Loïc Huder [a]
Toai Le Quang [a], Alexandre Artaud [a,b], Guy Trambly de Laissardière [c], Louis Jansen [a,b], Claude Chapelier [a] and Vincent Renard [a]
[a] Univ. Grenoble Alpes, CEA, INAC, PHELIQS, F-38000 Grenoble, France
[b] Univ. Grenoble Alpes, CNRS, Inst. NEEL, F-38000 Grenoble, France
[c] Univ. Cergy-Pontoise, CNRS, LPTM, F-95302 Cergy-Pontoise, France

loic.huder@cea.fr

Spectroscopic signature of uniaxial relative strain in twisted graphene layers

Strain alters the band structure of crystalline materials and can be an additional knob to tune the properties of 2D materials [1]. The prospect of assembling 2D layers into van der Waals heterostructures further widens the possibilities of band engineering since new artificial materials with designed properties are made available. Strain in such van der Waals heterostructures has been largely overlooked since it is generally assumed that those are exempt from strain owing to the weak van der Waals bonds between the layers. In this work, we show that even a small strain difference (relative strain) between the layers can qualitatively alter the band structure of one of the simplest van der Waals heterostructures: twisted graphene layers.

Twisted graphene layers (TGL) are archetypal because they were among the first reported van der Waals heterostructures and do demonstrate large tunability of the band structure. The misorientation of the layers indeed induces a moiré interference between them that depends on the rotation angle and allows important modifications of the electronic properties of the TGL. For large rotation angles, the system retains its linear Dirac-like dispersion at low-energies behaving like two single decoupled graphene layers [2]. Nevertheless, the interlayer coupling induces logarithmic divergences of the density of states called van Hove singularities (vHs) whose energy is tunable with the rotation angle. Small rotations angle are of special interest as new phenomena emerge: the van Hove singularities are very close to the Dirac point and the band structure is further affected by a renormalization of the Fermi velocity that cancels for a series of magic angles leading to electronic localization [3].

We have studied twisted graphene layers with a small rotation angle (Θ=1.26°). Scanning Tunneling Spectroscopy (STS) revealed additional peaks (Figure 1b) compared to expected vHs in the density of states close to the Dirac energy (Figure 2a). We interpret these peaks as resulting from the lifting of the degeneracy of vHs by a small difference in strain in the two layers. A commensurability analysis of the moiré pattern imaged by Scanning Tunneling Microscopy (Figure 1a) allows to determine that the relative strain in the TGL is mainly uniaxial and small (0.35%). This analysis allows to generate a moiré cell suitable for tight binding calculations where the atomic positions are fixed according to the measured strain. Tight-binding calculations of the local density of states using this cell reproduce the experimental data without adjustable parameter (Figure 2b). This points out that small differences in strain between the layers efficiently alters the properties of TGL. The spatial localization of the electronic states, expected for this small angle, was also shown to be preserved but weakened by the application of relative strain.

The influence of relative strain on the local density of states of TGL has strong implications for van der Waals heterostructures engineering as relative strain between the constituent layers could be exploited as an additional and more effective tuning parameter.

References

[1] Amorim et al., Physics Reports, 617 (2016) 1
[2] Lopes dos Santos et al., Physical Review Letters, 99 (2007) 256802
[3] Trambly de Laissardière, Mayou and Magaud, Nano Letters, 10 (2010) 804

Figures

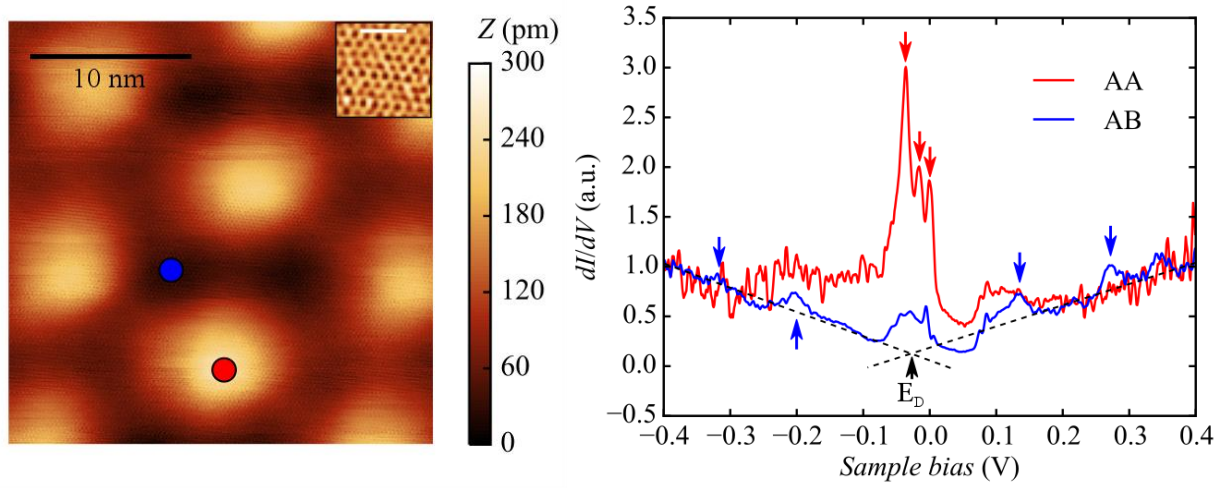

Figure 1: a) (26.37 x 26.37) nm² Scanning Tunneling Microscopy topograph of twisted graphene layers showing the moiré pattern. The twist angle between the graphene layers was estimated to be Θ=1.26°. The sample bias was V=-400 mV and the current setpoint was I=50 pA. Inset : Zoom of the image showing the honeycomb lattice of the carbon atoms in the top layer. The scale bar is 1 nm. b) Local density of states recorded by STS at the spots marked with colored dots in Fig.1a (red and blue dots for AA and AB regions respectively) showing multiple van Hove singularities in AA regions (red arrows) and peaks at higher energy in AB regions (blue arrows). The current setpoint is I=300 pA for a bias voltage of V=-400 mV. The position of the Dirac point E_D is estimated from the V shape of the high-energy density of states (dashed lines).

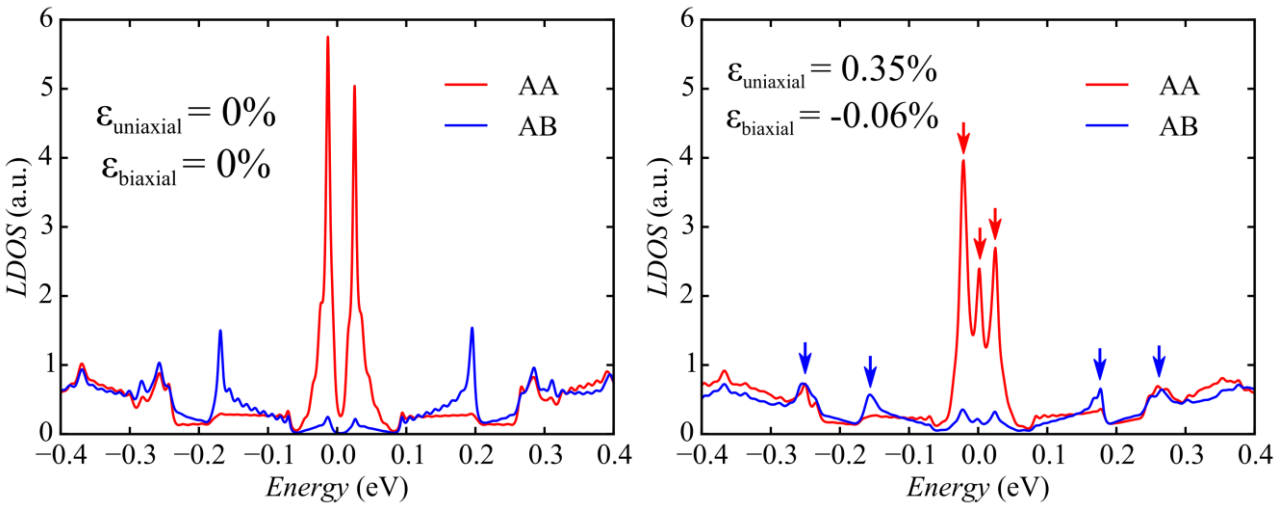

Figure 2: a) Local density of states calculated by tight-binding for twisted graphene layers without strain. Only two vHs are localized in AA regions near the Dirac point. b) Local density of states calculated by tight-binding on the atomic positions found by the commensurability analysis which include the relative strain. The three vHs localized in AA regions are in agreement with STS experiments as are the peaks at higher energy in AB regions.