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Effective mass and band gap of strained graphene

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ABSTRACT

The effective mass of strained graphene is investigated by tight-binding and density-functional theory calculations. For graphene strained in the zigzag direction, we find a strong anisotropy in the effective mass near the gap opening, with an abrupt increase of the effective mass at the critical strain in one direction and a smooth variation perpendicular to it. There is no band-gap opening for isotropic strain, but at an expansive strain of about 28%, the lower edge of the s-band reaches the Fermi level and makes the graphene metallic.

1. Introduction

In graphene, the energy dispersion relation is linear near the Dirac points, which makes the charge carriers in graphene massless and highly mobile [1–3]. While advantageous for electronic devices [4–7], these properties of graphene are also accompanied by the flaw that graphene has no band gap, putting limits to the on-off ratio of any device in the transistor geometry. Different schemes have been put forward to open and tune the band gap, such as using graphene nanoribbons, confining the electrons and holes in them, surface-induced gap opening, controlling the density of electrons, and applying strain and electric field [8–10]. While a band gap of 0.34 eV has been predicted for the single layer graphene between boron nitride layers [11] and for graphene placed on SiO_2 of 0.26 eV [12], these are larger values for the band gap than the 53 meV predicted band gap for graphene on BN [13] resulting from symmetry breaking. A band gap of 0.26 eV has been experimentally determined for graphene on SiC [14], and an even larger band gap found for graphene on MgO [15,16], where again the band gap is believed to be a result of symmetry breaking in the graphene.

In bilayer graphene, the hole mass is found to be 20–30% larger than the electron mass and both the electron and hole mass increase with the density giving hyperbolic bands [17]. Even with transferred graphene and graphene on BN substrates, the effective mass, while small, is found to be finite, in the range of 0.04–0.06 m_e [16,18–20]. There is often a suppression of the conductivity over a wide energy range and delocalization of electrons on opening the gap [21]. So in general, approaches to opening a band gap in graphene to modify graphene from a gapless semiconductor to a semiconductor with a gap also seem to have the effect of turning graphene into fairly ordinary graphite-like material when it comes to conductivity and mobility, although with a band gap.

The creation of a band gap with *strain* has been investigated both theoretically [7,22–26] and experimentally [26–28]. Pereira et al. [22], Gui et al. [23], as well as Naumov and Bratkovsky [25], using a tight-binding approach, were able to show that a band gap open for some types of uniaxial strain but not for isotropic (affine) strain. The effective mass for uniaxially strained graphene, which is really the key parameter in addition to the band gap, has sadly not been really considered in any of the model calculations of the strain induced graphene band gap, with only a few exceptions [24].

The purpose of this paper is twofold. First, we determine the effective mass for uniaxially strained graphene. Second, we have used density-functional theory (DFT) to investigate how the electronic structure of isotropically strained graphene is affected by the s, p_x, and p_y bands. The tight binding (TB) approach is satisfied due to the Hückel character of the electronic structure of graphene, meaning that the behavior near the Fermi level is determined by the p_z orbitals only. This means that all essential electronic parameters, including the effective mass, can be obtained to a fairly

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high accuracy from tight-binding calculations, but it also poses the question whether and how other bands interfere at large strains.

2. Background

The singular nature of the band structure of graphene makes *ab-initio* calculation very cumbersome, because the vicinity of the Dirac point requires a sampling of many *k*-points. An insufficiently dense mesh of *k*-points can give rise to unphysical band gaps in weakly strained graphene. Careful research [1] has shown that the Dirac point is topologically protected and a large uniaxial strain is necessary to open gap [22–25]. In this study, we used the tight-binding method of [1] to calculate the effective mass of graphene strained in the zigzag direction.

Fig. 1(a) shows the considered strain geometry. There are two mechanisms that give rise to changes in the electronic structure. First, the t' bonds (hopping integrals) in the zigzag direction are weakened compared to the t bonds in the armchair direction. Second, the strain changes the bond angles. As discussed in Ref. [1], these two mechanisms have similar effects, and our main focus will be on the ratio t'/t. In this case, a gap opens when t' gets smaller than $t/2$, which happens at a strain ε_o of slightly more than 20% [1]. On a tight-binding level approach to band structure, both the gap and the effective mass (see below) follow from the Hückel-type energy expression,

$$E = \left|t + 2t'\exp(3ibk_y/2)\cos\left(\sqrt{bk_x}/2\right)\right|, \tag{1}$$

where b is the unstrained C–C distance. In the context of our work, it is convenient to write,

$$t' = \frac{1}{2}(1-\eta)t, \tag{2}$$

where $\eta \sim (\varepsilon - \varepsilon_o)$ parameterizes the excess strain beyond the opening of the gap. In more detail, $\eta = -1$ describes unstrained graphene, $-1 < \eta < 0$ means strained graphene without gap, $\eta = 0$ is the point where the gap opens, and $\eta > 0$ corresponds to a band gap $E_g = 2\eta t$.

The physics of the band-gap opening is well understood in the terms of the location of the Dirac points in the Brillouin zone (BZ, Fig. 1(b)). In unstrained graphene, the Dirac points are at the K (and K') points at the boundary of the BZ, but the uniaxial strain shifts the Dirac points towards each other until they meet each other at M. Fig. 2 illustrates this shift by showing $E(k_x, k_y)$ for (a) unstrained and (b) strongly strained graphene.

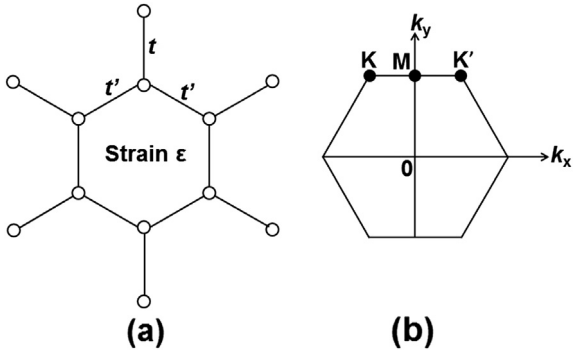

Fig. 1. (a). The uniaxial strain considered in this study. The strain weakens the t' bonds compared to the t bonds and eventually creates a band gap. (b). Brillouin zone of graphene. If t and t' are used to parameterize the strain, it is sufficient to consider the line K–M–K'.

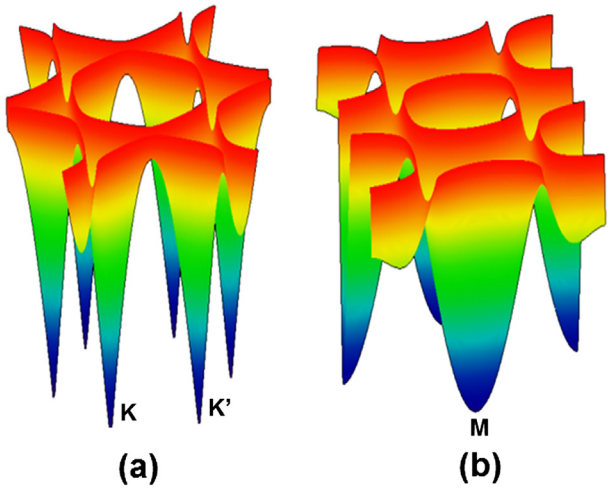

Fig. 2. Energy landscape $E(k_x, k_y)$ for (a) unstrained graphene ($\eta = 0$) and (b) graphene strained beyond the gap opening ($\eta = 0.1$). In unstrained graphene, M is a saddle point, but at the critical strain ($\eta = 0$), K and K' merge into M, and the curvature of the energy minimum at M determines the effective mass.

3. Effective mass

Because uniaxial strain shifts the Dirac points towards each other until they meet each other at M, the effective mass, as a result of the opening of a band gap, is obtained by expanding $E(k_x, k_y)$ around the minimum at the M point:

$$E = \eta t + \frac{3}{8}k_x^2 b^2 t + \frac{9}{8\eta}k_y^2 b^2 t. \tag{3}$$

This yields,

$$m^*_{xx} = \frac{4\hbar^2}{3b^2 t}, \tag{4a}$$

and,

$$m^*_{yy} = \frac{4\eta\hbar^2}{9b^2 t}. \tag{4b}$$

Near the opening of the band gap, the effective mass is strongly anisotropic, $m^*_{xx} \gg m^*_{yy}$. In more detail, m^*_{xx} immediately jumps to a "metallic" value $m_o = 4\hbar^2/3b^2 t$, whereas m^*_{yy} needs substantial excess strain (η) to reach m_o.

For strains less than that necessary for the opening of the band gap, both m^*_{xx} and m^*_{yy} are exactly zero, corresponding to an infinite curvature at the tip of the Dirac cone. Fig. 3 illustrates the physical origin of the theta-function-like transition at the critical strain ($\eta = 0$). Fig. 3 shows the band edges and wave vector dependent band gaps versus energy along the K–M–K' line, that is, along $\mathbf{k} = (k_x, 2\pi/3b)$. Note that the electrons are not allowed to fill the states in the white area between the holes (bright gray) and the occupied states (dark gray). The origin of this "forbidden region" near the M point is seen very easily by putting $k_x = 0$ and $k_y = 2\pi/3b$ in Eq. (1): the corresponding energy, $E = |t - 2t'|$, has no solutions unless $t' = t/2$. The physical reason behind this functional structure of the energy and behind the robust (topologically protected) nature of the Dirac points is well-known, namely the peculiar topology of the honeycomb lattice. This topology (three nearest neighbors always belong to different sublattices) is not easily destroyed by strain.

For strain well beyond that necessary to open up the gap in the band structure at the chemical potential, the tight-binding effective