**Reconstruction Dependent Interaction at the Graphene/ 6H-SiC(000-1) Interface probed by STM and ab-initio calculations.**

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Graphene single and multilayers grown by thermal decomposition on the 6H(4H)-SiC(000-1) face (in short SiC-C face) have demonstrated physical properties similar to those expected for ideal graphene ([1], see [2] for a review) and thus represent an appealing technique to prepare wafer scale graphene films directly on an insulating substrate. The structure of the interface has a determinant influence on the electronic properties of such samples, as demonstrated in the well documented case of graphene grown on the SiC-Si face: a strong graphene substrate interaction leads to highly perturbed first carbon plane (the so-called buffer layer) which lacks the characteristics Dirac cones of the material, and charge transfer results in a significant doping of the successive graphene planes. Moreover, the interfacial coupling is thought to be responsible for the unique orientation of the carbon planes found in multilayers on the Si face by imposing the orientation of each newly formed graphitic layer.

In spite of its relevance, the structure of the interface is not well established for the SiC-C face. Recent reports suggest that it depends on the growth conditions [3], and that it can be heterogeneous [4]. To address this point we have performed Scanning Tunneling Micoscopy (STM) and Spectroscopy (STS) experiments on partially graphitized samples prepared in-situ under UHV, coupled with ab-initio calculations. From an experimental point of view, the so called “transparency” of graphene [5] allows the investigation of the (buried) substrate structure at the interface from high-bias STM images whereas the low energy electronic structure of the graphene layer can be probed in low bias images [6]. Thus a complete description of the electronic structure of the interface can be achieved from variable bias STM/STS data.

Starting from the clean SiC(3x3) surface, we first obtain monolayer graphene islands on top of the unperturbed SiC(3x3) reconstruction (G/3x3 islands). At variance with the case of the Si face the (azimuthal) orientation of the graphene layer varies from one island to the other, i.e. a “rotational disorder” is found in the samples. No significant perturbations of either the substrate or the graphene layer structures were observed on G/3x3 islands with different orientations [7] (see Figure 1 as an example). This indicates that the graphene-SiC(3x3) interaction is quite weak, leading to an almost ideal system [7]. We shall present STM/STS measurements which allow the determination of parameters (graphene doping and interface defect density) relevant to the physical properties of the system [8]. Finally, owing to the coexistence of G/3x3 islands with area of bare SiC(3x3) surfaces we could perform a quantitative study of the high bias “transparency” of graphene, which indicates an enhancement of the tunnelling probability from/to the substrate surface states when they are buried below the carbon plane [8].

Further annealing below the graphitization temperature leads to the selective transformation below the graphene layer of the SiC(3x3) surface reconstruction into the SiC(2x2) one, leading to G/2x2 islands. This transformation results in an increase of the graphene substrate interaction [9]. The atomic structure of the SiC(2x2) surface is a simple adatom-restatom structure (see Figure 2-a), and the graphene-substrate coupling mostly involves Si adatoms [10]. The lattice mismatch and rotational disorder between graphene and SiC gives rise to moiré patterns [7], and thus the graphene-adatom stacking varies laterally within the period of the moiré. We shall present STM/STS data which show that the adatom graphene coupling depends on the local configuration, the energy and broadening of the adatom state being different for e.g. top and hollow graphene sites. This result can be qualitatively understood in the framework of a simple (non interacting) Anderson impurity model (see e.g. [12]). This stacking dependent interaction is correlated to perturbations in the low energy local density of states of graphene (see Figure 2-b). Ab-initio calculations allow a quantitative analysis of the full interface electronic structure in the case of small commensurate supercells.

**References**


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**Figures**

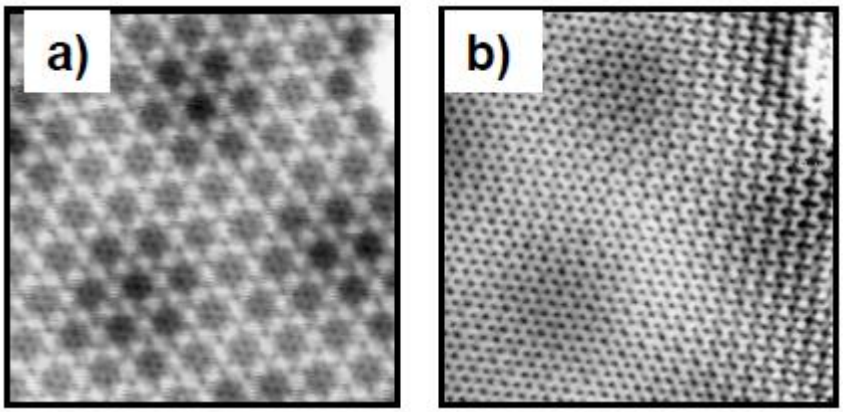


*Figure1 : STM images of the same spot on a G/3x3 island, images size: 7.5x7.5 nm². a) High bias image (sample bias: -2.0V) showing the structure of the SiC(3x3) reconstruction through the graphene layer. b) Low bias image (sample bias -50mV) showing the low energy features of graphene: honeycomb atomic contrast (left) superimposed to "standing wave patterns" due to electron scattering at the island edge (right).*

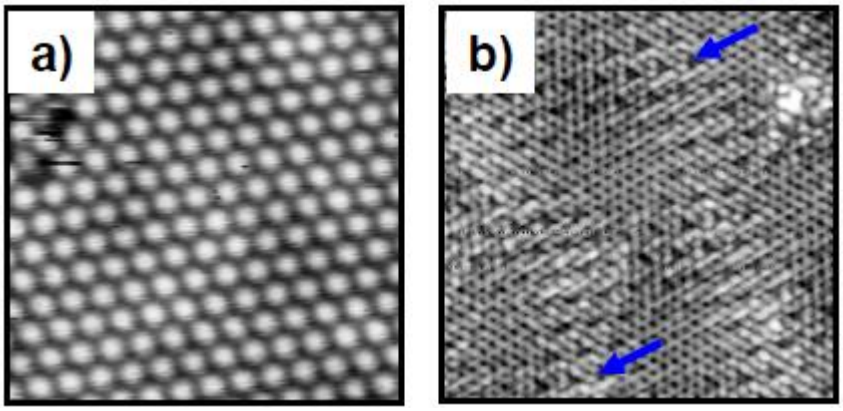


*Figure2 : STM images of the same spot on a G/2x2 island, images size: 7.5x7.5 nm². a) High bias image (sample bias: +2.5 V) showing the adatoms of the SiC(2x2) reconstruction through the graphene layer. b) Low bias image (sample bias -50mV) showing the perturbation to the low energy local density of state of graphene in G/2x2 islands. The perturbation leads to "switched-off" graphene atoms (some indicated by arrows), which do not show up in a weakly interacting system (e. g. G/3x3, figure 1-b). The perturbation is modulated in space with the (pseudo) period of the moiré pattern.*