Visualizing In-Plane Junctions in Nitrogen-Doped Graphene

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Controlling the spatial distribution of dopants in graphene is the gateway to the realization of graphene-based electronic components. Here, it is shown that a submonolayer of self-assembled physisorbed molecules can be used as a resist during a post-synthesis nitrogen doping process to realize a nanopatterning of nitrogen dopants in graphene. The resulting formation of domains with different nitrogen concentrations allows obtaining n–n’ and p–n junctions in graphene. A scanning tunneling microscopy is used to measure the electronic properties of the junctions at the atomic scale and reveal their intrinsic width that is found to be ≈7 nm corresponding to a sharp junction regime.

1. Introduction

Mastering the doping of materials is the foundation of microelectronics. The control of the bandstructure of crystals by traces of dopants allows the realization of p–n junctions that are fundamental building blocks for electronic devices. In the search for post-silicon technology, new promises have arisen with the discovery of graphene and 2D materials. Soon after the first isolation of graphene, its chemical doping was achieved by the interaction of pure graphene with C60 has also been widely studied. In the case of some key questions are still pending regarding the properties of in-plane junctions in chemically doped graphene. The structure of such junctions at the atomic scale and the width of the space charge region remain unknown. To answer these questions, an investigation of the structure and electronic properties at the atomic scale is needed, and can be achieved using STM in an ultra high vacuum (UHV) environment. In order to have an easy access to the junctions by STM, a distribution of junctions on the whole surface of a sample is desirable. Here, we address these questions, and in order to obtain a collection of junctions in a sample, we provide a new route to control the spatial distribution of nitrogen dopants in graphene using self-assembled monolayer islands of C60 molecules as a molecular resist during post synthesis nitrogen doping. One advantage of this strategy is that it is a post-synthesis method, which allows to treat any graphene sample independently of the growth method. This method leads to the formation of a large collection of domains on a sample, allowing us to address the junctions at the atomic scale by STM. Compared to conventional lithography.

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resist, the use of a physisorbed molecular monolayer deposited under UHV conditions makes it possible to avoid the presence of polymer residues and to achieve a significantly higher degree of cleanliness of the sample, which is mandatory for this study. One can, however, note that specific cleaning procedures can also be used to improve the cleanliness of the surface when photoresist chemical compounds are used.[17] It has to be noted that the junctions investigated here have a different nature from the electrostatic or substrate engineering junctions. In the present case, the junctions are obtained by a spatial variation of the concentration of dopants, an analogue of standard p–n junctions in semiconductors, whereas in other cases, the junctions are induced by the environment of a pristine graphene layer. One interest of chemically doped graphene is its stability and the possibility to be transferred on different substrates or devices. Moreover, previous work have shown that nitrogen dopants do not alter the bandstructure of graphene.[18]

2. Results and Discussion

We start with the demonstration that single layer C₆₀ islands can be used as a resist to pattern the concentration of nitrogen dopants in graphene. All STM measurements were performed under ultrahigh vacuum (UHV) conditions at low temperature (4.6 K) on multilayer graphene grown on the carbon rich SiC(000₁) (See Supporting Information). The deposition of a submonolayer of C₆₀ on graphene yields to compact C₆₀ monolayer islands possibly including a native second layer that appears as bright protrusions on top of the monolayer islands (Figure 1A; Figures S1 and S2, Supporting Information). The basic idea of the submonolayer molecular resist is sketched in Figure 1B. The C₆₀/graphene sample is exposed to activated nitrogen atoms produced by a plasma source.[19] The sp² carbon atoms of C₆₀ are expected to react with nitrogen similarly to the sp² carbon atoms of graphene, thus preventing the reaction of nitrogen with graphene. We have tested this idea by exposing a C₆₀/graphene sample to a nitrogen plasma source. An image of the sample after plasma exposure is shown in Figure 1C. Bright spots in the molecular island indicate that the C₆₀ molecules have been effectively reacting with nitrogen. Substitutional nitrogen atoms appear on the surrounding graphene as bright dots.[18–20]

In order to check the effect of C₆₀, we remove the C₆₀ island by nanoshaving (sweeping the molecules with the STM tip[21]). This procedure consists in scanning the surface with a reduced tip-sample distance (large current, low bias voltage) at high speed. Although the parameters may be adjusted during the procedure, we have used typically a sample bias voltage of 0.1 V and a current setpoint of 1 nA with a scanning speed of 1.7 µm s⁻¹. During the procedure, intermediate images were acquired to check the state of the sample. The surface after 3 h of molecule removal procedure is shown in Figure 1D. The C₆₀/graphene sample is exposed to activated nitrogen atoms produced by a plasma source.[19] The sp² carbon atoms of C₆₀ are expected to react with nitrogen similarly to the sp² carbon atoms of graphene, thus preventing the reaction of nitrogen with graphene. We have tested this idea by exposing a C₆₀/graphene sample to a nitrogen plasma source. An image of the sample after plasma exposure is shown in Figure 1C. Bright spots in the molecular island indicate that the C₆₀ molecules have been effectively reacting with nitrogen. Substitutional nitrogen atoms appear on the surrounding graphene as bright dots.[18–20]
Figure 2. Unipolar junction in nitrogen-doped graphene. (A) Large scale STM image of a n–n’ graphene junction area (~0.3 V, 100 pA). (B) dI/dV spectra measured at positions marked by crosses in (A). The inset shows series of spectra measured along the white line in (A). (C) dI/dV map at ~0.3 V measured simultaneously with the topography shown in (A). (D) Topographic STM image (~0.3 V, 200 pA) of a junction taken at a different location than the previous one. (E) dI/dV spectra measured at positions marked by crosses in (D). (F) Mapping of the Dirac point extracted from spectra measured over the sample area shown in (D). The white line indicate the line over which the profile shown in (G) has been measured, revealing the variation of the Dirac point position across the junction. (H) Top: 3D topographic STM image of the area (D) color coded with the conductance map at ~0.3 V. Down: Sketch of the Dirac cones on both sides of the junction and linescan of the conductance map across the junction. (I) Atomic structure of the n–n’ graphene junction used for charge redistribution, with 3 nitrogen atoms on one side and 1 nitrogen atom on the other side. The corresponding isosurface (10^-4eV/Å^3) is superimposed. The evolution of the calculated Dirac point energy along the n–n’ junction is represented below.

measurements give average efficiencies of 62% (Figure S3, Supporting Information). One advantage of physisorbed molecules resist its soft and noninvasive nature; the molecules can easily be removed without inducing any defect in graphene. A more general procedure can be used by removing the molecules by thermal annealing. Therefore, nanodomain patterning of nitrogen in graphene can be achieved in a three steps process (Figure 1E). A large scale STM image after annealing at 600 °C is shown in Figure 1F. Clearly, domains with low nitrogen concentration can be seen, which are a fingerprint of the C_60 islands before annealing. This shows unambiguously that physisorbed C_60 islands constitute an effective mask to induce nano-structuration of nitrogen dopants in graphene.

We now turn to the electronic properties of the junctions made of adjacent domains with different nitrogen concentrations. The graphene area shown in Figure 2A contains a larger concentration of nitrogen in the right part than in the left part. dI/dV spectra measured on each region are characteristic of n-doped graphene. The gap-like feature around the Fermi level corresponds to the well-known inelastic excitation of a phonon mode of graphene.[22] The Dirac point is marked by a dip in the dI/dV curve at the voltage V_D[28-20,22] below the Fermi level indicating the expected n-type doping. The spectra clearly show a larger downshift of the Dirac point on the high nitrogen concentration part (~0.21 V) (Figure 2B) than on the low nitrogen concentration part (~0.09 V). More understanding is provided by the spatial variation of the Dirac point obtained by a dI/dV mapping at an energy slightly below the Dirac point[23,24] or by measuring a dI/dV spectrum and extracting V_D at each pixel of an image.[28,23-26] In Figure 2C, we show a conductance map measured at ~0.3 V exhibiting a higher conductance on the low-doped region and a lower conductance on the high-doped region. This contrast is expected[22] since, at this bias voltage, the dI/dV signal lies around the minimum at V_D for the highly doped part, while it lies in the increasing part of the dI/dV curve for the weakly-doped part. This area constitutes a unipolar n–n’ junction. The clear contrast and sharp boundary between the two parts constituting the junction allows us to estimate the area of each domain and to estimate the nitrogen concentration that is found to be 0.22% on the high-doped part and 0.06% on the low-doped part. A closer view of another junction is shown in Figure 2D. The left part has a larger doping than the right part, the atomic resolution allows to identify each doping site in that image (Figure S4, Supporting Information). Using the conductance and the topographic image, we evaluated the nitrogen concentration following the same procedure as described above, and we obtained 0.28% on the high-doped region and 0.08% on the low-doped region. The difference in the doping level of the two parts is reflected in the spectra of Figure 2E. A quantitative mapping of the Dirac point position has been obtained by measuring a dI/dV spectrum and determining the Dirac point at each pixel of the image. The result is shown in Figure 2F. A
linescan over the junction shows the variation of the Dirac point (Figure 2G). The width \( d \) of the junction is calculated using a fitting profile with the function\(^{[21]} \)
\[
V(x) = V_0 + V_1 \tanh \left( \frac{x - x_0}{\Delta} \right)
\]
We take the value 4\( \Delta \) as an estimate of the barrier width (cutting the step profile at 96% of the values on both sides of the junction). We determine a width of the junction of 77 nm. A more systematic measurement on several linescans taken over three different mappings gives an average value of 71 nm with a standard deviation of 2.9 nm (Figure S5, Supporting Information). We also measured a conductance map on the same area (Figure 2H) together with a linescan. The width of the junction has been determined using the same fitting procedure, and a statistics of linescans measured on three different conductance maps gives an average value of 72 nm with a standard deviation of 1.6 nm (Figure S5, Supporting Information). This finding opens new opportunities for probing the transport properties in sharp junctions. Dual probe STM experiments could be envisaged for measuring the transport through such junctions for example. In transport devices, C\( \text{60} \) mask may possibly be patterned using atomic force microscopy followed by nitrogen plasma exposure in order to realize transport experiments through nitrogen-doped graphene junctions.

In order to simulate, the evolution of the Dirac point energy and to compare it to the experimental evolution shown in Figure 2F,G, we have designed a model \( n-n' \) graphene junction unit cell. Namely, we have considered a 116.4 Å \( \times \) 74.4 Å rectangular unit cell of graphene of about 3500 atoms, with 3 substituting nitrogen atoms on one side of the cell, and 1 substituting nitrogen atom on the other side, following the experimental conditions. The two groups of atoms are separated by a distance of 69.4 Å. This unit cell is represented in the top of Figure 21. Then we have calculated the projected density of states (PDOS) for successive slices of graphene along the length of the unit cell (see Experimental Section for details). These calculations have been performed using Density Functional Theory (DFT). For each calculated PDOS, we have extracted the position of the local Dirac point, similarly to what has been measured in the linescan of Figure 2F. The corresponding evolution of the Dirac point energy is represented in the red curve of Figure 21. The two pairs of blue vertical lines delimit the regions containing the group of three nitrogen atoms (on the left) and the single nitrogen atom (on the right). One can clearly observe a variation of the Dirac point energy, from an n-doped region on the left at \( \approx -0.22 \) eV, to an almost neutral region on the right at \( \approx -0.07 \) eV. These findings are in good agreement with the experimental evolution shown in Figure 2G. Some extra variations of the Dirac point energy are also observed in the vicinity of the nitrogen atoms, with a minimum at \( -0.36 \) eV (left side) and another one at \( -0.22 \) eV (right side). This can be related to the local redistribution of electronic density induced by the nitrogen atoms, as represented in the charge isosurface of Figure 2I. It is worth to notice that close to the charge redistribution of the nitrogen atoms is influenced by the potential gradient similarly to a standard semiconducting \( p-n \) junction (see Figure S6, Supporting Information).

In addition to the variation of the Dirac point, we have investigated the variation of interlayer interaction and local work function in a junction. On multilayer graphene, the rotational disorder between adjacent top layers eventually leads to the formation of moiré patterns and van Hove singularities (vHs)\(^{[28]} \).

In Figure 3A, we show a graphene area with a moiré pattern of periodicity \( \lambda = 1.64 \) nm. \( d \)\( \text{df/dV} \) spectra measured on the two parts with different doping levels show a shift of \( E_D \) and vHs in the same direction (see Figure 3B). It is worth to notice that the position of the vHs peaks are not symmetric with respect to \( E_D \). On the highly doped part, \( V_{D} = -0.2 \) V, and the peak positions of the vHs are \( E_{\text{vHs}} = 0.82 \) V and \( V_{\text{vHs}} = -0.83 \) V. This gives highly asymmetric positions with respect to \( V_D \), with \( V_{\text{vHs}} = 1.02 \) V and \( V_{\text{vHs}} = -0.63 \) V. After renormalization by the phonon inelastic excitation energy,\(^{[22]} \) the actual energies of the vHs with respect to the Dirac point can be obtained \( E_{\text{vHs}} = 0.90 \) eV and \( E_{\text{vHs}} = -0.63 \) eV (see Supporting Information). This result is different from the standard case where the energy position of the vHs at positive and negative energy \( E_{\text{vHs}} \) are symmetric with respect to the Dirac point \( E_D \) following the relation \( E_{\text{vHs}} = E_D + \frac{2}{2} \Gamma \sin(\theta/2) \approx \pm 1 \). In this relation, \( \hbar \) is the reduced Planck’s constant, \( \Gamma K \) is the length of the reciprocal vector at the \( K \) point, \( \Theta \) is the angle between the two graphene layers, \( v_F \) is the Fermi velocity of graphene, and \( t \) is the interlayer coupling energy. Here, the asymmetry is due to the fact that the top graphene layer is doped and interacts with the undoped underlying layer (see the inset in Figure 3B). Considering the Dirac energy of the top layer \( E_D \) and the Dirac energy of the layer below \( E_D \), the vHs energies become as (more details in Supporting Informations and Figure S7, Supporting Information): \( E_{\text{vHs}} = E_D + \frac{2}{2} \Gamma \sin(\theta/2) \approx \pm 1 \).

Taking \( v_F = 10^6 \) m \( s^{-1} \), \( t = 0.1 \) eV, \( \sin(\theta/2) = 0.123/\lambda \) and \( E_D - E_D = 0.2 \) eV, we obtain \( E_{\text{vHs}} = 0.84 \) eV and \( E_{\text{vHs}} = -0.64 \) eV in good agreement with the experimental values. Interestingly, these relations can be reversed to deduce the Dirac point energy when its direct determination is rendered difficult by the proximity with the phonon feature. On the lower doped part, the peaks of the vHs are at 0.83 and 0.74 V. The Dirac point can be deduced from the relations \( E_D = 2E_{\text{vHs}} - 2\hbar \Gamma \sin(\theta/2) \approx 2t + E_D \) and \( E_D = 2E_{\text{vHs}} + 2\hbar \Gamma \sin(\theta/2) - 2t - E_D \). We find a Dirac point at \( +0.18 \) eV in the first case and \( +0.12 \) eV in the second case. These values are quite close and more importantly they are positive. A close look at the spectroscopy in Figure 3B shows a minimum in the \( d\text{df/dV} \) curve above the Fermi level \( \approx +0.18 \) V in good agreement with the calculated value from the vHs. Actually, we often observe a natural p-doping in some area of our pristine graphene samples (Figure S8, Supporting Information). This is in agreement with previous observations of natural p-doping of graphene grown on the carbon side of SiC.\(^{[29–32]} \)

Further study is needed to fully understand the origin of this doping. The very low concentration of nitrogen atoms on the left region in Figure 3A makes it plausible that the remaining doping level in this area is dominated by the initial p-doping of the pristine graphene sample. Therefore, this junction is a \( p-n \) junction. Another example of a \( p-n \) junction can be found in the Supporting Information (Figure S9, Supporting Information). Such junctions are observed more rarely than the \( n-n' \) junctions described above. Further evidence of the nature of the junction is provided in Figure 3C showing a mapping of point spectra taken across the \( p-n \) junction. First, the shift of the vHs at negative bias is clearly observable. The variation of the \( E_{\text{vHs}} \) position
along the line extends over a distance of 5.5 nm as determined by the fitting curve (Figure 3D) in good agreement with the junction width determined above. Second, the Dirac point can be seen in Figure 3C as a dark trace at negative bias on the right side, shifting to positive bias on the left side. One can notice that across the junction, $-v_{Hs}$ varies from $-0.79$ to $-0.66$ eV (after renormalization by the phonon energy) corresponding to a variation of 0.13 eV. The Dirac point energy is varying from $-0.14$ to $0.12$ eV (after renormalization by the phonon energy) corresponding to a total variation of 0.26 eV that is twice the energy variation of the $v_{Hs}$ as expected from the relation above.

We now turn to the link between the work function and the doping level. In Figure 3E, we show another sample area with a n–n' junction. The variation of the local work function can be followed by measuring the first field emission resonance (FER) peak obtained by $dZ/dV$ spectroscopy measured in constant current mode. In Figure 3F, we show $dZ/dV$ spectra revealing a peak at 4.15 V on the low doping part and at 4.09 V on the high doping part. This indicates that the work function decreases when the n doping increases. A visualization of the variation of the work function is obtained by measuring spectra at each point of the image of Figure 3E and extracting the voltage value of the FER peak on each spectra. The resulting FER mapping is shown in Figure 3E and clearly reveals a higher work function on the lower doping level area. This variation follows qualitatively the variation of the Dirac point as can be seen from the $dI/dV$ spectra measured at the same location in Figure 3G and from the Dirac point mapping shown in Figure 3E. This variation is consistent with the expectation that increasing the n-doping level increases the Fermi energy and reduces the work function as sketched in Figure 3H.

We have employed DFT to characterize the junction and its transport properties. We consider in Figure 4A an ideal, sharply defined n–n' junction between two doped regions (0.06% N and 0.17% N ) within the virtual crystal approximation. The calculated potential shifts of the onsite $p_z$ orbitals yield a spatial...
The width of the junctions determined in the experiment corresponds to the intrinsic width of such in-plane junctions, since it is close to the low limit obtained from the calculations. In Figure 4B,C we consider the effect of a single N-atom placed near the “pristine” junction (Figure 4A), resulting in a change in transmission and corrugation in the potential (dashed lines in Figure 4C). We observe only minute changes in the transmission function for energies in the interesting energy region between the two Dirac points (zero points in Figure 4B), while the scattering resonances due to the N are located ≈0.5 eV away. We further show how the local bondcurrents are perturbed only in the vicinity of the N atoms (red lines in Figure 4C).

3. Conclusion

In summary, we have shown that a C_{60} island monolayer can be used as a mask during plasma exposure of a graphene sample to achieve a nanostructuration of nitrogen dopants in graphene. We have shown that the nanostructuration results in the formation of unipolar (n–n') and dipolar (p–n) junctions in graphene. The typical width of the junctions interface is 7 nm and corresponds to sharp junctions with a width lower than the Fermi wavelength. We foresee that the submonolayer molecular resist technique presented here can be very versatile and is not limited to graphene. Hence, one can expect it to be effective on any other substrate where molecular self-assembly can be achieved such as transition metal dichalcogenides or other 2D van der Waals materials. Other chemical doping or functionalization with other species than nitrogen can also be envisaged. Moreover, this method can also be expanded to the effect of surface functionalization on other properties of materials that can be investigated with local probes such as forces or chemical activity.

4. Experimental Section

Multilayer graphene samples were grown on a 6H-SiC wafer purchased from NovaSiC. The sample was first degassed under UHV conditions at 790 °C during 5 h. Further surface cleaning was achieved by annealing the sample at 850 °C for 15 min under a silicon flux of ≈1 mL min^{-1}. The synthesis was then realized by annealing the sample at 1250 °C during 5 min. After synthesis, the sample was transferred in air to the UHV system where low-temperature STM measurements were performed. The graphene sample was degassed under UHV at 850 °C before further measurements and sample preparation.

The nitrogen-doping was performed by exposing the graphene sample to a flux of nitrogen radicals produced by a remote radio-frequency plasma source fed with N₂. The pressure in the chamber during doping was 5.10^{-4} mbar, the plasma power was 100 W. The deposition of C_{60} molecules was achieved by sublimation using an effusion cell (Dr. Eberl MBE-Komponenten GmbH) under UHV at 400 °C onto the samples at the STM stage maintained at ~5 K. The graphene sample was then brought to room temperature allowing molecules to diffuse on the surface.

All STM measurements were performed with a low-temperature STM apparatus (Omicron) working at 4.6 K at a pressure <1 x 10^{-10} mbar. The dI/dV spectra were acquired using a lock-in detector at a frequency of ~823 Hz and a modulation amplitude of 35 mV. The measurements were performed with an electrochemically etched tungsten tip. Before measuring on graphene, the tip was calibrated on an Au(111) surface until it showed the Shockley surface state feature in the spectroscopic measurements.
Calculations of the Dirac point evolution (Figure 21) and charge isosurface along the model graphene unit cell have been performed using the very efficient Density Functional Theory (DFT) localized-orbital code Fireball.\[39,40] This method uses a self-consistent version of the Harris–Foulkes LDA functional,\[16,37] instead of the traditional Kohn–Sham functional based on the electronic density. In that respect, one approximates the total charge by a superposition of spherical charges around each atom. Also, Fireball used a localized optimized minimal basis set,\[38] and the self-consistency was achieved over the occupation numbers through the Harris functional. The LDA exchange–correlation energy was calculated using the efficient multi-center weighted exchange–correlation density approximation (McWEDA).\[19,40] Here, the cut-off radii for the wavefunctions’ radial part (for s, sp, and spd basis sets) defining the optimized basis set were the following (in atomic units): \( r_s = r_p = 4.5 \) and 4.2 for C and N atoms, respectively.

For the Dirac point evolution calculations, the graphene unit cell was divided in thin nanoribbons of 74.4 Å length (width of the graphene unit cell) and \( \approx 6 \) Å width. The PDOS of each nanoribbon was calculated and the minimum of the PDOS gives the values of the local Dirac point energy.\[25\]

Regarding the charge isosurface, the full isosurface charge of the doped graphene unit cell was calculated to which the full isosurface charge of the corresponding pristine graphene was subtracted, without nitrogen atoms. The difference gave authors the spatial repartition of the charge modification induced by the substituting nitrogen atoms.\[24\]

The DFT and transport calculations in Figure 4A were done using siesta/transiesta with the GGA-PBE functional,\[22\] periodic boundary conditions with 168 k-points (open boundary conditions) in the direction along (perpendicular to) the junction, and a SZP basis set.

Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest
The authors declare no conflict of interest.

Data Availability Statement
The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords
graphene, nitrogen dopants, p–n junctions, scanning tunneling microscopy

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