MODELING AND ANALYSIS OF SPIN SPLITTING IN STRAINED GRAPHENE NANORIBBONS

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KEYWORDS
Complex systems, graphene, coupled theory, Dirac energy bands, multiscale effects.

ABSTRACT

We study the influence of ripple waves, originating from the electromechanical effects, on band structures of graphene nanoribbons (GNRs). GNRs are complex systems that require novel approaches for their analysis, due to multiscale and multiphysics effects involved. Here, we develop a mathematical model and we show that the externally applied magnetic fields along z-direction in combination with pseudo-fields enhance the spin splitting of GNRs bands. In particular, we show that the strain tensor induce quantum confinement effect that turn to lead the opening of the bandgaps at Dirac point. Such finite band gaps are highly sensitive to the control parameters (period length, applied stress) of the ripple waves that help to design the optoelectronic devices for straintronic and spintronic applications.

INTRODUCTION

Graphene has a potential interest for future optoelectronic devices due to its unique electronic and physical properties (Sarma et al. 2011, Castro et al. 2009, Novoselov et al. 2005, Abanin et al. 2006, Barbier et al. 2006). Several observed quantum properties such as the half integer quantum Hall effect, non-zero Berry phase, as well as the measurement of conductivity of electrons in the electronic devices lead to novel applications in carbon based nanoelectronic devices (Sarma et al. 2011, Castro et al. 2009, Novoselov et al. 2005, Novoselov and Jiang et al. 2005, Novoselov et al. 2004, Zhang et al. 2005). One atom thick graphene sheet has the same properties as a two dimensional system that does not contain any band gap at two Dirac points (Novoselov et al. 2005). Further strain engineering of graphene by controlling the electromechanical properties via the pseudomorphic gauge fields are considered as a next generation optoelectronic devices (Shenoy et al. 2008, Choi et al. 2010, Bao et al. 2012, Cadelano et al. 2009, Bao et al. 2009). Small band gap opening is also expected due to implementation of strain tensor in the band structures of graphene through pseudomorphic vector potential.

Due to a range of multiscale effects associated with these properties, the development of new mathematical models and their efficient computational implementations are essential. In this paper we present a model that couples the Navier equations, accounting for electromechanical effects, to the electronic properties of zigzag graphene nanoribbons. We show that the ripple waves originating from the electromechanical effects strongly influence the band structures of GNRs. This response mechanism might be used for tuning the band gaps at the Dirac point in strained GNRs that can be utilized to design the optoelectronic devices for the application in straintronic (Levy et al. 2010).

Experimental studies on two dimensional images of graphene sheet taken from high resolution transmission electron microscope or scanning tunneling microscope show that in-plane and out-of-plane ripples waves varies by several degrees and reach to the nanometer scale (Sarma et al. 2011). These ripples in graphene are induced by several different mechanisms that have been widely investigated (Shenoy et al. 2008, Cadelano et al. 2009, Choi et al. 2010, Kitt et al. 2012, Carpio and Bonilla 2008, Cadelano and Colombo 2012). 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 (Bao et al. 2009, Bao et al. 2012, Cerda and Mahadevan 2003). Recently in Ref. (Prabhakar et al. 2014), in-plane oscillations and thermomechanics of relaxed-shape graphene due to externally applied tensile edge stress along both the armchair and zigzag directions in graphene quantum dots have also been explored. Here authors have shown that the level crossing between the ground and first-excited states in the localized edge states can be achieved with accessible values of temperature. The level crossing is absent in the states formed at the center of the graphene sheet due to the presence of threefold symmetry. More recently, in Ref. (Prabhakar and Melnik 2015), the

Proceedings 30th European Conference on Modelling and Simulation ©ECMS Thorsten Claus, Frank Herrmann, Michael Manitz, Oliver Rose (Editors)
ISBN: 978-0-9932440-2-5 / ISBN: 978-0-9932440-3-2 (CD)

authors of this work have investigated the influence of in-plane ripple waves in graphene nanoribbons. In this paper, we investigate the influence of both in-plane and out-of-plane ripple waves in zigzag graphene nanoribbons in presence of external magnetic fields along z-direction. In particular we present a model that couples the Navier equations, accounting for electromechanical effects, to the electronic properties of zigzag graphene nanoribbons. We show that the ripple waves originating from the electromechanical effects strongly influence the band structures of GNRs. This response mechanism might be used for tuning the band gaps at the Dirac point in strained GNRs that can be utilized to design the optoelectronic devices for the application in straintronics. Other novel applications of complex systems, such as GNRs, based on coupled physical effects are expected.

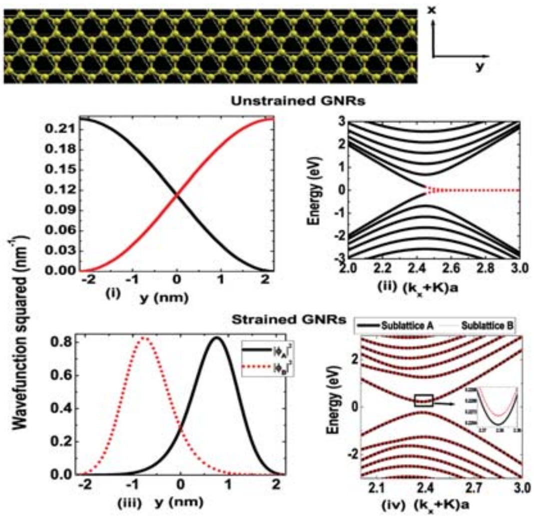

FIGURE 1: Schematics of zigzag graphene nanoribbons is shown in upper panel. (a) Ground state wavefunctions squared vs distance (y) in zigzag GNRs at k_x=0. These plots are obtained from Eqs. (23) and (24). (b) The band structures of GNR with the zigzag edge are obtained from Eqs.(19) (dotted lines) and (22) (solid lines). Here we choose the width of the GNR as L=3 $\sqrt{3}$ aN (N=6) to reproduce the results of Ref. (Brey and Fertig 2006). Band diagram of strained zigzag GNRs are shown in Fig. 1 (iii) and (iv). Here we clearly see the band gap openings due to strain tensor and highly asymmetric wavefunctions of graphene electrons of sublattices A and B are observed. The parameters are chosen as: τ_e=-100eV/nm, h_0=1nm and B=1T.

MATHEMATICAL MODEL

The total elastic energy density associated with the strain for the two dimensional graphene sheet can be written as (Landau and Lifshitz 1970, Carpio and Bonilla 2008, Cadelano and Colombo 2012) $2U_s = C_{iklm}\varepsilon_{ik}\varepsilon_{lm}$. 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 (Juan et. al. 2013, Carpio and Bonilla 2008, Bao et al. 2009, Shenoy et al. 2008, Cerda and Mahadevan 2003). Hence, the strain tensor components for graphene in the 2D displacement vector $u(x,y) = (u_x, u_y)$ can be written as

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

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

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

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

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

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

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

In the continuum limit, elastic deformations of graphene sheets under applied tensions are described by the Navier equations $\partial_j \sigma_{ik} + F_i / t = 0$, where F_i are applied tensions. Hence, the coupled Navier equations of electroelasticity can be written as: (Landau and Lifshitz 1970)

$$\left(C_{11}\partial_x^2 + C_{66}\partial_y^2\right)u_x + (C_{12} + C_{66})\partial_x\partial_y u_y + \frac{1}{2}\partial_x\left[C_{11}(\partial_x h)^2 + C_{12}(\partial_y h)^2\right] + C_{66}\partial_y(\partial_x h)(\partial_y h) + \frac{F_x}{t}, \tag{8}$$

$$\left(C_{66}\partial_x^2 + C_{11}\partial_y^2\right)u_y + (C_{12} + C_{66})\partial_x\partial_y u_x + \frac{1}{2}\partial_y\left[C_{12}(\partial_x h)^2 + C_{22}(\partial_y h)^2\right] + C_{66}\partial_x(\partial_x h)(\partial_y h) + \frac{F_y}{t}, \tag{9}$$

where t is the thickness of the single layer graphene, $F_x = \tau_e q\, sin(qx)$ and $F_y = \tau_e q\, sin(qy)$. 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, $\partial_x h = k h_0\, cos(kx)$,

$\partial_y h = kh_0 \cos(ky)$, where $k = 2\pi / l$, 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 (Meng et al. 2013, Guinea et al. 2008, Bao et al. 2009). Thus, we write Eqs.(8) and (9) as:

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

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

For zigzag GNRs elongated along x-direction and applying tensile edge stress along y-direction, we assume ε_{yy} is non-vanishing strain tensor component. Therefore, from Eq (9), we write the strain tensor as (Meng 2013):

$$\varepsilon_{yy} = \frac{\tau_e}{C_{22}t}\cos(qy) + \frac{1}{4}k^2h_0^2 + \frac{kh_0^2}{4L}\sin(kL) - \frac{2\tau_e}{qC_{22}tL}\sin\left(\frac{qL}{2}\right). \quad (12)$$

Now we turn to the influence of strain tensor on the electronic properties of zigzag graphene quantum dots.

In the continuum limit, by expanding the momentum close to the K point in the Brillouin zone, the Hamiltonian for π electrons at the K point reads as (Maksym and Aoki 2013, Krueckl and Richter 2012, Neto et al. 2009):

$$H = v_F\left(\sigma_x P_x + \sigma_y P_y\right) + \frac{1}{2}g_0\mu_B B\sigma_z, \quad (13)$$

In (13), $P = p - \eta A_s - eA$ with $p = -i\eta\partial_x$ being the canonical momentum operator, $A_s = (-\varepsilon_{yy}, 0)\beta / a$ is the vector potential induced by pseudomorphic strain tensor and $A = B(-y, 0)$ is the vector potential due to applied magnetic field, B along z-direction (Kitt et al. 2012, Guinea et al. 2008, Guinea and Horovitz et al. 2008, Juan et al. 2013). The last term is the Zeeman energy.

For strained graphene nanoribbons with zigzag edge (Sevincli et al. 2008, Zheng et al. 2007), we assume $H\psi = \varepsilon\psi$, where $\psi(r) = \exp(ik_x x)\left(\phi_A(y)\ \phi_A(y)\right)^T$ (Neto et al. 2009). Thus the two coupled equations can be written as

$$\left(k_x - \partial_y + \frac{\beta}{a}\varepsilon_{xx} + \frac{eB}{\eta}y\right)\phi_B = \left(\frac{\varepsilon - g_0\mu_B B/2}{\eta v_F}\right)\phi_A, \quad (14)$$

$$\left(k_x + \partial_y + \frac{\beta}{a}\varepsilon_{xx} + \frac{eB}{\eta}y\right)\phi_B = \left(\frac{\varepsilon + g_0\mu_B B/2}{\eta v_F}\right)\phi_B. \quad (15)$$

In the general case, exact solutions of (14) and (15) are not feasible to find. However for some special cases, e.g. for unstrained Hamiltonians without any source of external magnetic field, we can write two coupled equations as:

$$\left(k_x - \partial_y\right)\phi_B = \left(\frac{\varepsilon}{\eta v_F}\right)\phi_A, \quad (16)$$

$$\left(k_x + \partial_y\right)\phi_A = \left(\frac{\varepsilon}{\eta v_F}\right)\phi_B, \quad (17)$$

Now, we can apply operator $\left(k_x + \partial_y\right)$ to Eq.(16) and by using Eq.(17), we can arrive at the second order partial differential equation:

$$\left(\eta v_F\right)^2\left(k_x^2 - \partial_y^2\right)\phi_B = \varepsilon^2\phi_B. \quad (18)$$

The unstrained GNRs with zigzag edges support two different states such as surface waves (edge states) which exist at or near the edge and confined modes. Thus, we write the energy spectrum of the nanoribbons near the edge as:

$$\varepsilon_{n\pm}^{z} = \pm\sqrt{\left(\eta v_F\right)^2\left(k_x^2 - z^2\right)}, \quad (19)$$

where z is a real number which follows the solution of:

$$\exp(-2zL) = (k_x - z)/(k_x + z). \quad (20)$$

For $z = ik_n$, the transcendental Eq.(20) becomes

$$k_x = k_n\cot(k_n L), \quad (21)$$

and the energy spectrum of GNR for confined modes is given by

$$\varepsilon_{n\pm}^{zc} = \pm\sqrt{\left(\eta v_F\right)^2\left(k_x^2 + k_n^2\right)}, \quad (22)$$

Also the wavefunctions $\phi_A(y)$ and $\phi_B(y)$ for GNR with zigzag edge is given by

$$\phi_A = \frac{2iN}{\varepsilon_{n\pm}^{zc0}}\left\{k_x\sin(k_n y) - k_n\cos(k_n y)\right\}, \quad (23)$$

$$\phi_B = 2iN\sin(k_n y). \quad (24)$$

Since the wavefunctions do not admix the valleys for zigzagGNR, we assume $\left\langle\phi_A'(y)|\phi_A'(y)\right\rangle = \left\langle\phi_B'(y)|\phi_B'(y)\right\rangle = 0$ and apply the normalization condition $\left\langle\phi_A(y)|\phi_A(y)\right\rangle + \left\langle\phi_B(y)|\phi_B(y)\right\rangle = 1$ to find the constant N as:

$$|N|^2 = \frac{k_n\left(\varepsilon_n^{zc}\right)^2}{\tilde{\kappa} + 4k_n\left(k_n^2 L - k_x\sin^2(k_n L)\right)}, \quad (25)$$

where

$$\tilde{\kappa} = \left(k_x^2 - k_n^2 + \left(\varepsilon_n^{zc0}\right)^2\left\{2k_n L - \sin(2k_n L)\right\}\right) \quad (26)$$

At $k_x = 0$, Eqs.(23) and (24) can be written as

$$\phi_A = \mu\frac{i}{\sqrt{L}}\cos\left[\frac{(2n+1)\pi y}{2L}\right], \quad (27)$$

$$\phi_B = \mu\frac{i}{\sqrt{L}}\sin\left[\frac{(2n+1)\pi y}{2L}\right], \quad (28)$$

Where $n = 0, 1, 2\Lambda$. The wavefunctions and eigenvalues of the unstrained zigzag GNRs are shown in Figs. 1(i) and (ii).

For strained GNRs, we can apply the operator

$$\left(k_x + \partial_y + \frac{\beta}{a}\varepsilon_{xx} + \frac{eB}{\eta}y\right)$$

from left on (14) and the operator

$$\left(k_x - \partial_y + \frac{\beta}{a}\varepsilon_{xx} + \frac{eB}{\eta}y\right)$$

from left on (15) and cast these two coupled Eqs.(14) and (15) in two decoupled equations for sublattices A and B as:

$$(\eta v_F)^2\begin{bmatrix} -\partial_y^2+\left(\frac{\beta}{a}\right)^2\varepsilon_{yy}^2+\left(\frac{eB}{\eta}\right)^2 y^2+\frac{\beta}{a}\left(\partial_y\varepsilon_{yy}-\varepsilon_{yy}\partial_y\right) \\ +\frac{eB}{\eta}\left(\partial_y y-y\partial_y\right)+k_x^2+2\frac{\beta}{a}\varepsilon_{yy}k_x+2\frac{eB}{\eta}k_x y \\ +2\frac{\beta eB}{a\eta}\varepsilon_{yy}y+\frac{1}{4}\left(\frac{g_0\mu_B B}{\eta v_F}\right)^2 \end{bmatrix}\phi_B=\varepsilon^2\phi_B, \quad (29)$$

$$(\eta v_F)^2\begin{bmatrix} -\partial_y^2+\left(\frac{\beta}{a}\right)^2\varepsilon_{yy}^2+\left(\frac{eB}{\eta}\right)^2 y^2-\frac{\beta}{a}\left(\partial_y\varepsilon_{yy}-\varepsilon_{yy}\partial_y\right) \\ -\frac{eB}{\eta}\left(\partial_y y-y\partial_y\right)+k_x^2+2\frac{\beta}{a}\varepsilon_{yy}k_x+2\frac{eB}{\eta}k_x y \\ +2\frac{\beta eB}{a\eta}\varepsilon_{yy}y+\frac{1}{4}\left(\frac{g_0\mu_B B}{\eta v_F}\right)^2 \end{bmatrix}\phi_A=\varepsilon^2\phi_A, \quad (30)$$

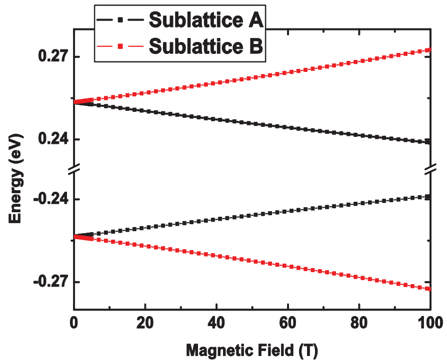

Figure 2: Bandstructures of strained GNRs of sublattices A and B vs magnetic fields. Here we choose the width of the GNR as L=3 $\sqrt{3}$ aN (N=6). The parameters are chosen as: τ_e =-100eV/nm, h_0=1nm and B=1T.

RESULTS AND DISCUSSIONS

The schematic diagram of the two-dimensional graphene sheet in a computational domain is shown in Fig. 1 (upper panel). For strained zigzag GNRs, by coupling strain tensor into the Dirac Hamiltonian through pseudomorphic vector potential, we assume that such strain tensor induce a parabolic confinement potential and thus we apply the Dirichlet boundary conditions at the two boundaries to let the wavefunctions to vanish at the boundary and solve numerically of two decoupled Eqs. (29) and (30) numerically based on finite element method (comsol 3.5). For GNRs considered here, typical numbers of elements depend on grid refinements and exceed 800. We solve the multiphysics problem, ensuring the convergence of the results. In Fig. 1(i), we have plotted the wavefucntions squared vs x for the lowest energy states of zigzag GNRs for $k_x = 0$. For the case $k_x = 0$, the wavefunctions correspond to the nodeless confined states. This is perfectly described by Eqs. (23), (24), (27) and (28). In Fig. 1(ii), we have plotted the band structures of zigzag GNRs and see that the finite width of the GNR breaks the energy spectrum into an infinite set of bands. Here the solid lines show the confined modes and dotted lines show the edge states of the surface waves that have vanishing energy at or near the edge of the zigzag GNRs. Figs. 1(iii) and (iv) correspond to the wavefunctions and the band diagram of strained zigzag GNRs. Here in Fig. 1(iii) we clearly see that the combination of strain tensor with magnetic fields shift the localization of wavfunctions to the zigzag edge. In Fig. 1(iv) we see that the the strain tensor induce opening of the finite band gap at Dirac point. In Fig. 2, we have plotted energy eigenvalues associated to sublattices A and B of electron hole like states vs magnetic field. Here we see that the spin-splitting energy difference enhances with magnetic field. We re-emphasized the importance of the analysis of coupled effects in such complex physical systems as GNRs.

CONCLUSIONS

Based on analytical and finite element numerical results, we have analyzed the band structures of strained and unstrained zigzag graphene nanoribbons in presence of externally applied magnetic field along z-direction. Our focus has been on coupled effects in such complex systems. In particular, we have shown that finite width of the unstrained GNR breaks the energy spectrum into an infinite set of bands. By implementing the contribution of strain tensor in the Dirac Hamiltonian, we have shown that in the combination of strain tensor and external magnetic field act like a shifted parabolic confinement potential. As a result, we have shown that the localization of wavefunctions of electrons move towards the edge of the zigzag boundary. We have also confirmed that the strain tensor induce opening of the finite band gap at Dirac point. Finally in Fig. 2, we have shown that the Zeeman spin splitting energy enhances with magnetic fields in strained GNRs. The developed model and associated methodology can be useful for the analysis of complex physical systems where coupled physical effects are essential.

ACKNOWLEDGEMENTS

The authors were supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada, the Canada Research Chair (CRC) program, and the Bizkaia Talent Grant under the Basque Government through the BERC 2014-2017 program, as well as Spanish Ministry of Economy and Competitiveness MINECO: BCAM Severo Ochoa excellence accreditation SEV-2013-0323.

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