66}\partial_x^2 + C_{11}\partial_y^2\right) u_y + \left(C_{12} + C_{66}\right) \partial_x \partial_y u_x - \beta_{22}\partial_y \Theta = 0. \tag{8}$$

3 Computational Details

The schematic diagram of the two-dimensional graphene sheet in a computational domain is shown in Fig. 1(a). We apply tensile edge stress along the armchair direction only to induce the oscillations in the strain tensor in the graphene sheet (see Fig. 1(a)). We have used the multiscale multiphysics simulation framework and solved the Navier equations (7) and (8) via the Finite Element Method to investigate the influence of thermo-electromechanical effects on the relaxed shape of graphene. For the waves along the armchair direction, we have used the Neumann boundary conditions at sides 1, 3 and employed $u(x, 0) = A\sin(kx)$ at sides 2 and 4. Here A is the amplitude and $k = 2\pi/\lambda$ with λ being the wavelength. These conditions are mechanical boundary conditions for displacement only. For thermal part of the model, we have imposed Dirchlet boundary conditions at sides $1, 2, 3$ and side 4 is connected to the heat bath of temperature T(x). We have chosen a $1.5 \times 0.5\ \mu\text{m}^2$ graphene sheet. All parameters for our simulations have been taken from Table 1.

C_{11}[N/m]	359.4
C_{12}[N/m]	41
C_{66}[N/m]	159.2
$\alpha_{11}[10^{-6}/\text{K}]$	-7
$\alpha_{22}[10^{-6}/\text{K}]$	-7
$\beta_{11}[10^{-3}\text{N}/(\text{m}\cdot\text{K})]$	-2.8
$\beta_{22}[10^{-3}\text{N}/(\text{m}\cdot\text{K})]$	-2.8
ν	0.165

Table 1: The material constants for graphene, used in our calculations, have been taken from Refs. [10, 12, 11]. The numerical values of the thermal coefficients β_{11} and β_{22} have been obtained from expressions $\beta_{11} = C_{11}\alpha_{11} + C_{12}\alpha_{22}$ and $\beta_{22} = C_{12}\alpha_{11} + C_{22}\alpha_{22}$.

4 Results and Discussions

Fig. 1(b) shows the relaxed shape of graphene under the applied tensile stress along the armchair direction. As can be seen, the relaxed shape graphene oscillates sinusoidally along the armchair direction. This relaxed shape of graphene due to applied tensile edge stress mimics the theoretically and experimentally reported results in Refs. [12, 11]. In practice, relaxed shapes of graphene can be observed in any optoelectronic devices made from two dimensional graphene sheet mounted on a substrate trenches. As a result, we find the out-of-plane ripple waves induced on the surface of the graphene sheet that might be implemented for making straintronic devices. In Fig. 2, we investigate the influence of temperature 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 out-of-plane oscillations of graphene sheet. We note that the increasing temperature from 0 K to room temperature enhances the amplitude of the waves.

5 Conclusion

In this paper, we have developed a model which allows us to investigate the influence of temperature on the relaxed shape of graphene sheet. We have shown that intrinsic edge stresses can have a significant influence on the morphology of graphene sheets. We have presented a model that couples the Navier equations, accounting for thermo-electromechanical effects, analyzed the in-plane oscillations of strain tensor of graphene sheet, and shown that the amplitude of the induced waves due to applied tensile edge stress increases with temperature.

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References

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva and A. A. Firsov, "Electric field effect in atomically thin carbon films", 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, "Two-dimensional atomic crystals", Proceedings of the National Academy of Sciences of the United States of America 102, 10451 (2005).

[3] S. Das Sarma, S. Adam, E. Hwang, and E. Rossi, “Electronic transport in two-dimensional graphene”, Rev. Mod. Phys. 83, 407 (2011).

[4] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov and A. K. Geim, “The electronic properties of graphene”, Rev. Mod. Phys. 81, 109 (2009).

[5] S. Prabhakar, R. Melnik, L. Bonilla and J. Raynolds, “Spin echo dynamics under an applied drift field in graphene nanoribbon superlattices”, Applied Physics Letters 103, 233112 (2013).

[6] M. Droth and G. Burkard, “Electron spin relaxation in graphene nanoribbon quantum dots” Phys. Rev. B 87, 205432 (2013).

[7] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, A. A. Firsov, “Two-dimensional gas of massless Dirac fermions in graphene”, Nature 438, 197 (2005).

[8] D. Huertas-Hernando, F. Guinea and A. Brataas, “Spin-orbit coupling in curved graphene, fullerenes, nanotubes, and nanotube caps”, Phys. Rev. B 74, 155426 (2006).

[9] Theory of Elasticity, L. D. Landau and E. M. Lifshitz, Pergamon Press Ltd. (1970).

[10] A. Carpio and L. Bonilla, “Periodized discrete elasticity models for defects in graphene”, Phys. Rev. B 78, 085406 (2008).

[11] W. Bao, F. Miao, Z. Chen, H. Zhang, W. Jang, C. Dames, C. Lau, “Controlled ripple texturing of suspended graphene and ultrathin graphite membranes”, Nature Nanotechnology 4, 562 (2009).

[12] V. Shenoy, C. Reddy, A. Ramasubramaniam and Y. Zhang, “Edge-Stress-Induced Warping of Graphene Sheets and Nanoribbons”, Phys. Rev. Lett. 101, 245501 (2008).

[13] E. Cerda and L. Mahadevan, “Geometry and Physics of Wrinkling”, Phys. Rev. Lett. 90, 074302 (2003).

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