

Erratum to: Influence of metal support in-plane symmetry on the corrugation of hexagonal boron nitride and graphene monolayers

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Erratum to

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The writings of the text on the last line, left column on the 4th page and the text on lines 8th, 10th, 11th and 16th in the 4th paragraph, left column and on lines from 1st to 8th in the 1st paragraph, right column on the 5th page, and the text on line 4th in the 1st paragraph, left column on the 9th page, and Fig. 3 and its caption on the 5th page in the original version of this article were unfortunately incorrect.

Instead of

“direction of the Rh(110) surface (Fig. 2(a)).”

“the hexagonal ring is 2.37 Å,” “3.80 Å and rotated either by 26.36° or 33.64° with respect to the Rh(110) [110],” “stripes is 13.19 Å for both plausible structures.”

“and LEED measurements. It should be noted that according to our tentative model, the lattice parameter of the 2D adlayer was 5.3% smaller than that of the truncated bulk h-BN. This could be because our simple schematics did not consider the small amount of buckling in the 2D adlayer, which would increase the interatomic distances within the h-BN monolayer. Further, it”

“substrate direction.”

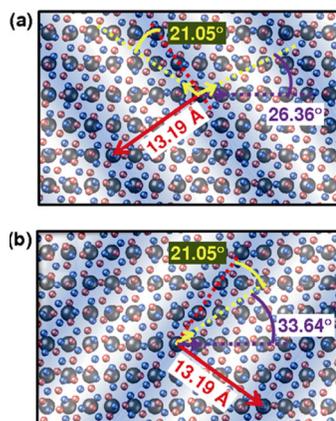


Figure 3 Atomic arrangement of h-BN/Rh(110) system. (a) and (b) Schematic representations of plausible atomic structures, as obtained from structural analyses displayed in Figs. 1 and 2, for the two domains observed at h-BN/Rh(110) interface. In both structures, honeycomb h-BN arrangement showing a periodicity of 2.37 Å was overlaid on rectangular Rh(110) lattice showing periodicities of 2.69 and 3.80 Å with relative orientation angles of (a) 26.36° and (b) 33.64° with respect to substrate [110] direction, respectively. Boron, nitrogen, and rhodium atoms are represented by salmon pink, blue, and grey spheres, respectively.

It should read

“direction in the reciprocal space of the Rh(110) surface (Fig. 2(a)).”

“the hexagonal ring is 2.51 Å,” “3.81 Å and rotated either by 26.28° or 33.72° with respect to the Rh(110) [001],” “stripes is 13.99 Å for both plausible structures.”

“and LEED measurements. It”

“substrate direction in the reciprocal space.”

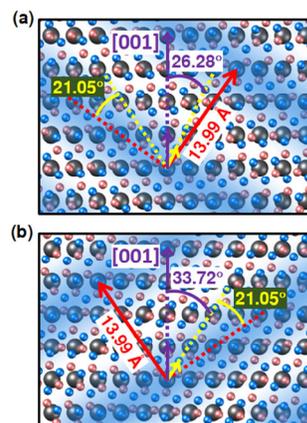


Figure 3 Atomic arrangement of h-BN/Rh(110) system. (a) and (b) Schematic representations of plausible atomic structures, as obtained from structural analyses displayed in Figs. 1 and 2, for the two domains observed at h-BN/Rh(110) interface. In both structures, honeycomb h-BN arrangement showing a periodicity of 2.51 Å was overlaid on rectangular Rh(110) lattice showing periodicities of 2.69 and 3.81 Å with relative orientation angles of (a) 26.28° and (b) 33.72° with respect to substrate [001] direction, respectively. Boron, nitrogen, and rhodium atoms are represented by salmon pink, blue, and grey spheres, respectively. In these schematics, the relative translation between h-BN and Rh(110) lattices has been arbitrarily chosen.

To make it easier to understand, herein, we list the revised text in Section 3.1 Structure of the h-BN/Rh(110) interface and Section 4 Conclusions along with Figure 3 and its caption.

3.1 Structure of the h-BN/Rh(110) interface

The prepared Rh(110) surfaces exhibited large terraces separated by monoatomic and multiatomic steps (Fig. S1 in the Electronic Supplementary Material (ESM)). In turn, STM images of h-BN monolayers grown on Rh(110) surfaces were characterized by a

stripe-like moiré pattern, as shown in Figs. 1(a) and 1(b). Along the STM study presented here a unique moiré pattern has been found on the h-BN monolayers grown on the Rh(110) surfaces. This pattern of quasi-1D regularly spaced stripes results from the superposition of the honeycomb structure of the h-BN monolayer with the rectangular lattice of the Rh(110) substrate. High-resolution STM images reveal the atomic periodicity of the h-BN lattice together with the moiré stripes (Fig. 1(b)). The spacing between stripes is $13 \pm 1 \text{ \AA}$, and the angle between the moiré fringes and the h-BN lattice is around 20° . Likewise, the STM-apparent corrugation measured across the moiré rows was systematically smaller than 30 pm . As an example, Fig. 1(c) shows a topography profile measured across three moiré stripes along the green line in Fig. 1(b).

LEED measurements reveal the existence of two possible orientations of the h-BN lattice with relative angles of around 28° and 36° with respect to the $[1\bar{1}0]$ direction in the reciprocal space of the Rh(110) surface (Fig. 2(a)). To simplify the interpretation of the LEED pattern, a schematic is shown in Fig. 2(b), where the Rh(110) spots are represented by white circles, the spots corresponding to the atomic periodicities of both h-BN domains are indicated by red and green circumferences, respectively, and the satellite spots due to the moiré pattern are denoted by yellow dots. Deeper examination of the LEED pattern showed that the two rotational domains are specular with respect to both the $[1\bar{1}0]$ and $[001]$ directions of the Rh(110) surface, since due to the hexagonal symmetry of h-BN and to the rectangular one of the substrate, a rotation angle of 36° is completely equivalent to -28° and vice versa. It means that both domains are isostructural, which is consistent with the existence of only one moiré pattern along the h-BN/Rh(110) interface (Fig. S2 in the ESM).

It should be noted that while the adsorption of some species on Rh(110) is known to induce surface reconstruction [52–56], the h-BN layer did not change the ordering of the underlying metal surface, which was inferred by comparing the LEED patterns obtained prior to (Fig. S1(b) in the ESM) and after (Fig. 2(a)) the growth of the h-BN monolayer, confirming that the Rh(110) surface showed the same periodicity in both LEED patterns.

STM imaging also showed the two possible h-BN lattice orientations with respect to the Rh(110) surface. Figure 2(c) shows a STM topograph acquired from the surroundings of a domain boundary between two h-BN flakes exhibiting different orientations with respect to the Rh(110) surface. The structural equivalence of these domains is reflected in the fact that the angle between the moiré stripes and the atomic periodicity of h-BN are identical (around 20°) for both flakes, within the precision limits of STM imaging. Finally, it is noteworthy to mention that the angle between the h-BN lattices of both flakes is around 9° , in good agreement with the angle between the LEED spots originating from the electron diffraction from the lattices of the two domains coexisting at the h-BN/Rh(110) interface, as shown in Figs. 2(a) and 2(b).

Plausible schematic representations of the atomic structures of the two rotational domains were constructed based on STM and LEED structural characterizations of the h-BN monolayers epitaxially grown on Rh(110) surfaces. As shown in Fig. 3, the superposition of a honeycomb arrangement of h-BN, in which the distance between the atoms at alternate positions of the hexagonal ring is 2.51 \AA , with a rectangular Rh(110) lattice showing periodicities of 2.69 and 3.81 \AA and rotated either by 26.28° or 33.72° with respect to the Rh(110) $[001]$ direction gave rise to a stripe-like superstructure commensurate across the stripes and incommensurate along them. For both orientations, the angle between the h-BN lattice and the moiré fringes is 21.05° . The spacing between the stripes is 13.99 \AA for both plausible structures. Therefore, the proposed atomic structures reproduce well all the experimental findings obtained by STM and LEED measurements. It should be mentioned that

orientations resulting from the rotation by an angle of 180° of the h-BN lattice for each one of the two domains also could be present at the interface.

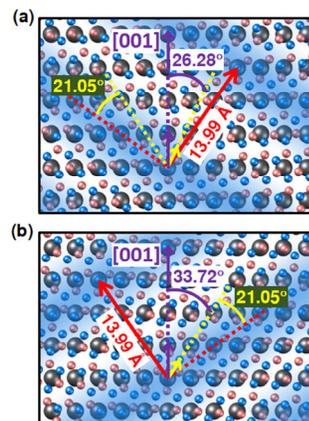


Figure 3 Atomic arrangement of h-BN/Rh(110) system. (a) and (b) Schematic representations of plausible atomic structures, as obtained from structural analyses displayed in Figs. 1 and 2, for the two domains observed at h-BN/Rh(110) interface. In both structures, honeycomb h-BN arrangement showing a periodicity of 2.51 \AA was overlaid on rectangular Rh(110) lattice showing periodicities of 2.69 and 3.81 \AA with relative orientation angles of (a) 26.28° and (b) 33.72° with respect to substrate $[001]$ direction, respectively. Boron, nitrogen, and rhodium atoms are represented by salmon pink, blue, and grey spheres, respectively. In these schematics, the relative translation between h-BN and Rh(110) lattices has been arbitrarily chosen.

4 Conclusions

The structural properties of h-BN monolayers grown on Rh(110) were studied by STM and LEED. The h-BN layer can adopt only two possible orientations with respect to the Rh(110) surface with relative angles of around 28° and 36° referred to the $[1\bar{1}0]$ substrate direction in the reciprocal space. For both orientations, which result in two specular domains with respect to the $[1\bar{1}0]$ and $[001]$ substrate directions, the superposition of the h-BN and Rh(110) lattices gives rise to a quasi-1D stripe-like moiré pattern showing a periodicity of $13 \pm 1 \text{ \AA}$ and rotated about 20° with respect to the 2D adlayer lattice. Consistent with the existence of only these two isostructural configurations, the analysis of the boundary between flakes exhibiting different rotational domains suggested the h-BN layer was significantly anchored to the substrate. Nevertheless, opposite to what happens in strongly interacting lattice-mismatched graphene/metal and h-BN/metal systems with (111)-oriented fcc substrates or (0001)-terminated hcp ones, STM images showed that the apparent corrugations of moiré stripes measured at the h-BN/Rh(110) and graphene/Rh(110) interfaces are rather small. This discrepancy has been explained in terms of the possible high symmetry chemical environments that can be found within the resulting moiré cells depending on substrate crystallographic orientation. On the basis of such considerations, lattice-mismatched interfaces of graphene and h-BN monolayers with substrates exhibiting hexagonal or pseudohexagonal symmetries, especially 3d and 4d transition metals showing half-filled d bands, are more likely to be strongly corrugated. In contrast, for other substrate symmetries the interface is expected to be rather flat. Thus, this report provides valuable information toward solving the long-standing problem of predicting the most relevant properties graphene and h-BN monolayers will exhibit after their growth on a given substrate. Likewise, such information could be used, for instance, to tune the electronic properties of metal-supported graphene or h-BN monolayers or to develop nanotemplates exhibiting different geometries and adsorbate affinities for growing superlattices of atoms, molecules, and clusters.