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Theory of Graphene on SiC(11-20)a Substrate

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1. Introduction

Thermal annealing of SiC substrate forms graphene on its surface. Graphene obtained by this method is expected for the graphene substrate for the industrial use [1]. In case of the SiC(0001) substrate, few layer graphene is controllably formed. We successfully obtain wafer-scale epitaxial bilayer graphene on this substrate by high temperature annealing in ultra-high vacuum. We also successfully obtain wafer-scale epitaxial monolayer graphene by high temperature annealing in Ar atmosphere. The quality of those graphene is high enough to observe carrier transport with high mobility [2,3].

Graphene can also be formed on different orientation of the SiC substrate. On SiC(000-1) substrate, multilayer graphene is obtained. In this case, the graphene is almost non-doped, while graphene formed on SiC(0001) substrate is n-doped [4]. In both cases, the first graphene layer on the bulk-truncated substrate acts as the buffer layer, and the second graphene layer acts as the monolayer graphene electronically.

Recently, we have also successfully obtain graphene on SiC(11-20)a substrate experimentally. It seems that the formed graphene is in the epitaxial relation to the substrate as on (0001) substrate.

In this contribution, we theoretically study the atomic and electronic structure of graphene on SiC(11-20)a substrate. We reveal that this surface also has a buffer layer and that the graphene is non-doped.

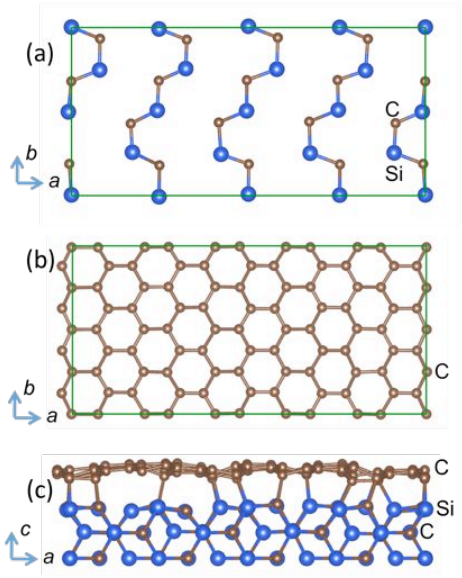

Fig. 1: (a) Top view of the atomic structure of the top-most layer of the SiC(11-20)a substrate. (b) Top view of the graphene. (c) Side view of the optimized atomic structure for SiC(11-20)a surface covered with one graphene layer.

2. Method

Our calculation method is the first-principles method with pseudopotentials, plane wave bases, and a density functional [5-8]. The cut off of the plane wave bases is 25Ry. We employ the repeated slab geometry. The thickness of the slab is three SiC layers, and the back-side of the slab is terminated by H atoms. We optimize the atomic structures, and calculate the electronic states.

3. Surface covered with one graphene layer

The bulk-truncated SiC(11-20) surface has the lateral unit cell with 5.31Å x 10.05Å. Four times of this unit cell in the a-direction [Fig. 1 (a)] well matches with the graphene 5√3 x 4 unit cell [Fig. 1 (b)]. In this case, graphene is only extended by 2% in the b-direction and by –0.1% in the a-direction. Therefore, epitaxial relation is expected as in the case of (0001) substrate.

We prepare this lateral unit cell, put one layer of graphene on the bulk truncated substrate, and fully optimize the atomic structure with fixing Si and C atoms on the back-side one layer.

After the structural optimization, the C atoms on the graphene layer largely move in the c-direction, while they almost remain in the a- and b-directions. The Si and C atoms on the top-most layer of the bulk truncated substrate move in the a- and b-directions as well as in the c-direction. The displacement of the Si and C atoms does not show any simple regularity as in the case of SiC(0001) substrate [9]. This comes from the fact that graphene has the three-fold symmetry while the SiC(11-20) substrate has the two-fold symmetry. It is

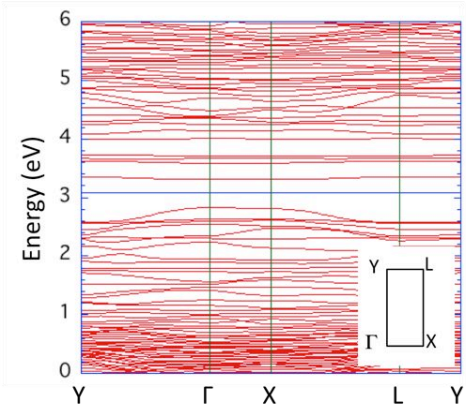

Fig. 2: Band dispersion relation of SiC(11-20)a surface covered with one graphene layer. The horizontal line around 3 eV represents the Fermi energy.

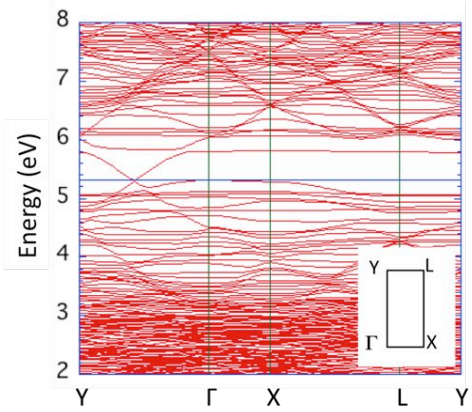

Fig. 3: Band dispersion relation of SiC(11-20)a surface covered with two graphene layers. The horizontal line around 5 eV represents the Fermi energy.

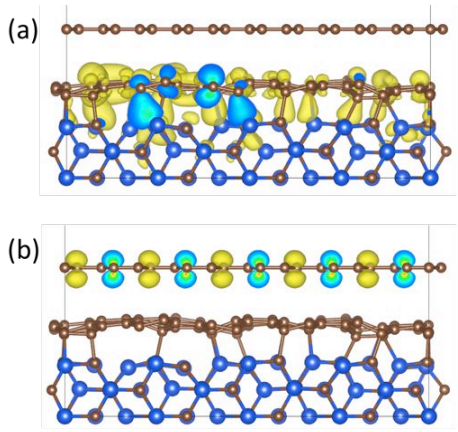

Fig. 4: Side views of distribution of squared wave functions of valence top band (a) at Γ point and (b) at the Dirac point for SiC(11-20)a surface covered with two graphene layers.

suggested that the STM image does not show any simple regular Moire pattern such as honeycomb for the case of SiC(0001) substrate.

The relatively large displacement of the C and Si atoms on the graphene layer and the top-most layer also indicates that the C atoms on the graphene layer have chemical bonds with the Si and C atoms on the substrate. This suggests that the graphene does not show the Dirac cone in its band structure.

The calculated result of the band dispersion relation actually confirms this point (Fig. 2). It is semiconductive with energy gap of 0.49 eV and does not show the Dirac cone.

4. Surface covered with two graphene layers

Next we put another graphene layer on the surface with one graphene layer. Because of the difficulty in calculating the van der Waals force between the graphene layers by our first-principles method, the second graphene layer is just located at the position with 3.35Å spacing from the average c-position of the first graphene layer. A-B stacking is also assumed for the first and second graphene layers.

The calculated band dispersion relation shows a clear Dirac cone (Fig. 3). This means that the second graphene layer acts as the monolayer graphene electronically, and that the first graphene layer acts as the buffer layer. In addition, the Fermi energy coincides with the Dirac point. This means that the graphene is electrically neutral non-doped as the case of SiC(000-1).

To check the origins of the bands around the Fermi energy, we also calculate the distribution of squared wave functions (Fig. 4). For the valence top band at Γ point, the wave function is localized on the first graphene layer and on the top-most layer of the SiC substrate [Fig. 4 (a)]. On the other hand, for the valence top band at the Dirac point, the wave function is surely localized only on the second graphene layer.

These results confirm that the second layer acts as the monolayer graphene, and the first layer acts as the buffer layer. These results also suggest that the reason of electrically neutral graphene is the absence of metallic interface states, which pins the Fermi energy position. Since the effective mass of the interface state is very heavy, only the Dirac carrier on the graphene must contributes to the carrier transport.

5. Conclusion

We study the atomic and electronic structure of graphene on SiC(11-20)a substrate by the first-princples calculation. We reveal that the first graphene layer has chemical bonds with the SiC substrate, and that it becomes the buffer layer. We also reveal that the second graphene layer acts as the monolayer graphene, and that it is electrically neutral non-doped.

Acknowledgment

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