Theoretical Study on C Adsorbate at Graphene/Cu(111) or h-BN/Cu(111) Interfaces

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To elucidate bottom-up fabrication of heterostructures of two-dimensional materials such as graphene and h-BN, C atom adsorption on Cu(111) surface partially covered with h-BN or graphene is studied by using the first-principles method with van der Waals correction. It is found that the C monomer more difficultly locates under h-BN than under graphene or on bare Cu, while the C monomer also more hardly diffuses under graphene than under h-BN or on bare Cu. In addition, formation of C dimers is more difficult under graphene than under h-BN or on bare Cu. These results suggest that we can control the heterostructure growth by modulating growth condition. It is further found that the shape of h-BN or graphene flake on the Cu surface depends on whether the edge is terminated with hydrogen (H) or not. Because the bond formation energy of edges with H atoms are different between h-BN and graphene, it is indicated that appropriate choice of H condition will lead us to the intentional formation of lateral and vertical heterostructures.

Keywords Graphene; h-BN; Cu surface; First-principles calculation; Crystal growth

I. INTRODUCTION

Two-dimensional materials such as graphene and h-BN are attractive because of their unique physical properties. Since graphene is a semiconductor and h-BN is an insulator, the heterostructures of these two materials give us new opportunities for electronic applications [1–3]. Therefore, the bottom-up fabrication of such heterostructures is highly demanded. Recently, a selective chemical vapor deposition (CVD) growth realizes a lateral heterostructure of graphene/h-BN [4–9]. After C-source gas is introduced and graphene islands are formed on the Cu(111) surface, BN-source gas is introduced and h-BN is grown along the edges of graphene islands. It is further found that a vertical heterostructure of graphene/h-BN can be realized just by changing the order of gas-source supply [10, 11]. If we could intentionally control to form both vertical and lateral heterostructures by CVD growth, we can obtain new opportunities for application of graphene [12].

For the fine control of fabrication, the detail mechanism

of crystal growth must be clarified in the atomic scale. Some mechanisms of graphene growth on the bare Cu surface and at the graphene/Cu interface has been theoretically reported [13–17]. On the other hand, the mechanism of graphene growth at h-BN/Cu interface has not yet been theoretically studied. In this contribution, we therefore investigate behavior of C adsorbate on the Cu surface partially covered with graphene or h-BN, in order to get a guiding principle on the fine control of heterostructure formation in the CVD growth [18]. We study the C adsorbate at the h-BN/Cu(111) interface as well as at the graphene/Cu(111) interface and on the bare Cu(111) surface by the first-principles method.

II. METHODS

We performed the first-principles calculation based on the density functional theory with the program package of PHASE/0 [19]. We employed the PAW method with the cutoff energy of 30 Ry. The $4 \times 4 \times 1$ Monkhorst-Pack grid was used for the k -point sampling. Because the graphene or

h-BN sheet is adsorbed on the Cu surface by the van der Waals interaction, we had to take the van der Waals correction into account. It is widely known that the selection of the correction method affects the calculated results [20–22]. In this study, we focused on the SCF vdW-DF1 method as the correction [23]. This correction method is reported to overestimate the distance between the graphene sheet and the Cu(111) surface [24, 25]. However, when the distance changes by about 0.2 Å around the most stable distance, the formation energy changes only by 0.01 eV. Therefore, we suppose that the SCF vdW-DF1 method does not affect the overall discussion in this work.

We employed the repeated slab geometry with four Cu atomic layers, one graphene or h-BN layer, and a vacuum region with the thickness of about 9.72 Å. The $2\sqrt{3} \times 2\sqrt{3}$ supercell of Cu(111) was used. This surface was covered with the $2\sqrt{3} \times 2\sqrt{3}$ supercell of graphene or h-BN, which was appropriately expanded to match the lattice periodicity to that of Cu(111). Therefore, the graphene and h-BN sheets were expanded by 4.09% and 2.33%, respectively. We fully optimized the atomic positions except for all outermost Cu atoms at the bottom surface to evaluate the formation energies. We also calculated the diffusion barriers by using the climbing image nudged elastic band method (CI-NEB) with seven replica images [26].

III. RESULTS AND DISCUSSION

First, we investigate how the h-BN layer stacks on the Cu(111) surface by calculating the stacking-position-dependence of formation energies. Since Cu is the face-centered-cubic (fcc) crystal, there are three high-symmetric sites on the surface; a T1 site on top of the outermost Cu atom, a T4 site above the second layer Cu atom, and an H3 site above the third layer Cu atom [Figure 1(a)]. Since a B or N atom of the h-BN layer can be located at one of these three sites, there are six possibilities for the candidates of stacking. We have calculated all of the six possibilities and found that B3N1 (B on H3 and N on T1) is the most stable for h-BN/Cu, as it is more stable by 0.001 eV than the second most stable of B2N1 (B on T4 and N on T1). The distance between the h-BN sheet and the Cu surface is 3.51 Å. For graphene/Cu, similar C stacking on H3 and T1 is the most stable, as it is more stable by 0.004 eV than C on T4 and T1. This result is consistent with the previous theoretical report on graphene/Cu(111) [15]. The distance between the graphene sheet and the Cu surface is 3.57 Å. We employ these stacked interfaces in the following studies. Our calculated results also clearly indicate that the van der Waals correction is important to stabilize the h-BN or graphene sheet on the Cu surface. When we calculate the stacked structures without the van der Waals correction and only within the generalized gradient approximation (GGA) [27], the formation energies are smaller by about 1.4 eV, and h-BN or graphene sheet can even rarely be bounded to the Cu surface.

Next, we put one C atom at various sites at the h-BN/Cu interface and investigate the most stable site for the C

Figure 1: Views of the super cell used in this study. (a) Top view of bare Cu surface and various high-symmetric sites. (b) A typical side view of a C adsorbate at the interface. (c) Top view of the h-BN/Cu surface and various high-symmetric sites. (d) A typical side view of a C adsorbate at the h-BN surface. The blue, green, and white spheres represent Cu, N, and B atoms, respectively.

monomer adsorption. Candidates of C adsorption sites directly on the Cu surface are T1, T4, H3, and a valley [Figure 1(a, b)]. For comparison, we also put it on the h-BN surface of h-BN/Cu or the graphene surface of graphene/Cu. Candidates of C adsorption sites on h-BN or graphene sheet are top N/C, top B/C, a bond center, and a hollow [Figures 1(c, d)].

The calculated results are summarized in Figure 2(a), and the close-up view is shown in Figure 2(b). Formation energies are calculated with an isolated C atom as the reference. We find that the C atom is preferably located on the center of the B–N bond (bond center) in case of adsorption on the h-BN surface. However, the adsorption energy is only 1.01 eV. At the interface, the C atom is preferably located on the H3 site (Cu H3) and forms a bond with a B atom in the h-BN sheet. The adsorption energy is larger by 3.07 eV than that for the adsorption on the h-BN surface. Therefore, the most stable site for the C monomer is Cu H3. The distance between the h-BN sheet and the Cu surface is about 0.34 Å for Cu H3. This indicates that graphene prefers to grow from the interface when the Cu surface is covered with h-BN.

Similarly, we put one C atom at various sites at the graphene/Cu interface. For comparison, we also put it on the graphene surface of graphene/Cu(111). We find that the C atom is preferably located on the center of the C–C bond (bond center) in the case of adsorption on the graphene surface. However, the adsorption energy is only 1.53 eV. At the interface, the C atom is preferably located on the H3 site (Cu H3) and forms a bond with a C atom in the graphene sheet. The adsorption energy is larger by 2.67 eV than that for the adsorption on the graphene surface. The distance

Figure 2: (a) Site-dependent adsorption energies of a C monomer for various surfaces. (b) A close-up view.

between the graphene sheet and the Cu surface is also about 0.34 Å for Cu H3. This also indicates that graphene prefers to grow from the interface when the Cu surface is covered with graphene. This is consistent with the previous theoretical report on graphene/Cu [15].

We further put one C atom at various sites on the bare Cu surface. Even on the bare Cu surface, we find that one C atom is also preferably located on the H3 site (Cu H3). Comparing the formation energies for the different surfaces, the C adsorbate at Cu H3 on h-BN/Cu is less stable by 0.1 eV than on bare Cu or on graphene/Cu. This suggests that the C atom is more difficultly located under h-BN than under graphene or on bare Cu.

Figure 3: Side views of the C monomer adsorbate (a) at the bonding position on the H3 site, (b) at the non-bonding position on the H3 site, and (c) at the subsurface position on the H3 site for h-BN/Cu.

If we check more details of the adsorption positions, we can find that C adsorption at the h-BN/Cu interface has a unique feature (Figure 3). The adsorbed C atom has a chemical bond with a B atom in the h-BN sheet. We find that the C atom can also position on the H3 site without bonding to a B atom in the h-BN sheet [H3 NB, Figure 3(b)]. This ‘non-bonding’ configuration (H3 NB) is less stable than the ‘bonding’ one and is regarded as a metastable configuration. The stability of this metastable configuration is confirmed by a vibrational analysis. The formation energies are -4.08 eV (H3) and -4.07 eV (H3 NB). The distance between the h-BN sheet and the Cu surface is about 0.35 Å for Cu H3 NB. A similar ‘nonbonding’ position is also found for the graphene/Cu interface. The formation energies are -4.19 eV (H3) and -4.05 eV (H3 NB). The distance between the graphene sheet and the Cu surface is also about 0.35 Å for Cu H3 NB. These make the diffusion path of the C adsorbate more complicated than that on the bare surface. The C adsorbate must diffuse from H3 via H3NB for both h-BN/Cu and graphene/Cu.

It is known for the C adsorption on bare Cu that the most stable position is not on the H3 site but at the subsurface H3 site (SS) between the topmost and second Cu atomic layers [14]. For the h-BN/Cu and graphene/Cu interfaces, the situations are the same. In our calculation, the subsurface positions [Figure 3(c)] are more stable by 0.42 eV for h-BN/Cu, 0.31 eV for graphene/Cu, and 0.34 eV for bare Cu than Cu H3. However, it is thought that the SS site is not much important for the CVD growth because of the physical reason, as discussed later.

Next, we evaluate the most preferable path for the lateral diffusion of the C adsorbate. The energy landscape for the lateral diffusion is shown in Figure 4(a). For h-BN/Cu, the C atom diffuses from the bonding position to the neighboring bonding position via the non-bonding position, the valley position, the position on the T4 site, the valley position, and the non-bonding position in sequence (H3-H3NB-valley-T4-valley-H3NB-H3). The barrier height is 0.14 eV, which is governed by the diffusion from the valley position to the position on the T4 site (the H3NB-valley transition). For graphene/Cu, the C atom diffuses from the bonding position to the neighboring bonding position via the non-bonding position, the valley position, the valley position, and the non-bonding position in sequence (H3-H3NB-valley-valley-H3NB-H3). The difference from h-BN/Cu comes from the unstability of the T4 site. The barrier height is 0.26 eV, which is governed by the diffusion from the bonding position on the H3 site to the non-bonding position (H3-H3NB transition). For bare Cu, the C atom diffuses from the position on H3 to the position on neighboring H3 via the valley position, the position on T4, and the valley position in sequence (H3-valley-T4-valley-H3). The barrier height is 0.11 eV, which is governed by the diffusion from the valley position to the position on the T4 site (the valley-T4 transition). This indicates that the C adsorbate more difficultly diffuses under graphene than under h-BN or on bare Cu. We also calculated the change in the height of the C adsorbates in the

Figure 4: Energy landscapes of (a) C-monomer lateral diffusion and (b) C-monomer direct vertical diffusion for various surfaces.

lateral diffusion. The results show that the z -coordinate of the C adsorbate first goes down by $0.39 \text{ \AA}$, next goes up by $0.42 \text{ \AA}$, then goes down again by $0.42 \text{ \AA}$, and finally goes up again by $0.39 \text{ \AA}$ for bare Cu. For h-BN/Cu, it first goes down by $0.64 \text{ \AA}$, next goes up by $0.15 \text{ \AA}$, then goes down again by $0.15 \text{ \AA}$, and finally goes up again by $0.64 \text{ \AA}$. For graphene/Cu, it first goes down by $0.70 \text{ \AA}$, next goes up by $0.13 \text{ \AA}$, then goes down again by $0.13 \text{ \AA}$, and finally goes up again by $0.70 \text{ \AA}$.

To elucidate the C adsorption site under the CVD condition, we further study the diffusion path for C direct vertical diffusion to the subsurface as well as its diffusion barrier [Figure 4(b)]. In case of h-BN/Cu, we find that the C atom diffuses from the bonding position on H3 to the subsurface position via the non-bonding position on H3 (H3-H3NB-SS). The barrier height is 0.33 eV , which is governed by the diffusion from the non-bonding position to the subsurface position (H3NB-SS transition). This barrier height is higher than that of 0.14 eV for the lateral diffusion. In the case of graphene/Cu, the C atom also diffuses from the bonding position on H3 to the subsurface position via the non-bonding position on H3 (H3-H3NB-SS). The diffusion barrier is 0.43 eV , which is also governed by the diffusion from the non-bonding position to the subsurface position (H3NB-SS

transition). This barrier height is higher than that of 0.26 eV for the lateral diffusion. In the case of bare/Cu, the C atom directly diffuses from the position on H3 to the subsurface position (H3-SS). The diffusion barrier is 0.43 eV , which is higher than that of 0.11 eV for the lateral diffusion. Therefore, the diffusion barrier for the direct vertical diffusion is higher by 0.17 eV or more than that for the lateral diffusion.

If we consider the diffusion via the valley position, we find that the barrier heights to the subsurface position are lower for any surfaces. The barrier heights are 0.21 eV , 0.31 eV , and 0.30 eV for h-BN/Cu, graphene/Cu, and bare Cu, respectively. Even though all of these barrier heights are lower than those of the direct vertical diffusion, they are still higher than those of the lateral diffusion. All these results suggest that the C atom diffuses along the interface or the surface rather than penetrates into the subsurface for any type of surface. Some of the previous theoretical studies on bare Cu or graphene/Cu proposed the subsurface diffusion of the C adsorbate rather than the surface or interface diffusion as we propose in this study [14, 17], while another theoretical study agrees with our study [15]. As the C atoms are supplied from the molecular gas to the surface in the CVD condition, it is necessary to calculate the vertical diffusion barriers with much larger cell sizes and with a different van der Waals correction method so as to confirm the preferable diffusion path rigorously.

To investigate the initial stage of nuclear formation, we also calculate the stable adsorption position of a C dimer. We find that one C atoms prefers to adsorb on the nonbond-

Figure 5: Most stable configuration of a C dimer at h-BN/Cu. (a) Top view and (b) front view.

ing position of the H3 site and the other on the position of the T4 site in any surfaces (Figure 5). The formation energy of the dimer is -2.51 eV for h-BN/Cu, -2.29 eV for graphene/Cu, and -2.56 eV for bare Cu. Therefore, the dimer formation is less preferable for graphene/Cu than for h-BN/Cu and for bare Cu, as the C monomer is the most stable for graphene/Cu.

Finally, we study the partially covered surface with a nanoribbon. For this purpose, we use a unit cell of $3 \times 4\sqrt{3}$ Cu(111) covered with a zigzag nanoribbon of the four-atomic-chain width. When the nanoribbon edges are bare, the ribbon are curled up and the edges are terminated by the Cu surface being independent of a h-BN or graphene nanoribbon, and of B-, N-, or C-edge [Figure 6(a)]. However, when the edges are completely terminated by H atoms, the ribbon keeps staying in parallel to the Cu surface [Figure 6(b)]. These results are consistent with the previous report on the graphene nanoribbon on Cu [14]. Furthermore, we calculate the bond formation energy of the H atom to the edge for a free-standing zigzag nanoribbon of the seven-atomic-chain width. The results show that the bond formation energies are -2.16 eV for N-edge of the h-BN nanoribbon, -2.22 eV for B-edge of the h-BN nanoribbon, and -0.09 eV for C-edge of the graphene nanoribbon, when the H atoms are provided from the H_2 gas. In the cases of nanoribbons on the Cu surface, the bond formation energies are changed to -1.08 eV for N-edge of the h-BN nanoribbon, -0.94 eV for B-edge of the h-BN nanoribbon, and -1.12 eV for C-edge of the graphene nanoribbon according to the calculations with a unit cell of $3 \times 6\sqrt{3}$ Cu covered with a zigzag nanoribbon of the seven-atomic-chain width. Since

Figure 6: Side views of the optimized atomic structures for h-BN zigzag nanoribbon on Cu(111). (a) Bare-edge nanoribbon and (b) H-terminated-edge nanoribbon.

our results indicate that the C adsorbate diffuses laterally on the Cu surface during the CVD growth, these results suggest the possibility of controlling the direction of the heterostructure growth by the H-termination. Lateral heterostructures could be realized when the bare edge is terminated by the Cu surface, because the theoretical studies have revealed that graphene flakes with bare edges can grow laterally on the Cu surface [14, 17]. On the other hand, vertical heterostructures could be realized when the edges are terminated by H, because C adsorbates could penetrate into the interface, form dimers, and grow into larger flakes. Since the bond formation energy of the edges with H atoms are different, appropriate choice of a H condition will also lead us to the intentional formation of lateral and vertical heterostructures [13, 14, 16, 17]. This is consistent with experimental findings [12, 28–31].

IV. CONCLUSIONS

To elucidate the bottom-up fabrication of heterostructures of two-dimensional materials, we investigate the C atom adsorption on the Cu(111) surface partially covered with h-BN or graphene by using the first-principles method with the van der Waals correction. We find that the C monomer is more difficultly located under h-BN than under graphene or on bare Cu. The C monomer also more difficultly diffuses under graphene than under h-BN or on bare Cu. In addition, C adsorbates more difficultly form dimers under graphene than under h-BN or on bare Cu. These results suggest that we can control the heterostructure growth by the growth condition. We further find that the shape of h-BN or graphene flake on the Cu surface depends on whether the edge is terminated with H or not. Because the bond formation energy of edges with H atoms is different between h-BN and graphene, we conclude that appropriate choice of H condition will lead us to the intentional formation of lateral and vertical heterostructures.

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