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

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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 [2,3]. In this work, we investigate the effects of uniaxial strain on the electronic properties of devices based on twisted graphene layers (see Fig. 1) [4,5]. First, we explore the effects of strain on the low-energy bands of twisted graphene bilayer. Second, we demonstrate that the strain engineering is an efficient technique to open finite transport gaps in vertical devices made of stack of twisted graphene layers.

Our calculations are based on the atomistic tight-binding model, similarly as in [6]. A unixial strain is applied in the in-plane direction (i.e., in the Oxy plane as schematized in Fig. 1). To compute the charge transport, the tight-binding Hamiltonian is solved using the Green's function formalism [5].

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 since the two graphene layers have different orientations, the strain can break 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 (see Fig. 3). 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, our study suggests the possibility of observing the van Hove singularities at reasonably low energy in a large range of twist angle (i.e., larger than 10°) [4].

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]. 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 open in this device (Fig. 4). Our study shows that besides its dependence on strain amplitude, this feature also depends on the twist angle and the strain direction. Important, we find that a finite gap as large as a few hundred meV can be achieved with a small strain of only a few percent (see Fig. 4(d)). On this basis, the ON/OFF current ratio as high as a few ten thousands and high thermoelectric power can be achieved in our proposed devices (see Fig. 5).

In summary, we demonstrate that strain engineering is a promising technique to modulate the electronic properties of twisted graphene bialyer systems and to enlarge their applications, e.g., in transistors, strain and thermal sensors. This can be also a useful approach for Van der Waals structures of other 2D planar materials.

References

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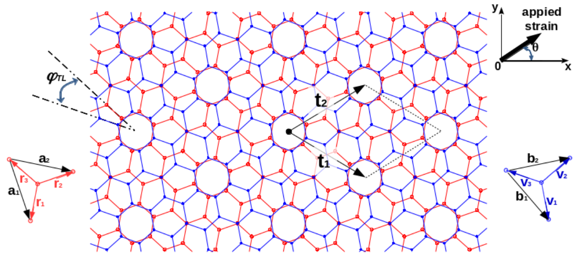

Fig. 1. Twisted graphene bilayer lattice considered in this work. The twist angle is ϕ_{TL} and a strain is applied along the direction θ.

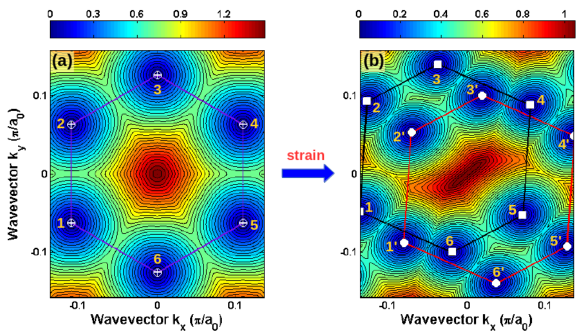

Fig. 2. Strain effects on the low-energy bands around the Dirac point.

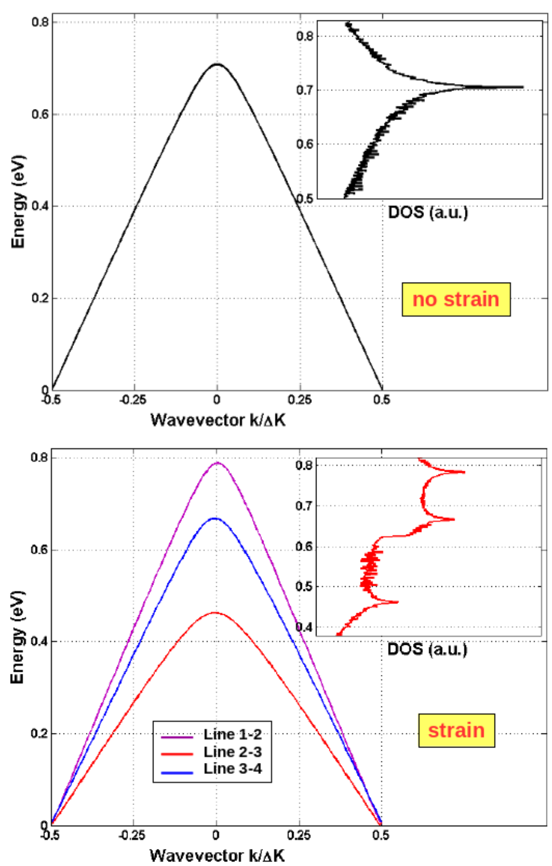

Fig. 3. Strain effects on the bands connecting two Dirac cones and the van Hove singularity points.

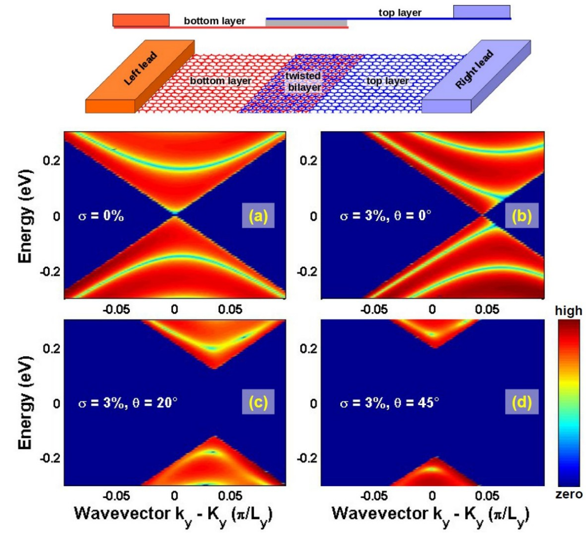

Fig. 4. (E-k_y)-maps of transmission probability showing the strain effects on the transport properties of vertical devices made of a stack of two twisted graphene layers.

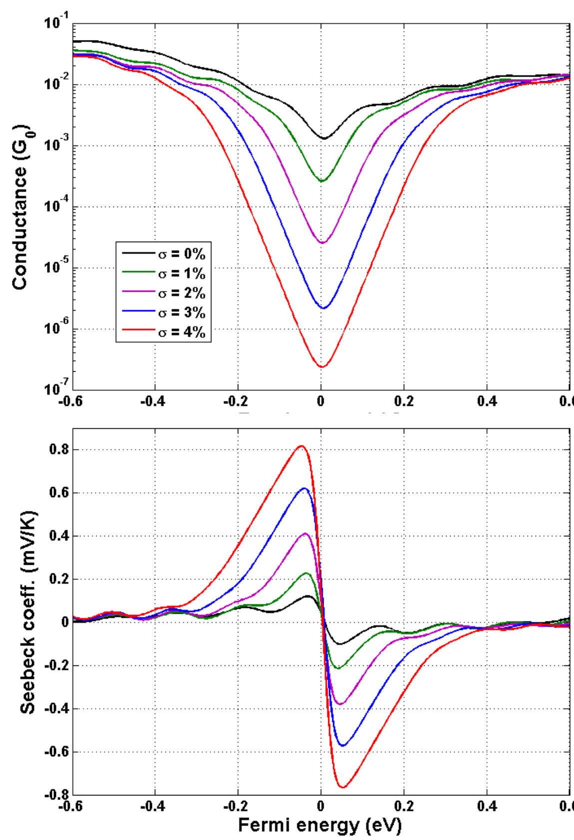

Fig. 5. Strain engineering to improve ON/OFF current ratio and Seebeck coefficient in vertical devices made of a stack of two twisted graphene layers.