Strain-induced conduction gap in vertical devices made of misoriented graphene layers

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Abstract

We investigate the effects of uniaxial strain on the transport properties of vertical devices made of two misoriented (or twisted) graphene layers, which partially overlap each other. We find that because of the different orientations of the two graphene lattices, their Dirac points can be displaced and separated in the $k$-space by the effects of strain. Hence, a finite conduction gap as large as a few hundred meV can be obtained in the device with a small strain of only a few percent. The dependence of this conduction gap on the strain magnitude, strain direction, channel orientation and twist angle are clarified and presented. On this basis, the strong modulation of conductance and significant improvement of Seebeck coefficient are shown. The suggested devices therefore may be very promising for improving applications of graphene, e.g., as transistors or strain and thermal sensors.

Keywords: graphene, strain engineering, energy-gap

(Some figures may appear in colour only in the online journal)
modulate the electronic structure of graphene nanomaterials. On this basis, many interesting electrical, optical and magnetic properties induced by strain have been investigated, e.g., see [18–32]. Remarkably, although the slightly strained (i.e., a few percent) 2D graphene remains semimetallic [19], strain has been demonstrated as a technique for strongly improving the applications of some particular graphene channels, for instance, graphene nanoribbons with a local strain [22, 25], has been demonstrated as a technique for strongly improving the applications of some particular graphene channels, for instance, graphene nanoribbons with a local strain and graphene strain junctions [26, 27].

Recently, the interest of the graphene community has also been oriented toward the investigation of twisted graphene few-layer lattices. They are actually few-layer graphene lattices where one layer is rotated relative to another layer by an arbitrary angle and can form a Moiré pattern. These graphene sections are still metallic (similarly, see the detailed explanation in [24, 27]). This feature is also expected to be observed here because the graphene lattices in the left and right sides have different orientations and hence their electronic structures should be, in principle, different when a strain is applied. Moreover, compared to the vertical devices [15] and strain hetero-channels [26, 27] previously studied, the advantages of these devices come from the use of a uniform strain and graphene materials only, which can make it a simple option for the fabrication process.

For the investigation of charge transport in the proposed devices, we employed atomistic tight-binding calculations as in [19, 26, 27, 40, 43]. Here, we assume that: (i) two (bottom and top) graphene sheets partially overlap each other and the transport (i.e., Ox) direction is perpendicular to this overlap section as shown in figure 1; (ii) the top sheet is rotated relative to the bottom one by a commensurate angle \( \theta \); (iii) a uniformly uniaxial strain is applied in the in-plane direction with an arbitrary angle \( \theta \) with respect to the transport direction. The commensurate angles are determined by \( \cos \phi_{12} = (n^2/2 + 3mn + 3m^2)/(n^2 + 3mn + 3m^2) \) [43], where \( n \) and \( m \) are coprime positive integers. The primitive vectors shown in figure 1 are determined as follows: \( \vec{l}_1 = m\vec{a}_1 + (n + m)\vec{a}_2 \) and \( \vec{l}_2 = -(n + m)\vec{a}_1 + (n + 2m)\vec{a}_2 \) if \( \text{gcd}(n, 3) = 1 \); \( \vec{l}_1 = \frac{n}{3} \vec{a}_1 + m\vec{a}_2 \) and \( \vec{l}_2 = -\frac{n}{3}\vec{a}_1 + \left(\frac{2n}{3} + m\right)\vec{a}_2 \) if \( \text{gcd}(n, 3) = 3 \) (where \( \text{gcd}(p, q) \) is the greatest common divisor of \( p \) and \( q \)). The detailed description of the two lattice types corresponding to \( \text{gcd}(n, 3) = 1 \) and 3 can be found in [43]. For simplicity, throughout the work, unless otherwise stated the channel orientation as schematized in figure 1 is considered, i.e., the transport direction is parallel to the vector \( \vec{L}_0 = \vec{l}_1 + \vec{l}_2 \). The strain causes changes in the C–C bond vector \( \vec{r}_{ij} \) according to

\[
\vec{r}_{ij}(\sigma) = \{1 + M_{ij}(\sigma, \theta)\}\vec{r}_{ij}(0)
\]

with the strain tensor

\[
M_{ij}(\sigma, \theta) = \sigma \left[ \begin{array}{c} \cos^2 \theta - \gamma \sin^2 \theta & (1 + \gamma) \sin \theta \cos \theta \\ (1 + \gamma) \sin \theta \cos \theta & \sin^2 \theta - \gamma \cos^2 \theta \end{array} \right]
\]

where \( \sigma \) represents the strain and \( \gamma = 0.165 \) is the Poisson ratio [45]. Taking into account the strain effects, the hopping parameters are adjusted accordingly as in [19], i.e.,

\[
t_{ij}(\sigma) = t_{ij}(0) \exp\left\{-3.37 \left[ \vec{r}_{ij}(\sigma)/\vec{r}_{ij}(0) - 1 \right]\right\}
\]

To compute the transport quantities (transmission probability and conductance) and extract the value of conduction gap, we used the non-equilibrium Green’s function technique and the bandstructure analysis described in [26, 27]. In particular, the conductance is computed from the standard Landauer formula:

\[
G(E_F) = \frac{e^2}{\pi h} \int_{-W}^{W} d\epsilon \int_{-\infty}^{\infty} dE T(\epsilon, k_x) \left[ -\frac{d\rho_F(\epsilon)}{d\epsilon} \right]
\]

where \( W \) is the channel width (i.e., its size along the Oy axis), the transmission probability \( T(\epsilon, k_x) \) is determined from the

![Schematic of vertical graphene devices investigated in this work (middle) and their side view (top). The bottom shows the zoom images showing the nearest-neighbor vectors \( \vec{\tau}_{1,2} \) and lattice vectors \( \vec{a}_{1,2} \) of the bottom (top) layer.](image-url)
In figure 2, we present $E - k_y$ maps showing the main effects of strain on the transmission probability of considered devices in two cases of $\phi_{TL} \approx 21.8^\circ$ (i.e., $n = m = 1$) and $\phi_{TL} \approx 27.8^\circ$ (i.e., $n = 3$, $m = 2$). First, the device remains metallic with a zero conduction gap in the case of unstrained layers (see figures 2((a), (e))). This is because the Dirac cones of graphene sections in the left and right sides are separated at the $k_y$-direction, similarly to what was explained in [27]. Therefore, the transport picture is dramatically changed as shown in figures 2((b),(d),(f)). In figure 2(b), although the Dirac cones are displaced, the device is still metallic with a zero conduction gap. This is essentially explained by the fact that the system is symmetric with respect to the overlap region (i.e., the Oy direction) even when the strain of $3\%$ with $\theta = 0^\circ$ is applied. Because of this symmetry, the Dirac cones of the left and right sides are still located at the same $k_y$-point, which explains the zero gap observed. This symmetry can be broken when the direction of applied strain changes, leading to the opening of a finite conduction gap as seen in figures 2((c),(d),(f)). In the case of $\phi_{TL} \approx 21.8^\circ$, finite gaps of $\sim 240$ meV and $390$ meV are achieved for the strain angles $\theta = 20^\circ$ and $45^\circ$, respectively. When changing the twist angle $\phi_{TL}$, we observed similar properties; however, the value of conduction gap for a given strain is dependent on $\phi_{TL}$. In particular, the gap of $\sim 305$ meV is obsered for the strain $3\%$, $45^\circ$ in the case of $\phi_{TL} \approx 21.8^\circ$ in figure 2(f). Thus, these data show the following important features: (i) the strain can induce a finite conduction gap in the device under study; and (ii) besides the strain magnitude, the gap is strongly dependent on the strain direction and twist angle. Similar features have been also reported in [27] for monolayer graphene strain junctions.

In figure 3, we display pictures showing the properties of conduction gap in the device discussed above with respect to the strain magnitude, strain direction and channel orientation while the twist angle $\phi_{TL}$ is $21.8^\circ$ is fixed. We first discuss the results in figure 3(a) obtained in the $L_0$-case where the transport direction is parallel to $\hat{L}_0 = \hat{t}_1 + \hat{t}_2$ and the strain magnitude $\sigma = 3\%$ is applied. It is shown that the conduction gap is a function of strain direction $\theta$ with two peaks at $\theta \approx \pm 45^\circ$ and zero values for $\theta = 0^\circ$ and $\pm 90^\circ$. The reason why the gap is zero at $\theta = \pm 90^\circ$ is essentially similar to that for which the zero gap is observed at $\theta = 0^\circ$ explained above. Figures 3((b),(c)) present the maps of conduction gap with respect to the strain magnitude and its applied direction in the tensile and compressive cases, respectively. In addition, it is shown that (i) the gap almost linearly increases with the strain magnitude; (ii) for a given magnitude, the compressive strain gives a larger gap than the tensile one; (iii) differently from the strain junctions in [27], both kinds of strain give a similar dependence of conduction gap on the strain direction. Finally, since it is due to the separation of Dirac cones in the $k_y$-axis, the conduction gap will also be dependent on the channel orientation. In figure 3((a), we additionally display the data.
obtained for two other channel orientations \( L_1 \) and \( L_2 \) (see the top-right images), compared to that of \( L_0 \). Note that in the two cases of \( L_{1,2} \), the transport direction is parallel to the armchair direction of the top and bottom layers, respectively, while as mentioned above, it is parallel to the vector \( \vec{L}_0 = \vec{t}_1 + \vec{t}_2 \) in the \( L_0 \)-case. Indeed, our calculations show that in general, a finite conduction gap can always be observed but its dependence on the strain direction is dramatically changed when changing the channel orientation. In particular, as seen in figure 3(a), the \( E_{\text{gap}}(\theta) \) function exhibits two similar peaks and two valleys in all cases but the position of these peaks/valleys strongly depends on the channel orientation.

Next, we explore the properties of conduction gap with respect to the twist angle \( \phi_{TL} \). In figure 4, we display the data obtained for two types of commensurate lattices [43] corresponding to \( \text{gcd}(n, 3) = 1 \) (lattice 01) and \( \text{gcd}(n, 3) = 3 \) (lattice 02). In addition, we consider separately the two regimes of large \( \phi_{TL} \) (>7.3°) in figure 4(a) and small \( \phi_{TL} \) in figure 4(c). In the regime of large \( \phi_{TL} \), we find that the similar \( E_{\text{gap}}(\theta) \) behavior with finite peaks is observed for all cases investigated: \( E_{\text{gap}} \) peaks are at \( \theta \approx \pm 45^\circ \) and zero values at \( \theta = 0^\circ \) or \( \pm 90^\circ \). More interestingly, two types of twisted lattices show opposite trends of conduction gap when increasing the twist angle, \( \phi_{TL} \): \( E_{\text{gap}} \)-peaks increase for the lattice type 02, while they are generally reduced in the case of the type 01. This phenomenon can be explained by the difference in the symmetry of these two lattice types. By way of illustration, we present a diagram in figure 4(b) showing the displacement and separation of Dirac cones of two graphene layers under strain of angle \( \theta = 45^\circ \). The diagram shows that although their displacement is similar for all cases, the separation of Dirac cones of two graphene layers have different behaviors, especially along the \( k_y \) direction. For the lattice type 02, this separation tends to increase when increasing the twist angle, while it reduces for the lattice type 01. These properties basically explain the results obtained.

In the regime of small \( \phi_{TL} \), we find as shown in figure 4(c) another trend of \( E_{\text{gap}}(\theta) \) in the case of lattices 01,
i.e., $E_{\text{gap}}$ quite surprisingly reduces around $\theta = \pm 45^\circ$ when decreasing $\phi_{TL}$, in contrast with the results obtained for large $\phi_{TL}$ in figure 4(a). This feature can be explained as follows (see also the diagrams in figure 4(d)). First, let us remember that (i) each graphene layer has two Dirac cones in the first Brillouin zone and (ii) the value of conduction gap is basically proportional to the smallest distance $\Delta k_y^D$ between Dirac cones of two layers in the $k_y$-axis, i.e., between the red and blue symbols in the first Brillouin zone schematized in the top diagram of figure 4(d) (similarly, see the detailed discussion in [27]). At $\theta = -90^\circ$ (similarly, at $\theta = 0^\circ$ or $90^\circ$), $\Delta k_y^D = 0$ and the gap is hence zero. When $\theta$ increases from $-90^\circ$, $\Delta k_y^D$ and, thus, $E_{\text{gap}}$ increase. The peak of $E_{\text{gap}}$ around $\theta = 45^\circ$ and its reduction when tuning $\theta$ from $45^\circ$ to $0^\circ$ are simply a consequence of the fact that the movement of Dirac cones changes its direction and the behavior of $\Delta k_y^D$ is reversed (i.e., from increasing to decreasing) around $\theta = 45^\circ$. These properties are observed in the cases of large $\phi_{TL}$ displayed in figure 4(a) but another peculiar feature appears in the cases of small $\phi_{TL}$: when the strain-induced displacement of Dirac cones is large enough, situations (1) and (2) (see the middle and bottom diagrams of figure 4(d)) can occur. In situation (1), the Dirac cone of the first Brillouin zone can reach its edge and then enter the second zone. Simultaneously, the Dirac cone of the second zone moves in the opposite direction to the first one. In situation (2), the two Dirac cones in the first Brillouin zone move in the opposite directions to the point of $k_y = 0$ and then exchange their places. Both situations can change the behavior of $\Delta k_y^D$ from increasing to decreasing or vice versa. Note that these situations occur only in the cases where the size of the Brillouin zone is small. That is exactly the case of small $\phi_{TL}$ considered here where the size of primitive cells is large. For instance, when increasing $\theta$ from $-90^\circ$ to $-45^\circ$, the behavior of $E_{\text{gap}}$ suddenly changes from increasing to decreasing as shown for $\phi_{TL} = 5.08^\circ$, $3.89^\circ$.

Figure 3. (a) Conduction gap as a function of strain direction ($\varepsilon = 3\%$) with different channel orientations $L_{0,1,2}$ (see the top-right images). The twist angle $\phi_{TL} \approx 21.8^\circ$ is considered here. The bottom shows the maps of conduction gap in the $L_0$-case with respect to the ((b) tensile and (c) compressive) strain and its applied direction. In these maps, the radius from the central point represents the strain magnitude ranging from 0 (center) to 4% (edge).
2.88° and 2.45° in figure 4(c). This is essentially because situation (1) occurs. In the case of 2.45°, the valleys of $E_{\text{gap}}$ around $\theta = \pm 45^\circ$ are observed because the situation (2) also occurs. Note that, in the case of lattices 02, because both the maximum displacement of Dirac cones along the $k_y$-axis and the size of the Brillouin zone tend to reduce when decreasing $\phi_{TL}$, the features discussed above are not observed. The evolution of maximum values of $E_{\text{gap}}$ when changing $\phi_{TL}$ is summarized in figure 5. When decreasing $\phi_{TL}$, the maximum value of $E_{\text{gap}}$ decreases monotonically for lattices 02 while it has a peak but also tends to zero for lattices 01. On this basis, it is suggested that to safely achieve a finite conduction gap without requiring good control of the twist angle, designing devices with $\phi_{TL}$ around/close to 30° should be a good option.

**Figure 4.** Conduction gap as a function of the strain direction of different twist angles $\phi_{TL}$: large $\phi_{TL}$ (a) and small $\phi_{TL}$ (c). (b) Diagram illustrating the strain-induced displacement of Dirac cones away from the $K$-point in the case of $\theta = 45^\circ$. Open (filled) squares denote the Dirac cones of the bottom (top) graphene layers. Two lattice types 01 and 02 (see text) are considered and, everywhere, the strain $\sigma = 3\%$ is applied. (d) Diagram showing the pictures of the movement of Dirac cones along the $k_y$-axis when changing the strain (see text). The red and blue colors distinguish the Dirac cones of two different layers. Filled and empty symbols show the position of Dirac cones in the first and second Brillouin zones, respectively.

**Figure 5.** Evolution of maximum values of conduction gap presented in figure 4 with respect to the twist angle $\phi_{TL}$. 
Now, we would like to discuss some possible applications of this type of hetero-channel. First, the devices can be used to improve the performance of graphene transistors with the advantage of utilizing a uniform strain and graphene materials only, compared to the vertical devices [15] and strain hetero-channels [26] previously studied. Indeed, as shown in figure 6(a), with a significant conduction gap, these devices can exhibit a very high ON/OFF current ratio, i.e., up to a few ten thousands for a small strain of only 4%. The twist angle is $\phi_{TL} \approx 21.8^\circ$ and $\theta = 45^\circ$. $G_0 = e^2/\hbar L_y$.

Finally, we would like to make some additional remarks. First, in this kind of device, the overlap region between the two layers can have important effects on the transport properties. As in the study on vertical structures with Bernal stacking [44], the size of this region determines, on the one hand, the coupling strength between layers and, on the other hand, the confinement effects (see figure 2) because the electronic structure in the bilayer region is very different from that of the left and right monolayer graphene sections. However, our calculations show that the change in the size of this overlap region does not dramatically change the ON-current (i.e., beyond the gap) except that it can give rise to peaks and shallow valleys in the conductance as seen in figure 6. Second, we would like to point out that besides the use of a uniform strain, the vertical devices studied here have the additional advantage of being able to achieve the same values of conduction gap as the unstrained/strained graphene junctions in [27], but with smaller strain. For instance, a strain of $\sim 4\%$ is enough to achieve a conduction gap of $\gtrsim 500 \text{ meV}$, while a strain of $\gtrsim 6$-$7\%$ is required in the latter channels. This improvement comes from the fact that the Dirac cones are displaced by strain in both the left and right graphene sections, while in strained/unstrained junctions, the displacement of Dirac cones occurs only in the strained graphene section. Similar improvement can be achieved in channels made of differently strained graphene lattices, e.g., compressive/tensile strained junctions [27]. However, the control of this complicated strain profile may be a practical issue. Third, besides the case of uniform strains studied here, similar effects can still be obtained in these devices if the strain is applied to only one layer or two different strains to two layers [51]. In such cases, the properties of $E_{\text{gap}}$ should, of course, be strongly dependent on the strain configurations.

In conclusion, we have investigated effects of uniaxial strain on the transport properties of vertical devices made of two misoriented (twisted) graphene layers. It was shown that strain can induce the displacement of Dirac cones of both layers and because of their different orientations, these Dirac cones can be separated in the $k$-space. As a consequence, the device channel can be tuned from metallic to semiconducting by strain. A conduction gap larger than 500 meV can be achieved in the device with a small strain of only $\sim 4\%$. The dependence of this conduction gap on the strain magnitude, strain direction, channel orientation and twist angle has been clarified. The twist angle $\phi_{TL} \approx 30^\circ$ is a good option for a large conduction gap, which is less sensitive to the different types of twisted layers. On this basis, an ON/OFF current ratio as high as a few thousands and a strong improvement of Seebeck coefficient can be achieved. The study has hence demonstrated that these vertical devices are very promising for enlarging the applications of graphene in transistors, strain sensors and thermoelectric devices.

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