Strain effects on the electronic properties of devices made of twisted graphene layers

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***Abstract*—The effects of uniaxial strain on the electronic and transport properties of twisted graphene bilayer structures are investigated by means of atomistic simulation. It is shown that the strain-induced modulation of band structure makes it possible to break the degeneracy and to modulate the position van Hove singularities. It is even possible to observe low-energy saddle points for a large range of twist angles. It is shown also that the strain-induced separation of Dirac points of the two lattices may generate a finite transport gap as large as a few hundreds of meV for a small strain of a few percent.**

Keywords—Graphene; Strain; Van Hove singularity; Conduction gap

I. INTRODUCTION

Graphene is one of the most attractive materials for beyond-CMOS electronics because of its specific electronic properties, which are a consequence of its two-dimensional honeycomb lattice and relativistic-like charge carriers at low energy [1]. To enlarge its range of applications, the modulation of electronic structure of graphene nanomaterials has been the subject of intense research. Recently, the interest of the graphene community has also been oriented toward the investigation of twisted graphene multilayer lattices, a specific type of Van der Waals structures of graphene. These lattices appear as promising materials providing various possibility of modulating their electronic properties by changing the twist angle [2-4]. In this work, we investigate the effects of uniaxial strain on the electronic properties of devices based on twisted graphene layers (see Fig. 1) [5,6]. First, we explore the effects of strain on the low-energy bands of twisted graphene bilayer, emphasizing the modulation of the energy position of van Hove singularities. Second, we demonstrate that the strain engineering is an efficient technique to open finite transport gaps in vertical devices made of stacks of twisted graphene layers.

II. MODEL

Our calculations are based on an atomistic nearest-neighbor tight-binding model, including the effect of strain on bond lengths and hopping parameters for interlayer and in-plane couplings following the approach described in [7,8]. A unixial strain is applied in the in-plane direction, i.e., in the O*xy* plane as schematized in Fig. 1 [6]. To compute the charge transport in the ballistic approximation, the tight-binding Hamiltonian is solved using the Green's function formalism [9].

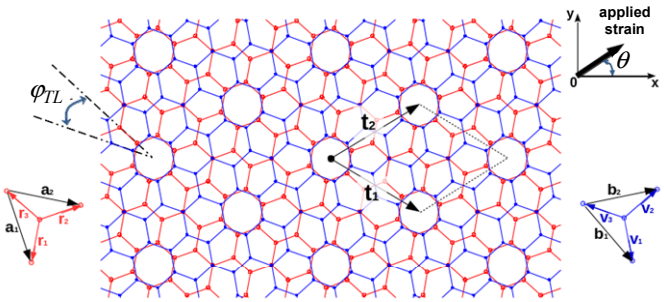

Fig. 1. Twisted graphene bilayer lattice considered in this work. The twist angle is φ_{TL} and a strain is applied with an angle θ with respect to the transport direction O*x*.

III. MODULATION OF VAN HOVE SINGULARITIES

In Fig. 2, we display two sub-figures showing the effects of strain on the low energy bands of twisted graphene bilayer. Interestingly, it is shown that due to the different orientation of the two graphene layers, the strain can break the degeneracy of the bands around the Dirac points. As a consequence, the number of Dirac cones can double (right panel of Fig. 2) and the van Hove singularity points [2] are separated in energy, which is a consequence of the irregularity of hexagons connecting the Dirac cones when strain is applied. It is well illustrated also in Fig. 3 where we plot the low-energy bands along some specific directions of k-space. Three saddle points may be achieved in strained lattices, instead of one without strain. Compared to the unstrained case, some of these saddle points are formed at lower energy and others are formed at higher energy. Besides their dependence on the twist angle, the mentioned phenomena are also dependent on both the strain amplitude and its applied direction. By choosing appropriately the amplitude and direction of strain, this study demonstrates the possibility of observing the van Hove singularities at reasonably low energy, even lower than 0.3 eV, for a large range of twist angles, i.e. for angles larger than 10° [4].

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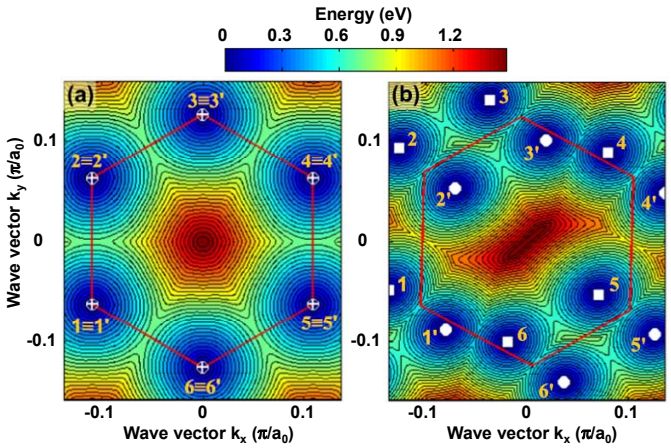

Fig. 2. Map of the lowest positive energy bands of twisted graphene bilayer with a twist angle φ_{TL} = 9.43° (a) without strain and (b) with a strain (σ,θ) = (6%, 20°).

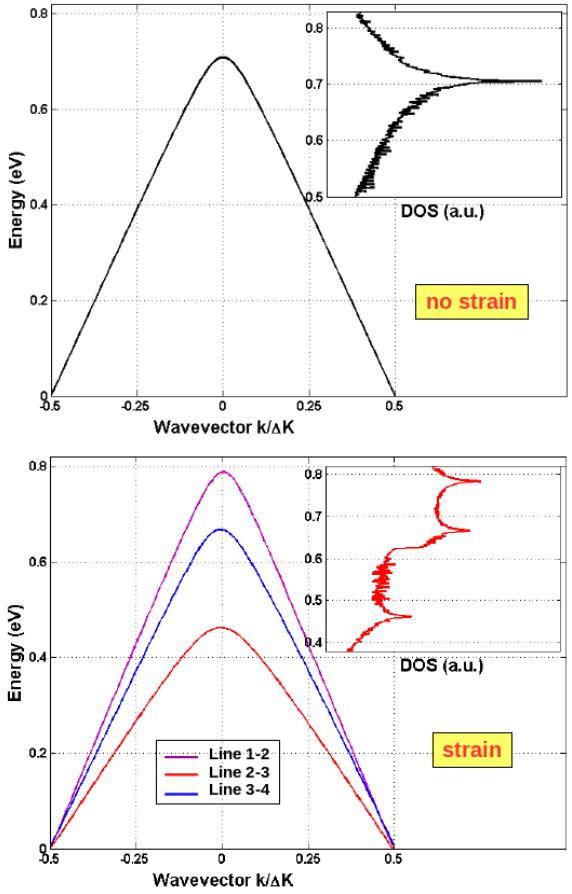

Fig. 3. Profile of conduction bands joining the Dirac points along the lines defined in Fig. 2. The structure and strain considered here are the same as in Fig. 2. The insets show the density of states with clear van Hove singularities.

IV. Conduction Gap

Next, we investigate the effects of strain on the transport properties of vertical devices made of twisted graphene bilayers (see the schematic view on top of Fig. 4) [5].

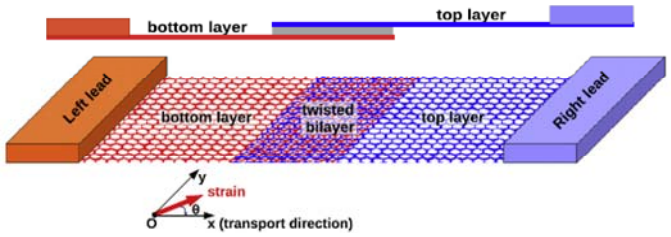

Fig. 4. Schematic side and top view of a vertical device made of two partially overlapped graphene layers.

Again, because of the different orientations of the two graphene layers, the Dirac cones of left and right graphene sections can be separated in the k-space and hence a finite transport gap can appear in this device, as shown in the maps of transmission probability displayed in Fig. 5. This study demonstrates that besides its dependence on strain amplitude, this feature also depends on the twist angle and the strain direction. For the strain angle $\theta = 0$ (Figs. 5(a) and (b)), the strain cannot open any gap because the Dirac cones of both sections are displaced similarly. However, for a strained angle of 20° (Fig. 5(c)) or 45° (Fig. 5(d)), a large transport gap is opened and may reach a few hundreds of meV for a small strain of only a 3%.

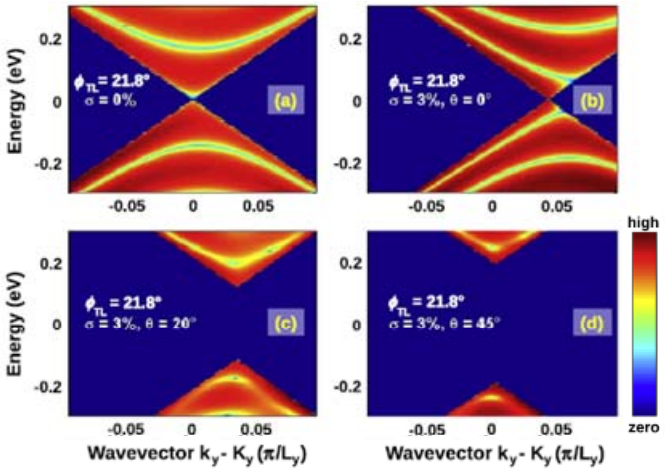

Fig. 5. (E – ky) maps of transmission probability of devices around the Dirac point for different strain angles and amplitudes. The twist angle is φ_{TL} = 21.8°. $L_y = \|\vec{t}_2 - \vec{t}_1\|$ is the size of the unit cell in the Oy direction.

Thanks to this effect, an ON/OFF conductance ratio as high as a few ten thousands is obtained in this device (see Fig. 6). This effect could be used to improve the performance of graphene electronic devices on 2D graphene layers. Compared with strained hetero-devices previously suggested requiring local strain to form a strained/unstrained junction [10], this vertical design offers the practical advantage of working with just a uniform strain over the full device. Additionally, it does not require any nanostructuring strategy as in the graphene nanomesh transistor [11]. Compared to other vertical devices previously demonstrated [12,13], this configuration has the additional advantage to be based on a single type of material.

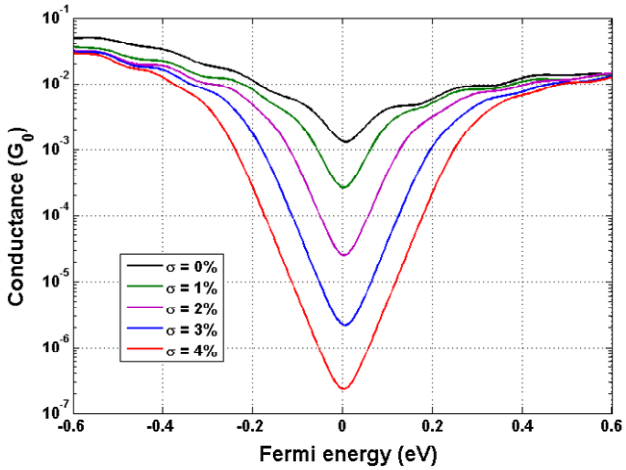

Fig. 6. Room temperature conductance for different strain amplitudes as a function of fermi energy. Parameters: $\varphi_{TL} = 21.8°$, q = 45°, $G_0 = e^2W/hL_y$.

V. Conclusion

The effects of uniaxial strain on the bandstructure and the transport properties of twisted graphene bilayers has been investigated using atomistic simulation including the detailed arrangements of carbon atoms. It has been shown that the strained-induced breaking of degeneracy of the band structure near the Dirac cones may strongly change the energy landscape. It makes it possible to observe van Hove singularities in the density of states at low energy for a wide range of twist angles. Additionally, the strain-induced separation of Dirac points of the two layers can generate a finite transport gap that may reach a few hundreds of meV for a small strain of a few percent, which opens a possible route to improve device performance.

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