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ABSTRACT

The influence of ripple waves on the band diagram of zigzag strained graphene nanoribbons (GNRs) is analyzed by utilizing the finite element method. Such waves have their origin in electromechanical effects. With a novel model, we demonstrate that electron-hole band diagrams of GNRs are highly influenced (i.e. level crossing of the bands are possible) by two combined effects: pseudo-magnetic fields originating from electroelasticity theory and external magnetic fields. In particular, we show that the level crossing point can be observed at large external magnetic fields ($B \approx 100T$) in strained GNRs, when the externally applied tensile edge stress is on the order of -100 eV/nm and the amplitude of the out-of-plane ripple waves is on the order of 1nm.

1. INTRODUCTION

Graphene is an attractive material for future optoelectronic devices.[1–3] One atom thick graphene sheet is considered purely a two dimensional system that does not possess any band gap at two Dirac points.[1] The measurement of the half integer quantum Hall effect, non-zero Berry phase, as well as the conductivity of electrons in graphene lead to novel applications in carbon-based nanoelectronic devices.[1,4–8] Due to strain engineering achievements for graphene-based optoelectronic devices, it is possible now to predict a small gap opening.[9,10] In this paper we present modeling results demonstrating that the electron-hole band diagrams of GNRs are highly influenced (i.e. level crossing of the bands are possible) by combining these two effects: pseudo-magnetic fields originating from electroelasticity theory and external magnetic fields.

Experimental studies on two dimensional graphene structures predicted that in-plane and out-of-plane ripples waves can vary by several degrees and reach to the nanometer scale.[11] These 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.[9,10] Recently in Ref.,[9] 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. The 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. Furthermore, the authors of this work have investigated the influence of in-plane ripple waves in graphene nanoribbons.[10] In this paper, we continue this line of research and investigate the influence of both in-plane and out-of-plane ripple waves in two dimensional graphene sheets by solving a model based on two dimensional Navier's equations.

2. MATHEMATICAL MODEL

We start from the total elastic energy density associated with the strain for the two dimensional graphene sheet that can be written as[12–14] $2U_s = C_{iklm}\varepsilon_{ik}\varepsilon_{lm}$. 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 representation, the strain tensor components can be written as

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

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where u_i and h are in-plane and out-of-plane displacements, respectively.[13,1516–18] 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[19]

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

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

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

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 tension components. Hence, the coupled Navier equations of electroelasticity can be written as:[12]

$$\left(C_{11}\partial_x^2+C_{66}\partial_y^2\right)u_x+\left(C_{12}+C_{66}\right)\partial_x\partial_y u_y+\frac{1}{2}\partial_x\left[C_{11}\left(\partial_x h\right)^2+C_{12}\left(\partial_y h\right)^2\right]+C_{66}\partial_y\left(\partial_x h\right)\left(\partial_y h\right)+\frac{F_x}{t}=0, \tag{8}$$

$$\left(C_{66}\partial_x^2+C_{11}\partial_y^2\right)u_y+\left(C_{12}+C_{66}\right)\partial_x\partial_y u_x+\frac{1}{2}\partial_y\left[C_{12}\left(\partial_x h\right)^2+C_{22}\left(\partial_y h\right)^2\right]+C_{66}\partial_x\left(\partial_x h\right)\left(\partial_y h\right)+\frac{F_y}{t}=0, \tag{9}$$

where t is the thickness of the single layer graphene, $F_x=\tau_e q\sin\left(qx\right)$ and $F_y=\tau_e q\sin\left(qy\right)$. 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 directions in the plane of two dimensional graphene sheet.[16,20,21] Thus we write Eqs. (8) and (9) as:

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

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

For zigzag GNRs elongated along x-direction and applying tensile edge stress along y-direction, we assume that ε_{yy} is a non-vanishing strain tensor component. Thus, from Eq. (9), we write the strain tensor as:[20]

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

The next step is to analyze the influence of strain tensor on the electronic properties of graphene quantum dots, armchair GNRs and zizag GNRs.

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:[5,22,23]

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

In (13), $P=p-\hbar A_s-eA$ with $p=-i\hbar\partial_x$ being the canonical momentum operator, $\mathbf{A_s}=\left(-\varepsilon_{yy},0\right)\beta/a$ is the vector potential induced by pseudomorphic strain tensor and $\mathbf{A}=B\left(-y,0\right)$ is the vector potential due to applied magnetic field along z-direction.[15,21,24,25] The last term is the Zeeman energy.

For strained graphene nanoribbons with zigzag edge,[26,27] we consider the Hamiltonian model $H\psi=\varepsilon\psi$, where

$\psi(r) = \exp(ik_x x)(\phi_A(y)\ \ \phi_B(y))^T$.[5] Thus the two coupled equations can be written as

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

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

For strained GNRs, we can apply the operator $\left(k_x + \partial_y + \frac{\beta}{a}\varepsilon_{xx} + \frac{eB}{\hbar}y\right)$ from left on (14) and the operator $\left(k_x - \partial_y + \frac{\beta}{a}\varepsilon_{xx} + \frac{eB}{\hbar}y\right)$ from left on (15) and cast these two coupled Eqs. (14) and (15) in two decoupled equations for sublattices A and B as:

$$\begin{aligned}(\hbar v_F)^2\Big[-\partial_y^2 + \left(\frac{\beta}{a}\right)^2\varepsilon_{yy}^2 + \left(\frac{eB}{\hbar}\right)^2 y^2 + \frac{\beta}{a}(\partial_y\varepsilon_{yy} - \varepsilon_{yy}\partial_y) \\ + \frac{eB}{\hbar}(\partial_y y - y\partial_y) + k_x^2 + 2\frac{\beta}{a}\varepsilon_{yy}k_x + 2\frac{eB}{\hbar}k_x y + 2\frac{\beta}{a}\frac{eB}{\hbar}\varepsilon_{yy}y + \frac{1}{4}\left(\frac{g_0\mu_B B}{\hbar v_F}\right)^2\Big]\phi_B = \varepsilon^2\phi_B,\end{aligned} \tag{16}$$

$$\begin{aligned}(\hbar v_F)^2\Big[-\partial_y^2 + \left(\frac{\beta}{a}\right)^2\varepsilon_{yy}^2 + \left(\frac{eB}{\hbar}\right)^2 y^2 - \frac{\beta}{a}(\partial_y\varepsilon_{yy} - \varepsilon_{yy}\partial_y) \\ - \frac{eB}{\hbar}(\partial_y y - y\partial_y) + k_x^2 + 2\frac{\beta}{a}\varepsilon_{yy}k_x + 2\frac{eB}{\hbar}k_x y + 2\frac{\beta}{a}\frac{eB}{\hbar}\varepsilon_{yy}y + \frac{1}{4}\left(\frac{g_0\mu_B B}{\hbar v_F}\right)^2\Big]\phi_A = \varepsilon^2\phi_A.\end{aligned} \tag{17}$$

3. RESULTS AND DISCUSSIONS

In Fig. 1, we present a schematic diagram of the two-dimensional graphene sheet in a computational domain is shown in (upper panel). For strained zigzag GNRs, by coupling strain tensor into the Dirac Hamiltonian through pseudomorphic vector potential, we assume that such strain tensor induces 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 two decoupled Eqs. (16) and (17) numerically based on the finite element method.[28] 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(lower panel), we have plotted the band diagram of strained graphene nanoribbons for electron-hole states vs k_x at $\tau_e = 100eV/nm$, $h_0 = 1nm$ and $B = 65T$. Here we find that the bands are splitted due to externally applied magnetic fields. By considering $k_x = 0$, the interplay between pseudo-spin due to non-vanishing strain tensor and external magnetic fields comes into effect which provides the crossing of the bands in GNRs. In Fig. 2, we have plotted the bandstructures of strained graphene nanoribbons of electron-hole states vs magnetic fields at Dirac point ($k_x = 0$). Here we find that the band splitting of GNRs can be observed at $B \approx 40T$ and the band crossing can also be seen at $B \approx 80T$.

4. CONCLUSIONS

We have developed a mathematical model of equilibrium systems of graphene nanoribbons under external tensions that allows us to investigate the influence of ripple waves in the band diagram of graphene nanoribbons. In Fig. 1, we have shown that the interplay between pseudo-spin, due to non-vanishing strain tensor, and external magnetic fields, provides the level crossing of the bands. In Fig. 2, we have shown that the band splitting and band crossing can be observed at suitably chosen realistic applied magnetic fields. Our findings can be helpful for the design of design of graphene-based straintronic and optoelectronic devices.

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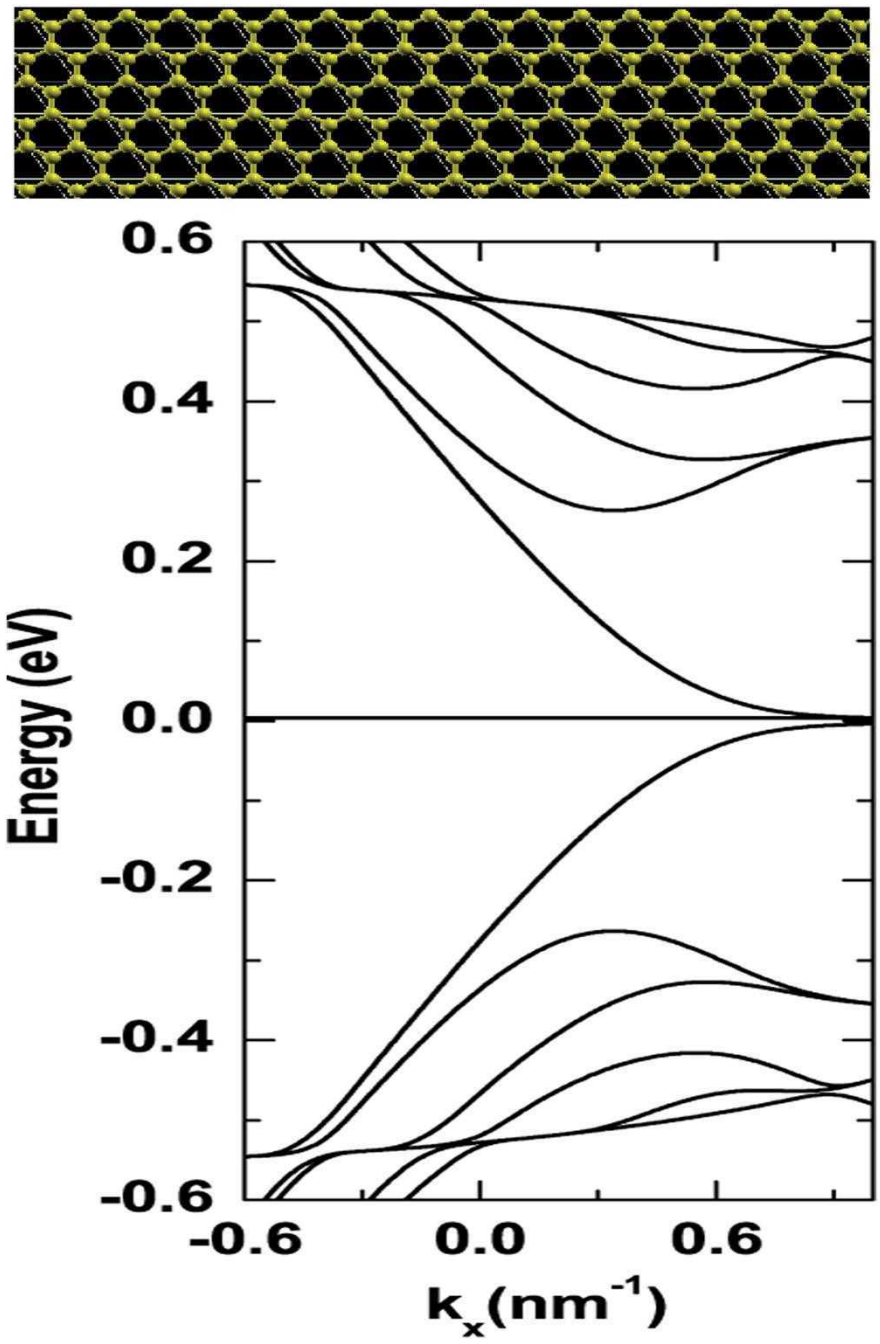

Figure 1. (Upper panel) Schematics of zigzag graphene nanoribbons. (Lower panel) Bandstructures of strained graphene nanoribbons of electron-hole states vs k_x. The parameters are chosen as: $\tau_e = -100eV/nm$, $h_0 = 1nm$, L=$3\sqrt{3}$aN with N=60, a=0.142nm, $\ell = 3.5L$, $\iota = L$ and $B = 65T$. At $k_y = 0$, splitted bands can be seen. Interplay between pseudo-spin, due to strain tensor, and external magnetic fields comes into effect largely at $k_x = 0$ that forced the bands to become degenerate.

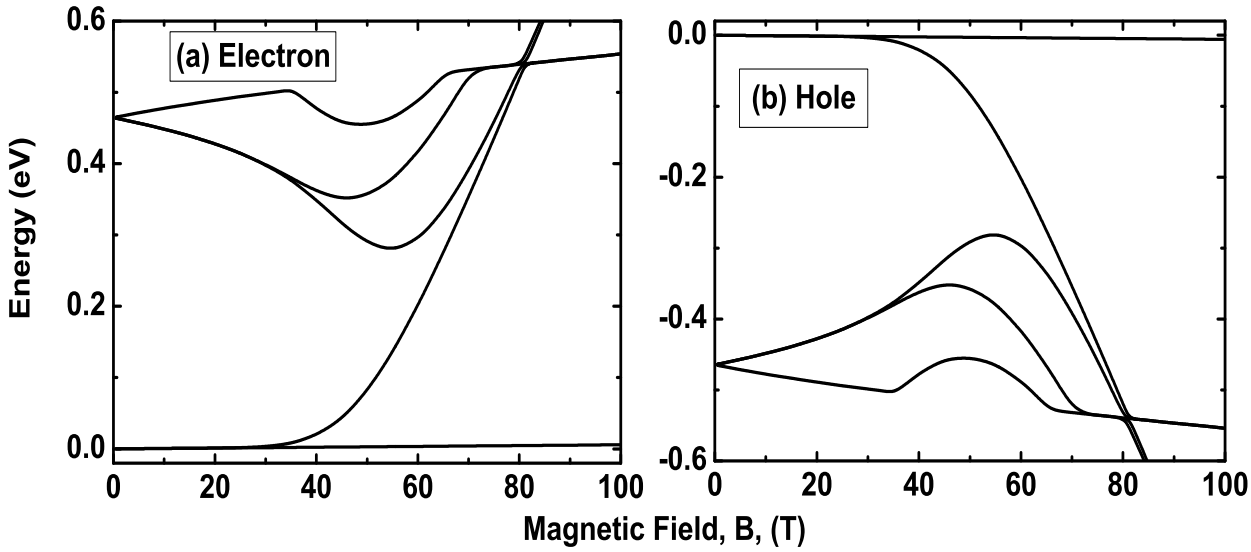

Figure 2. Bandstructures of strained graphene nanoribbons of electron-hole states vs magnetic fields at Dirac point ($k_x = 0$). The bands splitting can be seen at $B \approx 40T$ and the band crossing can be seen at $B \approx 80T$ The parameters are chosen as: $\tau_e = -100eV/nm$, $h_0 = 1nm$, L=$3\sqrt{3}$ 3 a N with N=60, a= 0.142 nm, $\ell = 3.5L$ and $\iota = L$.

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