Conduction gap in graphene strain junctions: direction dependence

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Abstract

It has been shown in a recent study (Nguyen et al 2014 Nanotechnology 25 165201) that unstrained/strained graphene junctions are promising candidates to improve the performance of graphene transistors which is usually hindered by the gapless nature of graphene. Although the energy bandgap of strained graphene still remains zero, the shift of Dirac points in the k-space due to strain-induced deformation of graphene lattice can lead to the appearance of a finite conduction gap of several hundred meV in strained junctions with a strain of only a few per cent. However, since it depends essentially on the magnitude of the Dirac point shift, this conduction gap strongly depends on the direction of applied strain and the transport direction. In this work, a systematic study of conduction-gap properties with respect to these quantities is presented and the results are carefully analyzed. Our study provides useful information for further investigations to exploit graphene-strained junctions in electronic applications and strain sensors.

Keywords: energy gap, graphene, strain, tight binding approach

1. Introduction

In spite of being an attractive material with excellent electronic properties [1], practical applications of graphene in conventional semiconductor devices are still questionable due to its gapless nature. In particular, the ON/OFF current ratio is low while the saturation of current is poor in pristine graphene transistors [2]. Many efforts of bandgap engineering in graphene [11–14, 16] have been made to solve these issues. The pioneer technique proposed [11] is to cut two-dimensional (2D) graphene sheets into one-dimensional (1D) narrow nanoribbons. In 2D graphene sheets, some options such as Bernal-stacking of graphene on hexagonal boron nitride substrate [12], nitrogen-doped graphene [13], graphene nanomesh lattice [14, 15] and Bernal-stacking bilayer graphene [16] have been explored. However, the possibility to open a sizable bandgap in graphene as large as those of standard semiconductors is still very unlikely. In particular, it requires very good control of lattice geometry and edge disorder in narrow graphene nanoribbons (GNRs) [17] and in graphene nanomesh lattices [18], while the bandgap opening in bilayer graphene by a perpendicular electric field may not be large enough for realistic applications [19]. Other methods should be further verified by experiments.

On the other hand, graphene was experimentally demonstrated to be able to sustain a much larger strain than conventional semiconductors, making it a promising candidate for flexible electronics (see in a recent review [20]). For instance, a graphene sheet on an unstretched polydimethylsiloxane substrate can endure and show good recovery of sheet resistance after 6% stretching [21]. On a pre-stretched polydimethylsiloxane substrate, graphene even showed stable sheet resistance up to 11%, and there was only one order change in this resistance up to 25% stretching. Especially, there are two recent works [22, 23] demonstrating techniques to generate extreme strains (>10%) in graphene in a controlled and nondestructive way. Garza et al [22] demonstrated the generation of uniaxial strains by pulling graphene using a tensile-MEMS while Shioya et al [23] achieved both biaxial strained and isotropic compressive strained states of graphene using thin-film-shrinkage methods. Interestingly, strain engineering has been suggested to
be an alternative approach to modulating efficiently the electronic properties of graphene nanomaterials [24]. In particular, the bandgap has periodic oscillations in the armchair GNRs [25], while the spin polarization at the ribbon edges (and also the bandgap) can be modulated by the strain in the zigzag cases. In 2D graphene sheets, a finite gap can open under large strains; otherwise, it can remain close to zero but the Dirac points are displaced [24, 26–29]. Many interesting electrical, optical, and magnetic properties induced by strain in graphene have been also explored; e.g. see [24, 30–38].

In addition, local strain is a good option to improve the electrical performance of graphene devices [24, 39–42]. For instance, it has been shown to enhance the ON current in a GNR-tunneling field effect transistor [39] and to fortify the transport gap in GNR-strained junctions [42]. In a recent work [43], we investigated the effects of uniaxial strain on the transport in 2D unstrained/strained graphene junctions and found that due to the strain-induced shift of Dirac points, a significant conduction gap of a few hundred meV can open with a small strain of a few percent. Note that the mentioned conduction gap is the energy window within which the Fermi energy can be varied and the junction remains insulating. This type of strained junction was then demonstrated to be an excellent candidate to improve the electronic operation of graphene transistors. Hence, it motivates us to further investigate the properties of this conduction gap so as to optimize the performance of graphene devices. On the one hand, the effects of strain should be, in principle, dependent on its applied direction. On the other hand, as a consequence of the shift of Dirac points along the perpendicular axis, the conduction gap is predicted to depend also on the transport direction. These properties of the conduction gap will be clarified fully in the current work.

2. Model and calculations

In this work, the \( \pi \)-orbital tight-binding model constructed in [27] is used to investigate the electronic transport through the graphene-strained junctions schematized in figure 1, where

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**Figure 1.** Schematic of unstrained/strained graphene junctions investigated in this work.

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**Figure 2.** Dependence of graphene bandgap on the applied strain and its direction: tensile (a) and compressive (b). The radius from the central point indicates strain strength ranging from 0 (center) to 30% (edge of maps), while the graphene lattice is superimposed to show visibly the strain direction. The orange circle corresponds to the strains of \( \sigma = 23\% \).
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Conductance (G0 = e2W/hLx) as a function of energy in graphene-strained junctions for σ = 4% with different strain directions. The transport along the armchair direction (ϕ = 0) is considered. The data obtained in a uniformly strained graphene is displayed for the comparison.

Based on this tight-binding model, the two methods described below can be used to investigate the conduction gap of strained graphene part of the structure (see figure 1). Here, we investigate a 2D graphene channel, i.e., the lateral size of unit cells along the Ox direction, Oy axis is parallel (resp. perpendicular) to the transport direction and, e.g., ~ a few tens of nm, as studied in [43]) of the active region. We assume a 1D profile of applied strain, i.e., the strain tensor, is a function of position along the transport direction while it is constant along the perpendicular one. Note that here, Ox (resp. Oy)—axis is parallel (resp. perpendicular) to the transport direction. The transport direction, ϕ, and strain direction, θ, are determined as schematized in figure 1. Based on this tight-binding model, the two methods described below can be used to investigate the conduction gap of strained junctions.

Green’s function calculations. First, we split the graphene sheet into the smallest possible unit cells periodically repeated along the Ox/Oy directions with the indices p/q, respectively (similarly, see the details in [45]). The tight-binding Hamiltonian can therefore be expressed in the following form:

\[ H_{\text{tb}} = \sum_{p,q} \left( H_{p,q} + \sum_{p_i,q_i} H_{p,q \rightarrow p_i,q_i} \right) \]

where \( H_{p,q} \) is the Hamiltonian of cell \( \{p, q\} \), and \( H_{p,q \rightarrow p_i,q_i} \) denotes the coupling of cell \( \{p, q\} \) to its nearest neighbor cell \( \{p_i, q_i\} \). We then Fourier transform the operators in equation (2) as follows:

\[ c_{p,q} = \frac{1}{\sqrt{M_{\text{cell}}}} \sum_{\kappa_x} e^{i\kappa_x p} \hat{c}_{p,x} \]

where \( M_{\text{cell}} \) is the number of unit cells and \( \kappa_x \equiv k_x L_y \) with the size \( L_y \) of unit cells along the Ox direction. The Hamiltonian (2) is finally rewritten as a sum of \( \kappa_x \)-dependent 1D components:

\[ H_{\text{tb}} = \sum_{\kappa_x} \hat{H}(\kappa_x) \]

\[ \hat{H}(\kappa_x) = \sum_p \hat{H}_{p \rightarrow p+1}(\kappa_x) + \hat{H}_{p}(\kappa_x) + \hat{H}_{p \rightarrow p-1}(\kappa_x) \]

With the Hamiltonian in this form, the non-equilibrium Green’s function formalism can easily be applied to compute transport quantities in the graphene-strained junction with different transport directions. In particular, the conductance at zero temperature is determined as:

\[ G(\epsilon_F) = \frac{e^2 W}{\pi h L_x} \int_{BZ} d\kappa_x T(\epsilon_F, \kappa_x) \]

where \( W \equiv M_{\text{cell}} L_y \) and \( T(\epsilon_F, \kappa_x) \) is the transmission probability computed from the Green’s functions. The integration over \( \kappa_x \) is performed in the first Brillouin zone. As in [18], the gap of conductance (conduction gap) is then measured from the obtained data of conductance.

Bandstructure analysis. To determine the conduction gap of strained junctions, we find that another simple way based on the analysis of graphene bandstructures could be efficiently used. It is described as follows. Since the conductance is computed from equation (5), the appearance of a conduction gap is essentially governed by the gaps of transmission probability, which is determined from the energy gaps in the unstrained and strained graphene sections. These energy gaps can be defined directly from the graphene bandstructures. Therefore, our calculation has two steps, similar to that in [43]. From the graphene bandstructures obtained using the tight-binding Hamiltonian above, we first look for the energy gaps \( E_{\text{unstrain}}(\kappa_x) \) and \( E_{\text{strain}}(\kappa_x) \) for a given \( \kappa_x \) of two graphene sections. The maximum of these energy gaps determines the gap \( E_{\text{cond}}(\kappa_x) \) of transmission probability through the junction. Finally, the conduction gap \( E_{\text{cond.gap}} \) is obtained by looking for the minimum value of \( E_{\text{cond}}(\kappa_x) \) when varying \( \kappa_x \) in the whole Brillouin zone.
In particular, the energy bands of strained graphene are given by

\[ E(\vec{k}) = \pm |t_1 e^{i\vec{k} \cdot \vec{a}_1} + t_2 e^{i\vec{k} \cdot \vec{a}_2} + t_3|, \]  

where the plus/minus sign corresponds to the conduction/valence bands, respectively. For a given direction \( \phi \) of transport, in principle, the vectors defining the sizes of unit cells along the \( Ox \) and \( Oy \) directions, respectively, can be always expressed as

\[ \vec{L}_x = n_1 \vec{a}_1 + n_2 \vec{a}_2 \] \[ \vec{L}_y = m_1 \vec{a}_1 + m_2 \vec{a}_2 \]

with 

\[ \cos \phi = \frac{\vec{L}_x \cdot \vec{L}_y}{||\vec{L}_x|| ||\vec{L}_y||} \] \[ \sin \phi = \frac{\vec{L}_x \times \vec{L}_y}{||\vec{L}_x|| ||\vec{L}_y||} \]

while 

\[ \vec{L}^0_{x,y} = \vec{a}_1 \pm \vec{a}_2. \]

Note that \( n_{1,2} \) and \( m_{1,2} \) are integers, while 

\[ \frac{m_1}{m_2} = \frac{n_1 + 2n_2}{n_2 + 2n_1}, \]

i.e., \( \vec{L}_x \cdot \vec{L}_y = 0 \). In other words, we have the following expressions

\[ \vec{a}_1 = \frac{-m_2 \vec{L}_x + n_2 \vec{L}_y}{n_2 m_1 - n_1 m_2}; \quad \vec{a}_2 = \frac{m_1 \vec{L}_x - n_1 \vec{L}_y}{n_2 m_1 - n_1 m_2} \]  

On this basis, the energy bands can be rewritten in terms of 

\[ k_{x,y} = \vec{k} \cdot \vec{L}_{x,y}(\equiv k_x, L_x) \]  

by substituting equations (7) into (6). This new form of energy bands is finally used to compute the conduction gap of strained junctions.

As a simple example, in the case of \( \phi = 0 \) (armchair direction), we calculate the conduction gap as follows. First, equation (6) is rewritten in the form

\[ E_{\phi=0}(\vec{k}) = \pm |t_1 e^{i\vec{k} \cdot \vec{a}_1} + t_2 e^{i\vec{k} \cdot \vec{a}_2} + t_3| \]

with the vectors \( \vec{L}_{x,y} \equiv \vec{L}^0_{x,y} \). Using this new form, the energy

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**Figure 4.** Local density of states (left panels) and corresponding transmission coefficient (right panels) for three different wave-vectors \( k_y \) obtained in an unstrained/strained graphene junction of \( \sigma = 4\% \), and \( \theta \equiv \phi = 0 \). On the top is a schematic of graphene bandedges illustrating the strain-induced shift of Dirac points along the \( k_y \)-direction.
gap of strained graphene for a given $\kappa_y$ is determined as

$$E_{\text{strain}}^{\text{gap}}(\kappa_y) = \frac{1}{2} \sqrt{(t_1 - t_2)^2 + 4t_1t_2 \cos^2 \frac{\kappa_y}{2} + t_3^2}$$

while $E_{\text{unstrain}}^{\text{gap}}(\kappa_y)$ is given by the same formula with $t_1 = t_2 = t_3 \equiv t_0$. The gap of transmission probability through the junction is then determined as $E_{\text{junc}}^{\text{gap}} = \max\{E_{\text{strain}}^{\text{gap}}(\kappa_y), E_{\text{unstrain}}^{\text{gap}}(\kappa_y)\}$ and, finally, the conduction gap is given by $E_{\text{cond}}^{\text{gap}} = \min\{E_{\text{junc}}^{\text{gap}}(\kappa_y)\}$ for $\kappa_y$ in the whole Brillouin zone.

Note that beyond the energy gaps mentioned, transmission through the junctions also depends on the size of the transition zone between unstrained and strained graphene sections. As shown in [42, 43], a short (i.e., smaller than about 5–6 nm) transition zone can have significant effects on the transmission probability; i.e., it can be slightly degraded compared to the case of junctions with a long transition zone. In this work, we mainly focus on the properties of the conduction gap with the assumption that the transition zone is long and hence the mentioned effect is negligible.

### 3. Results and discussion

First, we re-examined the formation of the bandgap of graphene under a uniaxial strain. From equation (9), it is shown that a strain-induced finite-bandgap appears only if $E_{\text{strain}}^{\text{gap}}(\kappa_y) > 0$ for all $\kappa_y$ in the first Brillouin zone, i.e., $\kappa_y \in [-\pi \frac{L_y}{L}, \pi \frac{L_y}{L}]$; otherwise, the bandgap remains zero. Hence, the condition for the bandgap to be finite is either

$$|t_1 - t_2| > |t_3| \quad \text{OR} \quad |t_3| > |t_1 + t_2|,$$

and the corresponding values of the bandgap are

$$E_{\text{gap}} = 2\left(|t_1 - t_2| - |t_3|\right) \quad \text{OR} \quad 2\left(|t_3| - |t_1 + t_2|\right).$$

This result was actually reported in [27, 46]. We remind that, as displayed in figure 2(a), a finite bandgap opens only for strains larger than $\sim 23\%$ and the zigzag (not armchair) is the preferred direction for bandgap opening under a tensile strain [27]. We extend our investigation to the case of compressive strain and find [see in figure 2(b)] that (i) the same gap threshold of $\sigma \approx 23\%$ is observed but (ii) the preferred direction to open the gap under a compressive strain is the armchair, not the zigzag, as is the case of tensile strain. This implies that the properties of graphene bandstructure at low energy should be qualitatively the same when applying strains of $[\sigma, \theta]$ and of $[-\sigma, \theta + 90^\circ]$. This feature can be understood by considering, for example, strains of $[\sigma, \theta = 0]$ and of $[-\sigma, \theta = 90^\circ]$. Indeed, these strains result in the same qualitative changes on the bond-lengths, i.e., an increased bond-length $r_3$ and reduced bond-lengths $r_{1,2}$. However, for the same strain strength, because of the exponential

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**Figure 5.** Maps of conduction gap in unstrained/strained graphene junctions: tensile (a, c) and compressive cases (b, d). The transport is along the armchair $\phi = 0$ (a, b) and zigzag $\phi = 30^\circ$ directions (c, d). The strain strength ranges from 0 (center) to 6% (edge of maps) in all cases.
dependence of hopping energies on the bond-lengths, the compressive strain generally induces a larger bandgap than the tensile one, as can be seen when comparing the data displayed in figures 2(a) and (b). We would like to emphasize again that a large strain is necessary to open a bandgap in graphene. This could be an issue for practical applications, compared to the use of graphene-strained junctions proposed in [43].

We now go to explore the properties of the conduction gap in graphene-strained junctions. In figure 3, we display the conductance as a function of energy computed from equation (5) using the Green’s function technique. As discussed above, a small strain of a few percent (e.g., 4% here) cannot change the gapless character of graphene, i.e., there is no gap of conductance in the case of uniformly strained graphene though Dirac points are displaced as experimentally demonstrated in [28, 29]. However, similar to the result reported in [43], a significant conduction-gap of a few hundreds meV can open in the unstrained/strained graphene junctions. The appearance of this conduction gap, as mentioned previously, is due to the strain-induced shift of Dirac points in a mechanism described as follows. Actually, the bandedges as a function of wave-vector $k_y$ in the $k$-space with the change in the transport direction $\phi$.

![Figure 6](image_url)

**Figure 6.** Map showing the dependence of conduction gap on the directions $(\theta, \phi)$ for $\varepsilon = 4\%$. The top is a diagram illustrating the rotation of Dirac points in the $k$-space with the change in the transport direction $\phi$. The bottom is a diagram illustrating the conduction gap ($\kappa_y = \cos 2\theta \cos 2\phi$, $\kappa_x = \frac{1}{2}$) with respect to the strain, its applied direction, and the direction of transport. Note that due to the lattice symmetry, the transport directions $\phi$ and $\phi + 60^\circ$ are equivalent while the applied strain of angle $\theta$ is identical to that of $\theta + 180^\circ$. Hence, the data obtained for $\phi$ ranging from $-30^\circ$ to $30^\circ$ and $\theta \in [0^\circ, 180^\circ]$ covers the properties of the conduction gap in all possibilities.

In figure 5, we present the maps of conduction gap with respect to the strain and its applied direction in two particular cases where the transport is either along the armchair ($\phi = 0^\circ$) or the zigzag ($\phi = 30^\circ$) directions. Both tensile and compressive strains are considered. Let us first discuss the results obtained in the armchair case. Figures 5(a) and (b) show that (i) a large conduction gap of up to $\sim 500$ meV can open with a strain of 6% and (ii) again the conduction gap is strongly $\theta$-dependent; in particular, its peaks occur at $\theta \approx 47^\circ$ and $137^\circ$ for tensile strain and at $\theta \approx 43^\circ$ and $137^\circ$ for compressive strain. In principle, the conduction gap is larger if the shift of Dirac points in the $k_y$ axis is larger, as in previous discussion about figures 3 and 4. We notice that the strain-induced shifts can be different for the six Dirac points of graphene [47] and the gap is zero whenever one Dirac point is observed at the same $\kappa_y$ in the two graphene sections. From equation (9), we find that the Dirac points are determined by the following set of equations:

$$
\cos \frac{\kappa_y}{2} = \pm \frac{1}{2} \sqrt{\frac{t_1 - (t_1 - t_2)^2}{t_2}},
$$

$$
\cos \frac{\kappa_x}{2} = \frac{t_1 + t_2}{|t_2|} \cos \frac{\kappa_y}{2},
$$

$$
\sin \frac{\kappa_x}{2} = \frac{t_2 - t_1}{|t_2|} \sin \frac{\kappa_y}{2},
$$

which simplify into $\cos \frac{\kappa_y}{2} = \pm \frac{1}{2}$ and, respectively,
\[
\cos \left( \frac{\theta}{2} \right) = \mp 1 \quad \text{in the unstrained case. Hence, the zero con-}
\]
\[
\text{duction gap obtained above satisfies the condition}
\]
\[
\frac{t_1^2 - (t_1 - t_2)^2}{4t_1t_2} = \frac{1}{4},
\]

i.e., there is no shift of Dirac points along the \( \kappa_y \)-axis. Additionally, it is shown that the effects of a strain \( \{\sigma, \theta\} \) are qualitatively similar to those of a strain \( \{-\sigma, \theta + 90^\circ\} \), i.e., the peaks and zero values of conduction gap are obtained at the same \( \theta \) in these two situations. To understand this, we analyze the strain matrix \( M_j(\sigma, \theta) \) and find that in the case of small strains studied here, the relationship between the bond lengths under these two strains is approximately given by

\[
r(\sigma, \theta) - r(-\sigma, \theta + 90^\circ) \approx \sigma (1 - \gamma) \eta_0,
\]

which is \( \theta \)-independent for all \( C-C \) bond vectors. It implies that there is a fixed ratio between the hopping energies \( t_1(\sigma, \theta) \) and \( t_1(-\sigma, \theta + 90^\circ) \) and hence a similar shift of Dirac points happens in these two cases.

Next, we analyze the properties of conduction gap displayed in figures 5(c) and (d) where the transport is along the armchair/zigzag directions considered in (a, b)/(c, d), respectively. The strains \( \sigma_c = -2\% \) and \( \sigma_t = 2\% \) are applied in (a, c) while \( \sigma_c = -1\% \) and \( \sigma_t = 3\% \) in (b, d).
conduction gap for $\phi = 30^\circ$, compared to the case of $\phi = 0$, as mentioned. Again, we found the same qualitative behavior of the conduction gap when applying the strains of $\{\sigma, \theta\}$ and $\{-\sigma, \theta + 90^\circ\}$.

We now investigate the conduction gap with respect to different transport directions $\phi$. We display a $(\theta, \phi)$-map of conduction gap for $\sigma = 4\%$ in figure 6 together with an additional diagram, in the top, illustrating the rotation of Dirac points in the $k$-space with change in transport direction. It is clearly shown that (i) a similar scale of conduction gap is obtained for all different transport directions, (ii) there is a smooth and continuous shift of $E_{\text{cond.gap}}$ with varying $\phi$, and (iii) the same behavior of $E_{\text{cond.gap}}$ is also observed when comparing the two transport directions of $\phi$ and $\phi = 30^\circ$, similar to the comparison for the case of $\phi = 0^\circ$ and $30^\circ$. The data plotted in figure 6 additionally shows that $E_{\text{cond.gap}}$ takes the same value in both cases of $\{\phi, \theta\}$ and $\{-\phi, -\theta\}$ with a remark that the strains of $-\theta$ and $180^\circ - \theta$ are identical. Moreover, the relationship between the values of $\theta$ and $\phi$ at peak or zero conduction gaps is almost linear. For instance, the relationship for conduction gap peaks is approximately given by $\theta = \theta_A - \eta_s \phi$. For tensile strains, $\eta_s$ takes the values of $\approx 1.5667$ and $1.4333$ for two peaks at $\theta_A = 0$ and $90^\circ$, respectively. On the opposite, it is about $1.4333$ and $1.5667$ for $\theta_A = 0$ and $90^\circ$, respectively, in the case of compressive strains. All these features are essentially consequences of the rotation of Dirac points in the $k$-space with respect to the transport direction $\phi$ as illustrated in the diagram on the top of figure 6 and of the lattice symmetry of graphene.

As an alternative, we investigate another kind of strained junctions based on compressive and tensile-strained graphene sheets. The idea is that in this type of strained junction, the shifts of the Dirac points are different in two graphene sections of different strains, which offers the possibility of using smaller strains to achieve a similar conduction gap, compared to the case of unstrained/strained junctions. In figure 7, we display the maps of the conduction gap with respect to the directions of compressive ($\theta_i$) and tensile ($\theta_t$) strains in two cases of transport direction: $\phi = 0$ (armchair) and $30^\circ$ (zigzag) for given strain strengths. Indeed, as seen in figures 7(a) and (b), with smaller strains $\{\sigma_i, \sigma_t\} = \{-2\%, 2\%\}$ or $\{-1\%, 3\%\}$, similar conduction gap of about $310\text{meV}$ can be achieved while it requires a strain of $4\%$ in the unstrained/strained junctions studied above. However, since the shift of the Dirac points is strongly dependent on the direction of applied strains and the transport direction, the properties of conduction gap in this case are more complicated. In particular, our calculations show that the preferred transport directions to achieve large conduction gaps are close to the armchair one. Otherwise, the conduction gap is generally smaller, similarly to the data for $\phi = 30^\circ$ compared to $\phi = 0$, as displayed in figure 7. Additionally, the preferred directions of applied strains for $\phi = 0$ are $\theta_i = \theta_t = 0$ or $90^\circ$.

In addition to the uniaxial strains studied above, we notice that generally, the conduction gap can occur in any strained junction and, of course, is strongly dependent on the type of strain. As an illustration, we display in figure 8 the maps showing the dependence of the conduction gap on the strain and the transport direction for two strain models: pure shear strain [figure 8(a)] and combined uniaxial-shear strain [figure 8(b)]. The strain tensor has the form [26] $M_{ij}^{\text{shear}} = \sigma (\delta_{ii} \delta_{jj} + \delta_{ij} \delta_{ji})$ for shear strains and $M_{ij}^{\text{comb}} = \sigma (\delta_{ii} \delta_{jj} + \delta_{ij} \delta_{ji} + \delta_{ji} \delta_{jj})$ for combined strains. It is shown that compared to uniaxial strain cases, (i) it requires smaller shear (or combined) strains to achieve the same conduction gap and (ii) its dependence on the transport direction is very different. The former is consistent with the fact that the threshold deformation required to achieve a finite bandgap in graphene is lower for shear/combined strains than for a uniaxial strain [26, 27], because the similar difference between the three nearest $C - C$ bond lengths ($\eta_{1,2,3}$) can be obtained with weaker shear/combined strains. Regarding the transport-direction dependence, the shear strain gives a peak conduction gap at $\phi \approx 30^\circ$ (zigzag) and a zero gap at $\phi = 0$ (armchair directions). In contrast, for a uniaxial strain with
\[ \theta = 0, \text{ the conduction gap is zero and maximum for the zigzag and armchair transport directions, respectively. In the case of combined strains, it has a peak at } \phi \approx -20^\circ \text{ and a zero value at } \phi \approx 10^\circ. \] We would like to emphasize an additional point that the ‘bandstructure analysis’ used in this work is a simple and efficient way to calculate the conduction gap in these types of graphene junctions with different strain models.

Finally, we have one remark that, based on the analogy between strain and magnetic field for generating the shift of Dirac points in graphene, one might expect to achieve the same effects by creating a junction of graphene sections having different vector potentials, e.g., using a ferromagnetic stripe on top of graphene. However, previous studies in the literature have shown that to obtain the same effects as with a strain of a few percent, very large magnetic fields, i.e., from a few tenths to hundreds Teslas [36, 48, 49], are required, making it very difficult to be realized in practice. Therefore, the strain could be a more realistic technique to achieve a finite conduction gap in this type of junctions.

4. Conclusion

Based on tight-binding calculations, we have investigated the strain effects on the transport properties of graphene-strained junctions and discussed systematically the possibility of achieving a large conduction gap with respect to the strain strength, its applied direction and the transport direction. It has been shown that due to the strain-induced displacement of Dirac cones away from the \( K \)-point, a finite conduction gap higher than 500 meV can be achieved for a uniaxial strain of only 6%. However, since it is essentially due to the shift of Dirac points along the \( k_x \)-axis, this conduction gap is strongly dependent not only on the strain strength, but also on the direction of applied strain and the transport direction. As an important result of the work, a full picture of these properties of the conduction gap has been presented and explained. The study could be a useful guide and provides an efficient calculation method for the investigation of graphene-strained junctions in electronic applications, e.g., as recently proposed in [43], and for other applications as strain sensors.

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