Electronic structure of defected trilayer graphene

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ABSTRACT
Gated trilayer graphene shows energy gap and three topologically protected gapless states when the stacking order changes from ABC to CBA. Here we investigate such a trilayer, but with a part of the internal layer cut and removed forming a region in trilayer built of only two not connected single graphene layers. We demonstrate that the electronic structure of this region is almost the same as of the gated trilayer. Curiously, the topological gapless states that appear due to difference in the stacking order of the adjacent trilayers localize mostly in these single graphene layers. Thus, strong disorder in the internal layer of gated trilayer graphene does not lead to destruction of its fundamental electronic properties.

KEYWORDS
Multilayer graphene; topological states

1. Introduction

Multilayer graphene systems are intensively investigated in the search for tunable energy gap [1–3], which is important for electronic applications of graphene. Different electronic properties of multilayers are achieved by gating and proper stacking arrangements of layers. Of special interest are systems containing various stackings, i.e., stacking domain walls that give rise to novel transport properties of graphene multilayers [3–6]. Multilayers focus also attention due to superconductivity discovered recently in moiré superlattices with twisted layers [7–9].

Gated trilayer graphene (TLG) opens energy gap in the ABC stacking [10, 11]. Very recently it has been shown that when TLG contains the ABC/CBA stacking domain wall, three topological valley-protected states appear in the energy gap, connecting the conduction and valence band continua [12]. Such states, which occur also in gated bilayer with AB/BA stacking domain wall [13–17], can provide one-dimensional currents along defined directions and thus can be useful in graphene-based electronics [18–21].

If a strip of the internal layer is cut along the zigzag direction and removed, one gets a TLG with a part built of only two disconnected single graphene layers (2SGL), as shown in Fig. 1. In this paper we investigate the electronic structure of 2SGL. We demonstrate that its spectrum is similar to the energy spectrum of gated trilayer with ABC/CBA stacking domain wall: it exhibits energy gap separating the conduction

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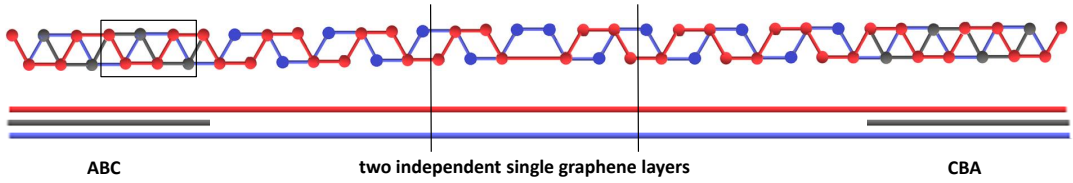

Figure 1. Top: schematic representation of the investigated trilayer graphene with a part of internal layer (grey) cut and removed. The system extends to infinity in the horizontal (armchair) direction and is periodic in the vertical (zigzag) direction. Bottom: schematic horizontal view along the armchair direction. Black solid lines mark the region of two disconnected layers (red and blue), where the LDOS is calculated. Black rectangle shows the example of four-atom unit cells of each layer used for calculation of the layer-resolved local density of states.

and valence band continua and two topological states in the gap. It means that the electronic structure of the adjacent trilayers is induced in the 2SGL. Surprisingly, the gap states are largely localized in the region of 2SGL. This suggests that the main features of gated TLG with stacking domain walls, important for its electronic applications, are robust to deformations and defects in the internal layer.

2. Model and Methods

The investigated trilayer graphene is schematically shown in Fig. 1. The width of the defected region, i.e., the 2SGL strip, is $W = 7$, measured in the units of graphene primitive unit cells. Thus, the pristine graphene trilayers on the left and right sides of the 2SGL are separated by 2.82 nm. The ABC/CBA stacking change in the trilayers is achieved by different lengths of the top and bottom layers of 2SGL. The system is infinite in both, the armchair and zigzag directions, but is periodic only in the zigzag direction.

We work in the π-electron tight binding approximation. Intra-layer and inter-layer hopping parameters $\gamma_0 = 2.7$ eV and $\gamma_1 = 0.27$ eV are used, respectively [22, 23]. Only the neighbor layers in TLGs are connected by γ_1; the outer layers are not connected. Voltages $-V$ and $+V$ are applied to the top and bottom layers, respectively. Two values of V are considered, $V = 0.1$ and $V = 0.5$ eV, because as demonstrated in [12, 24] the gapless states localize in different layers depending on the value of V vs γ_1.

Local density of states (LDOS) is calculated in the central part of the 2SGL, marked in Fig. 1 by two vertical solid lines. The width of the region where the LDOS is calculated equals two graphene unit cells, i.e., 0.8 nm. The LDOS is compared to the density of states calculated in the wider region that contains 2SGL and two adjacent strips of trilayers on the right and left side of 2SGL, i.e., in the entire structure shown at the top panel of the figure. To distinguish this density of states from the LDOS we call it *the density of states of the system* (SDOS). The LDOS and SDOS are calculated using the surface Green function matching technique [25]. Since TLG is periodic in the zigzag direction the LDOS and SDOS are k-dependent, where k is the wavevector corresponding to this periodicity. To determine the localization of the gapless states we calculate also the layer-resolved LDOS for individual states at the Fermi level i.e., in the center of the energy gap.

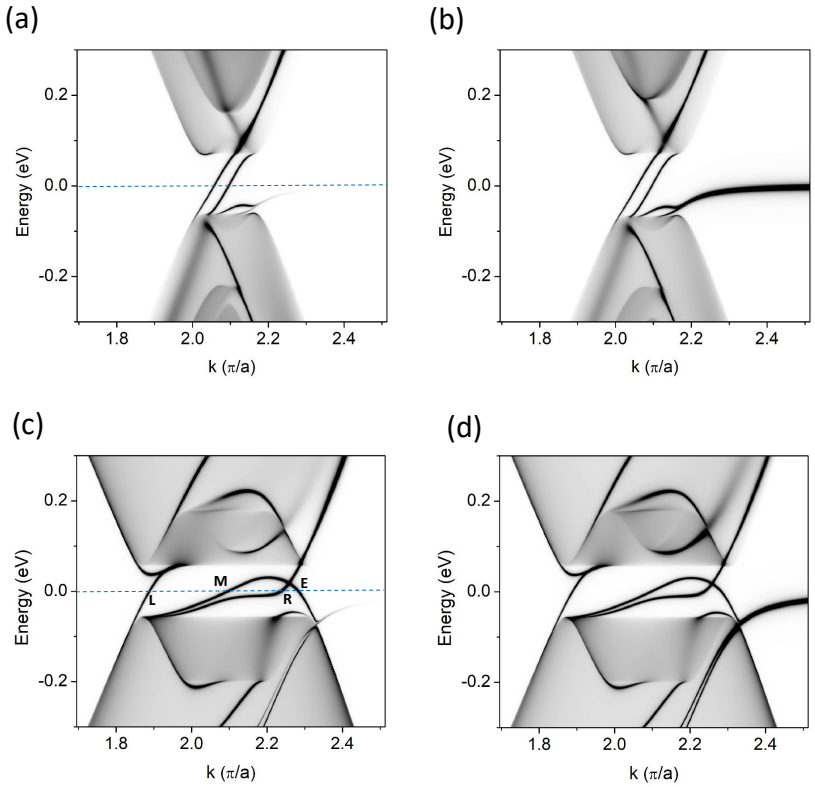

Figure 2. (a) and (c) LDOS calculated in the center of the region of two not connected single graphene layers, marked in Fig. 1 by two solid lines; (b) and (d) SDOS calculated in the entire structure shown in Fig. 1; (a) and (b) - $V = 0.1$ eV, (c) and (d) - $V = 0.5$ eV. The LDOS and SDOS are visualized close to the cones, i.e., close to $E = 0$ and $k = \frac{2}{3}\pi/a$, where a is the period of lengths in the zigzag direction, set here as $a = 1$.

3. Results and discussion

We first consider the case of $V = 0.1$ eV. In Fig. 2 (a) we present LDOS calculated in the very center of the 2SGL strip. For comparison, the SDOS calculated in the entire structure shown in Fig. 1, is presented in Fig. 2 (b).

First, we note the similarity between SDOS and LDOS of the defect-free TLG with the ABC/CBA stacking order change, investigated in Ref. [12]. It contains the valence and conduction band continua separated by the energy gap and two gapless states connecting these continua. One topological gapless state is missing in comparison to the defect-free TLG [12] and this is due to the broken and discontinuous internal layer. Additionally, a couple of energetically almost degenerate zigzag edge states is also visible in the SDOS. These states, which begin at the cone and extend to the Brillouin zone edge at $E = 0$, are due to two zigzag edges of the truncated internal layer [26, 27].

The most striking effect is a remarkable similarity of LDOS to SDOS. Let us recall that LDOS is calculated in the center of the 2SGL, i.e., at two not connected single graphene layers and away from the adjacent trilayers. It means that the energy spectrum of the gated trilayers is induced in the 2SGL. We have checked that the band continua of the LDOS are present also for $W > 7$ but are weakening for large separation of the trilayers. However, the gapless states persist in the region of the energy

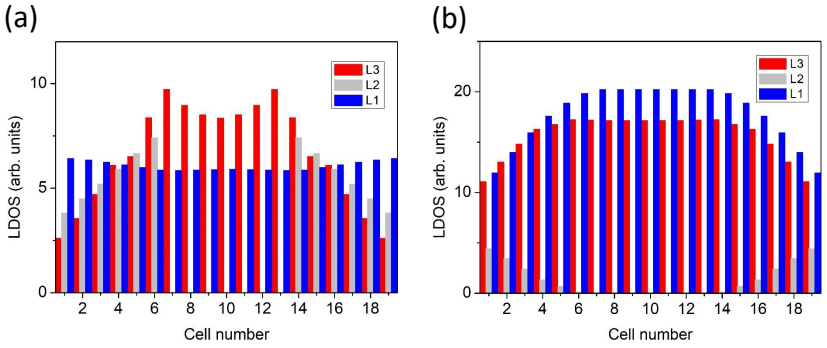

Figure 3. Layer-resolved density distribution of the gapless states (at $E = 0$) shown in Fig. 2 for $V = 0.1$ eV. (a) left state, (b) right state. Vertical bars represent densities calculated at four-atom unit cells (as shown in Fig. 1) in each layer. Lower layer (L1) - blue, middle layer (L2) - grey, upper layer (L3) - red. Six unit cells are taken into account in the left and right TLG, so the 2SGL part starts at cell number 7.

gap, even for very wide 2SGL. Similar effect was observed in Ref. [28] for gated bilayer with a part of one layer cut and removed.

In Fig. 3 the layer resolved densities of both gapless states are presented. They are calculated for k-values corresponding to the Fermi level ($E = 0$), marked in Fig. 2 (a) by points where the blue broken line crosses the gapless states. The left state has the density maximum localized in the top layer of 2SGL with a significant component in the bottom layer [29]. The density maximum of the right state also localizes mainly in the 2SGL and is equally distributed between the top and bottom layers, similarly as the middle gap state in the case of the defect-free TLG [12]. Comparing these densities with the layer-resolved densities of three gapless states present in defect-free TLG with stacking domain wall we can deduce that it is the rightmost gapless state (relating to that case) that disappears due to the disconnected internal layer.

We next consider the case of $V = 0.5$ eV, i.e., $V > \gamma_1$. The LDOS and SDOS are presented in Figs. 2 (c) and (d), respectively. Also for this gate voltage the LDOS is indistinguishable form the SDOS, except the zigzag edge states that appear in SDOS. Similarly as for $V = 0.1$ eV, two gap states connecting the valence and conduction band continua are also present. Comparing this spectrum with the LDOS of defect-free TLG [12] we can deduce that for this gate voltage it is the middle gap state (of the defect-free TLG) that for $k > \frac{2}{3}\pi$ bends down, crosses the right gap state and couples to the zigzag-edge states.

The layer resolved densities of the gap states calculated at the Fermi level are presented in Fig. 4. The left state (L) is localized almost exclusively in the bottom layer with the strong maximum density at the center of 2SGL. The middle gap state (M), similarly as in the case of the defect-free TLG, is almost equally distributed between the bottom and the top layer and is also localized in the 2SGL. The maximum density of the right gapless state (R) is located in the center of the upper layer of 2SGL, with strong component at the zigzag edges of the disconnected internal layer. The middle state, after crossing the right gapless state (E), changes its localization to the upper layer of 2SGL with some contribution at the zigzag edges of the internal layer. We have checked that this contribution becomes dominant when the state couples to the zigzag-edge state at the right side of the valence band continuum.

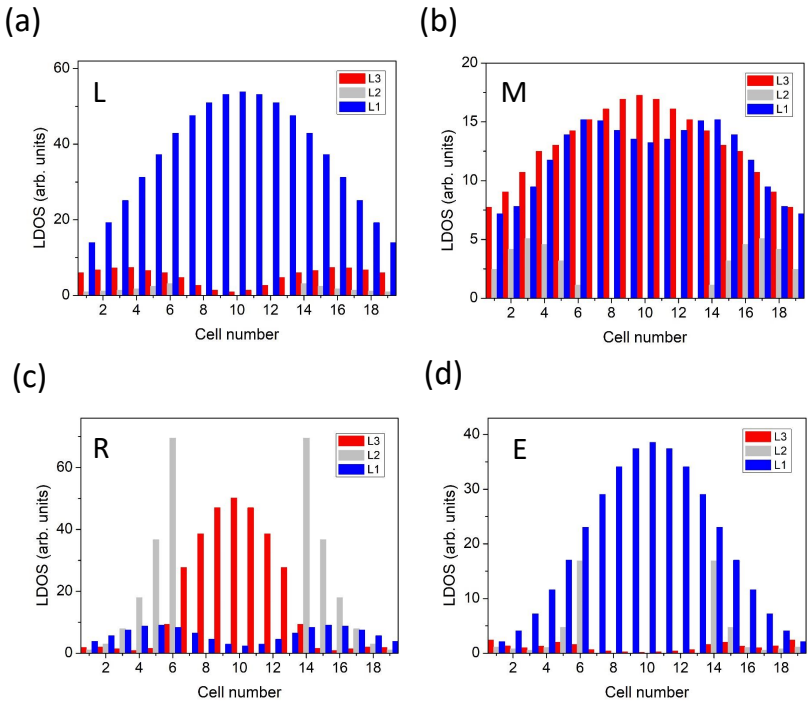

Figure 4. The same as in Fig. 3 but for $V = 0.5$ eV. (a) and (c) - left and right gapless states, respectively. (b) and (d) the third state in the gap that for $k > \frac{2}{3}\pi$ couples to the zigzag-edge states of the middle layer.

4. Conclusions

We have investigated the electronic structure of defected gated trilayer graphene with stacking domain wall ABC/CBA and the wide strip of the internal layer cut along the zigzag direction and removed. The destructed region of TLG consists of two separated single graphene layers, 2SGL. We have calculated the local density of states in the center of 2SGL and demonstrated that it is almost indistinguishable from the DOS of the entire system. Moreover, the electronic structure of defected TLG is not much different from the energy spectrum of defect-free TLG. In particular, two topologically protected gapless states, that appear due to the stacking order change in the trilayers adjacent to 2SLG, are still present and localize mainly in the defected region, i.e., in the single graphene layers. They appear here like *phantom* states, since such states should be absent in the energy spectrum of two disconnected single graphene layers. It means that the main features of the electronic structure of TLG with the stacking order change can persist when its internal layer is strongly defected. This is an important observation that proves that the essential properties of gated TLG with stacking domain wall, important for its electronic applications, are preserved when natural defects and cracks appear in TLG.

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