Conduction gap in unstrained/strained graphene junctions: direction dependence

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Graphene has been expected to be an excellent candidate for electronic applications. However, its applications are still limited because of the lack of bandgap between the valence and the conduction bands, making graphene transistors very difficult to have a high ON/OFF current ratio and a good saturation of current. Many techniques to open the bandgap in graphene have been suggested such as cutting a graphene sheet into nanoribbons [1], applying an electric field perpendicular to a bilayer graphene sheet [2], removing periodically some carbon atoms on a pristine graphene sheet to create a nanohole lattice called graphene nanomesh [3] or even stacking graphene sheets on hexagonal boron nitride substrate [4]. In a recent work, it was demonstrated that a small strain of 5% is sufficient to generate a significant conduction gap, i.e. an energy gap of transmission, in unstrained/strained graphene junctions, which makes this kind of junction a very good candidate to improve the performance of graphene transistors [5]. This conduction gap is essentially due to the strain-induced shift of Dirac point and, in principle, is strongly dependent on both the direction of applied strain and the direction of transport. In this work, we have performed a systematical study of the conduction gap and its direction dependences.

A nearest-neighbor tight-binding Hamiltonian was used. The application of a strain causes the following changes in the C-C bond vectors $\vec{r}_i(\sigma)=M_s\vec{r}_i(0)$ [6] with

$$M_s = 1+\sigma\begin{bmatrix}\cos^2\theta-\gamma\sin^2\theta & (1+\gamma)\sin\theta\cos\theta\\ (1+\gamma)\sin\theta\cos\theta & \sin^2\theta-\gamma\cos^2\theta\end{bmatrix}$$

where σ describes the strain and γ = 0.165 is the Poisson's ratio. The hopping parameter linking atoms is defined by $t_i = t_0\exp[-3.37(r_i(\sigma)/r_i(0)-1)]$, where $t_0=2.7eV$ and $r_i(0)=0.142nm$ are the hopping energy and the C-C distance, respectively, in the unstrained case. We consider the conduction gap of the structures schematized in Fig. 1. Our calculations are based on the non-equilibrium Green's function (NEGF) method and the analysis of the bandstructure.

First, our results show that a significant conduction-gap opens in unstrained/strained graphene junctions even with a small strain ranging from 0% to 6%. As shown in Fig. 2, it gets a value of ~ 300 meV for σ = 4%, and can have higher values for larger strains. Moreover, we found that the conduction gap depends strongly on the direction of both applied strain and transport. We display in Fig. 3 a map of conduction gap, in both cases of tensile and compressive strain, as a function of the strain direction θ, for a transport along the armchair direction, i.e. ϕ = 0°. It is shown that the conduction gap is strongly dependent on the strain direction θ. For instance, it is maximum and reaches ~ 450 meV (resp. ~ 500 meV) for $\theta=90°$ and is zero at $\theta=47°$ (resp. 43°) in the case of tensile (resp. compressive) strain. Similarly, the results obtained for the transport along the zigzag direction ϕ = 30° or -30° are presented in Fig. 4. Here, the zero gap appears at $\theta=90°$ while it is maximum for $\theta=47°$ (reps. 43°) in the case of tensile (resp. compressive) strain. For other transport directions, we find that there is a smooth shift of the peaks (zero points) of the conduction gap when the transport direction ϕ varies between armchair (0°) and zigzag (30° or -30°) cases.

We also found that a conduction gap can open in the tensile/compressive strain junctions. Similarly, the gap is strongly dependent on the strength and direction of strains.

To summarize, a systematical study of the conduction gap of unstrained/strained graphene heterojunctions has shown that the gap is strongly

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dependent on the amplitude of strain, on its direction, and on the direction of transport. The study provides a good guide for the strain-induced gap engineering in such junctions likely to improve the performance of graphene transistors.

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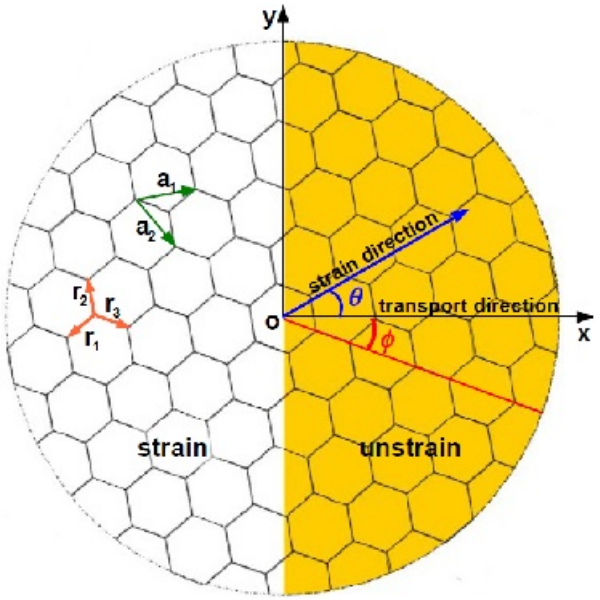

Fig. **1**. Schematic view of unstrained/strained graphene junctions considered in this work.

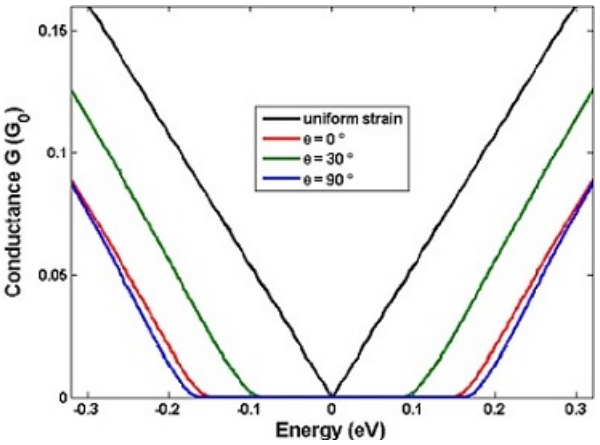

Fig. **2.** Conductance as a function of energy in graphene strain junctions with different strain directions: σ = 4%.

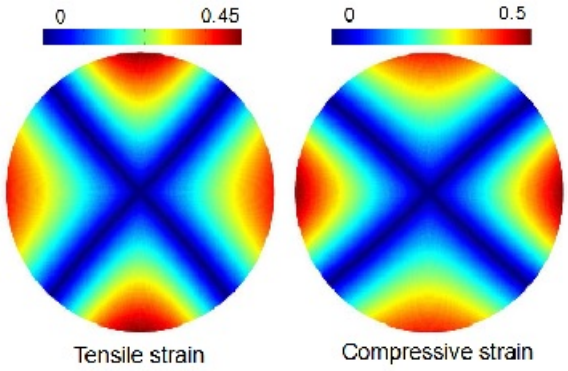

Fig. **3**. Conduction gap (in eV) according to strain angle θ in the case of the transport along the amrchair direction: strain ranges from 0% (center) to 6% (disk edge).

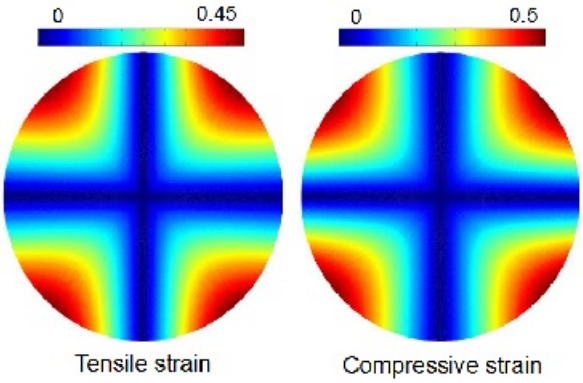

Fig. **4**. Conduction gap (in eV) according to strain angle θ in the case of the transport along the zigzag direction: strain ranges from 0% (center) to 6% (disk edge).

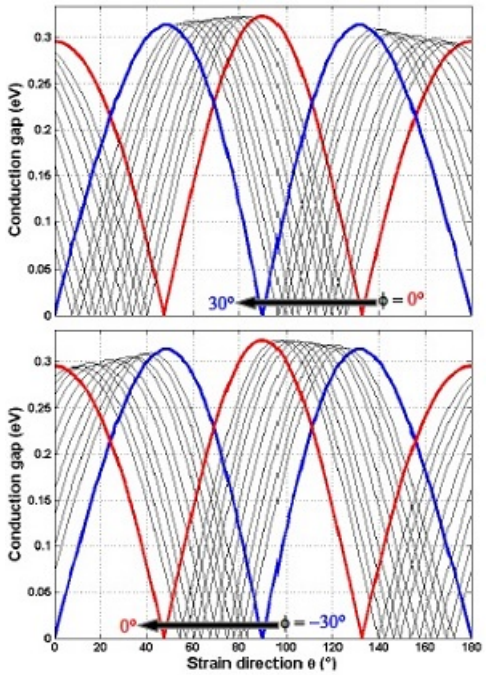

Fig. **5**. Conduction gap for different transport directions as a function of strain direction: σ=4%