Transport properties and applications of disoriented graphene systems: twisted bilayers and grain boundaries

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To modulate the electronic and transport properties of graphene, a very attractive route consists in arranging properly two graphene sections of different orientation. One may think about twisted graphene bilayers [1] and grain boundaries separating two crystalline graphene domains [2]. Strain may be also used as an additional degree of freedom to tune differently the bandstructure of the two sections [3].

In the present work we investigate these different options and their possible applications, by means of atomistic calculations combining Green's functions (GF) and tight-binding (TB) formalisms, and including strain effects [4]. We show in particular the possibility to tune in a wide range the conductance gap, which allows improving the behavior of devices like tunnel diodes and transistors. In the case of polycrystalline graphene we show additionally the possibility to manipulate valley-polarized currents and the optical-like behavior of Dirac particles, even at room temperature.

We first investigated vertical structures made of two disoriented graphene layers that partially overlap each other, as schematized in Fig. 1. We considered both cases of commensurate and incommensurate systems [5]. To include the uniaxial strain effects, the hopping parameters of the TB model were adjusted as described in [6,7].

In commensurate systems, 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 (Fig.2). Hence, a finite gap of transmission (conduction gap) as large as a few hundred meV can be obtained in the device with a small strain of only a few percent. This gap is strongly dependent on the strain amplitude σ, the strain orientation (θ angle) and the rotation angle ϕ between the two layers. In incommensurate systems the misalignment of Dirac cones may appear even without strain and can be enhanced by strain (Fig. 3). Such conduction gap can be used to enhance the performance of graphene FET or the Seebeck coefficient [8].

Systems containing a single grain boundary (GB) separating two graphene domains of different orientations (Fig. 4) may offer similar properties [9]. It may be used for instance to enhance the negative differential conductance in PN tunnel diodes under the effect of uniform strain (Fig.4). A peak-to-valley ratio of 792 has been achieved for a strain of 4% at room temperature.

By looking carefully at the transmission in such GB systems, we can observe that it is modulated differently by strain in the two valleys of graphene D and D' [9]. Indeed the relationship between reflected and incident angles of de Broglie electron waves (see Fig.5) is valley-dependent. In devices as schematized in Fig. 6, this breaking of inversion symmetry may lead to directionally-separated and valley-polarized currents, even at room temperature (Fig. 7). In addition, the refraction index can be modulated electrically and take negative values. It makes it possible to control the valley filtering and the electronic optics properties of polycristalline graphene.

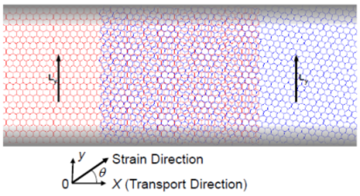

Fig. 1. Schematic of a device made of a vertical stack of misaligned graphene layers.

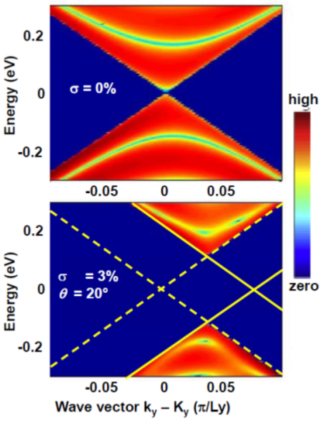

Fig. 2. (E-ky) maps of transmission probability in a particular bilayer structure for two strain configurations.

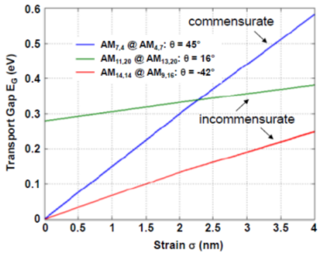

Fig. 3. Strain effects on the conductance gap in different devices with commensurate or incommensurate layers.

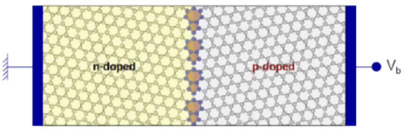

Figure 4. PN tunnel diode made of a grain boundary separating two crystalline graphene domains.

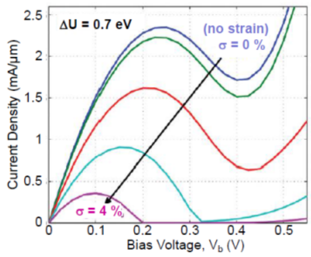

Fig. 4. *I-V* characteristics for different strain amplitudes σ, with strain direction $\theta = 45°$, T = 300 K.

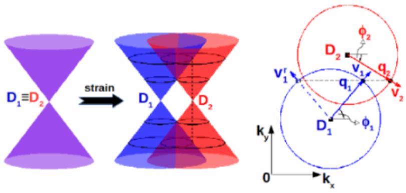

Fig. 5. Diagrams illustrating the strain effects on the band structure of graphene domains and the momentum conservation rule.

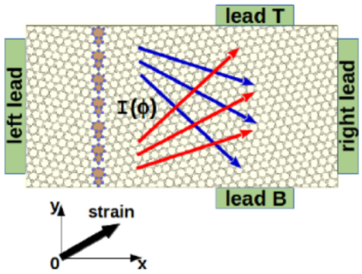

Fig. 6. Schematic view of a multiple electrode device made of a grain boundary system for measuring the directional polarized currents.

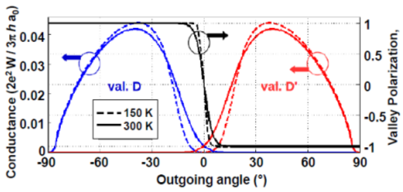

Fig. 6. Conductance (left axis) and valley polarization (right axis) as a function of outgoing angle ϕ_2 for a Fermi level E_F = 0.3 eV and two temperatures.

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