Elemental structure in Si(110)-''16×2'' revealed by scanning tunneling microscopy

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Atomic structures of the clean Si(110)-''16×2'' surface are studied by scanning tunneling microscopy (STM). High-resolution STM images reveal that the elemental structure in the ''16×2'' is a pair of pentagons. In the empty-states images the elemental structure is clearly resolved in ten protrusions, while in eight in the filled-states images. In order to clarify the atomic arrangement of the pentagons, we pay attention to the disordered area where the elemental structures are isolated on the bulk-terminated surface. The bulk-terminated surface structure, on which the pentagons are located, is well understood by the rotational-relaxation structural model. In consideration of the registry of the pentagon for the rotational-relaxation structure, a ''tetramer-interstitial'' model is proposed for the elemental structure, together with three other possible structural models.

I. INTRODUCTION

Various reconstructions such as 2×1, 5×1, 7×1, 9×1, 4×5, and ''16×2'' (the basic translation vectors **a**=[001] and **b**=1/2[110] are used here) have been reported on Si(110) surfaces by low-energy electron diffraction and reflection high-energy electron diffraction.[1–5] Recently it was revealed by Auger electron spectroscopy (AES) that the above reconstructions other than the ''16×2'' were induced by 2~7% nickel impurities.[6] Scanning tunneling microscopy (STM) studies[7–11] have revealed that the ''16×2'' structure consists of zig-zag chain protrusions due to the topmost atoms aligned up and down alternatively in monatomic height. Similar up-and-down structure have been reported on Ge(110),[12] SiGe/Si(110),[13] and Sn/Si(110) surfaces,[14] those belong to the same IV group in the periodic table as Si. Then, it is probable that the up-and-down structure is the most stable form of clean (110) surfaces of the diamond structure. To date some structural models for the ''16×2'' have been proposed using adatoms, dimers, trimers, and missing rows,[10,15,16] and these models were discussed by using angle-resolved ultraviolet photoelectron spectroscopy,[17] temperature-programmed desorption,[18] and theoretical studies such as total-energy minimization approach.[15,19] However the precise atomic arrangement has not been elucidated yet.

In this paper, we present atomistic study of the ''16×2'' structure by use of STM. High-resolution STM images reveal that the elemental structure in the ''16×2'' is a pair of pentagons. In order to determine the atomic arrangement of the pentagon we pay attention to a less ordered region of the ''16×2'' where the lattice arrangement of the substrate can be simultaneously observed. On the basis of the atomistic analysis, we propose structural models for the elemental structure in the ''16×2.''

II. EXPERIMENT

The experiments were performed in ultrahigh vacuum (UHV) with a base pressure of about 1×10^{-8} Pa. The specimen used was a phosphorus-doped *n*-type Si(110) wafer of 2.04-2.44 Ω·cm cut to a size of $15\times2\times0.3\,\mathrm{mm}^3$. It was degassed for fifteen hours at 600 °C and cleaned by flashing at 1200 °C followed by annealing at 600 °C. Then, the surface showed a ''16×2'' structure. The temperatures were measured using a previously calibrated optical pyrometer and STM observations were performed at room temperature. Electrochemically etched tungsten tips were used, and prior to STM observations, the oxide layer covered on the tip surface was removed by electron bombardment below a pressure of about 1×10^{-6} Pa.

III. RESULTS AND DISCUSSION

Figure 1(a) shows an image of the Si(110)-''16×2'' surface obtained at a sample voltage of −1.01 V and a constant current of 0.20 nA. The image shows protrusions of parallel zig-zag chains that are arranged up and down alternatively in monatomic height with the periodicity of (5,11)×(2,2). The chains are oriented along the [112] and/or [112] directions, forming two domains.[5] There exist disordered regions in the lower left and lower right in Fig. 1(a). Figure 1(b) shows an enlarged image of the area where ordered and disordered regions are coexisting. It is revealed that both regions consist of the same elemental structures indicated by two types of elliptic circles with different orientations, right side up (*R*) and left side up (*L*). They are crystallographically equivalent. When *R* (or *L*) arranges sequentially along the [112] (or [112]) direction, the chainlike structure in the ''16×2'' is completed. Then, it is important to clarify the atomic arrangement of the elemental structure.

Figure 2 shows high-resolution filled (a) and empty (b) states images of the ''16×2'' structure. The elemental structure is clearly resolved in ten protrusions in the empty states, while in eight in the filled states. From the shape we call the element a pair of pentagons (''PP'' hereafter). A similar structure consisting of eight protrusions was reported on the 5×1 surface and then was called ''two tetramers''[7] or ''octet.''[20] Van Loenen *et al.* suggested that the ''octets'' are stacked in the [112] or [112] direction to form the ''16×2'' structure.[9] Table I shows the constituent elements of the ''16×2,'' and the expected number of protrusions in a structural unit corresponding to the PP for previously proposed structural models. The models were composed of adatoms, dimers, trimers, and missing rows.[10,15,16,21] However,

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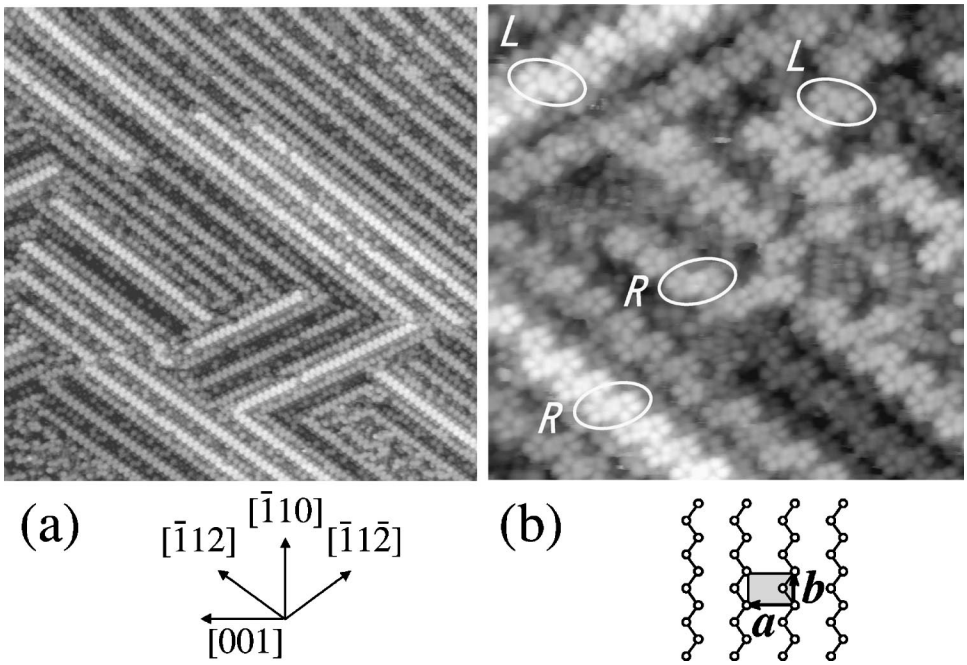

FIG. 1. STM topographic images of a clean Si(110) surface. (a) A wide scan image ($V_s=-1.01$ V, $I=0.20$ nA, 90 nm×90 nm); (b) an enlarged image ($V_s=0.52$ V, $I=0.19$ nA, 17 nm×17 nm). The elemental structures are indicated by elliptic circles, *R* and *L*. At the lower part the bulk-terminated Si lattice and the 1×1 unit cell are shown.

none of structural models can explain the number of protrusions in the PP observed in this study. Then, we explore structural model of the PP.

In order to determine the atomic structure of the PP, we pay attention to a disordered region where an individual PP is imaged isolatedly on the bulk-terminated surface, because it is possible to know directly the registry of the PP with respect to the substrate. Figure 3(a) shows a drift-corrected STM image obtained at the filled states, where several isolated PP's together with the underlying substrate structure along the [110] direction [indicated by *X*-*X*, *Y*-*Y* in Fig. 3(a)] are observed. A similar underlying structure was observed on the 5×1 surface and called ''tube'' by Becker Swartzentruber, and Vickers.[7] The bulk-terminated Si lattice

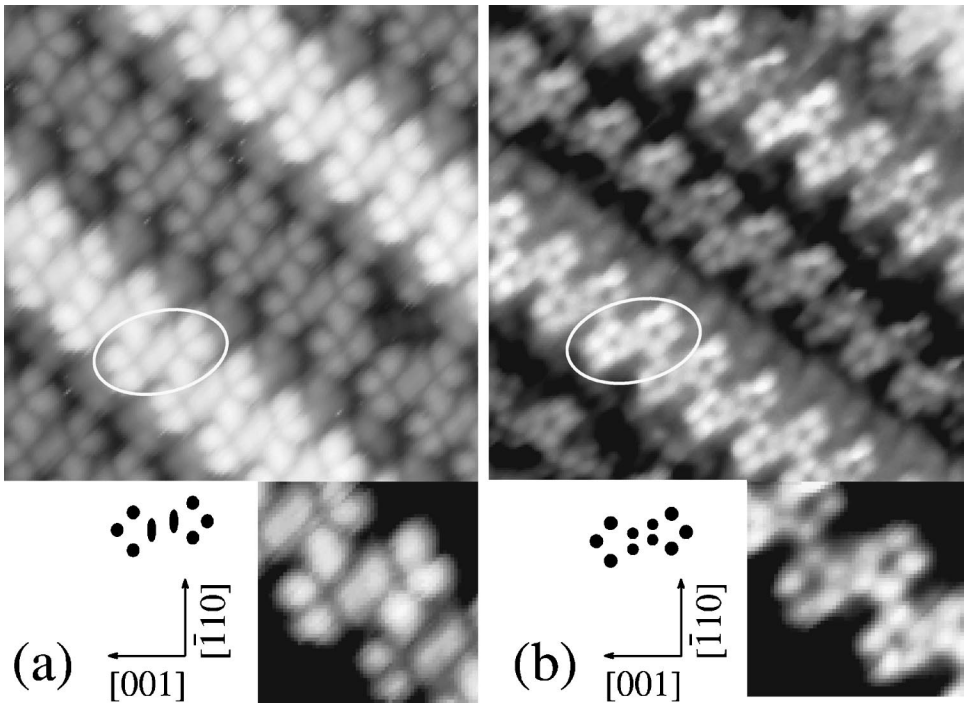

FIG. 2. High-resolution STM topographic images of the ''16×2'' structure in the filled states [(a) $V_s=-1.00$ V, $I=0.19$ nA, 10 nm ×10 nm] and in the empty states [(b) $V_s=1.20$ V, $I=0.20$ nA, 10 nm×10 nm]. The elemental structure in the ''16×2'' is indicated by the elliptic circle and schematically shown at the lower part. Magnified STM images are also shown.

TABLE I. The elements and the expected number of STM protrusions in the elemental structure corresponding to the PP for previously proposed structural models.

Model	Elements	Number of expected protrusions in a structural unit corresponding to a pair of pentagons
Dimer adatom[a]	Adatoms, dimers	8 (8 adatoms)
Rumpling[b]	Dimers, trimers	9 (5 dimers and 4 trimers)
Missing row-adatom[c]	Adatoms, missing row	8 (adatoms)
Stretched-hexagon[d]	Adatoms	7 (5 adatoms and 2 shared adatoms)
Tetramer-interstitial[e]	Adatoms, interstitials	10 (8 adatoms and 2 substrate atoms)

[a]Reference 15.
[b]Reference 10.
[c]Reference 16.
[d]Reference 21.
[e]This work.

is superimposed in Fig. 3(a), supposing that a chain of atoms along the [110] direction is located between X-X and Y-Y. The height difference between the PP and the ''tube'' is measured at about 0.1 nm, which corresponds to half the lattice spacing of (110) bulk layers. The value is almost the same as reported by Lutz Feenstra, and Chu (0.07 nm).[20] In the present high-resolution image of the ''tube,'' the periodicity of $\mathbf{b}(|\mathbf{b}|=0.384\,\mathrm{nm})$ along the [110] direction can be clearly imaged. Moreover, the location of the ''tube'' in the [001] direction shifts whenever it meets the PP. For example, between the PP's labeled as R and L, the ''tube'' is located on X-X but otherwise on Y-Y. The value of the shift is measured as about 0.14 nm.

As the candidates for the structure of the ''tube'' we examine two types of atomic configurations, the row of adatoms and the rotational-relaxation (RR) structure.[22,23] In the

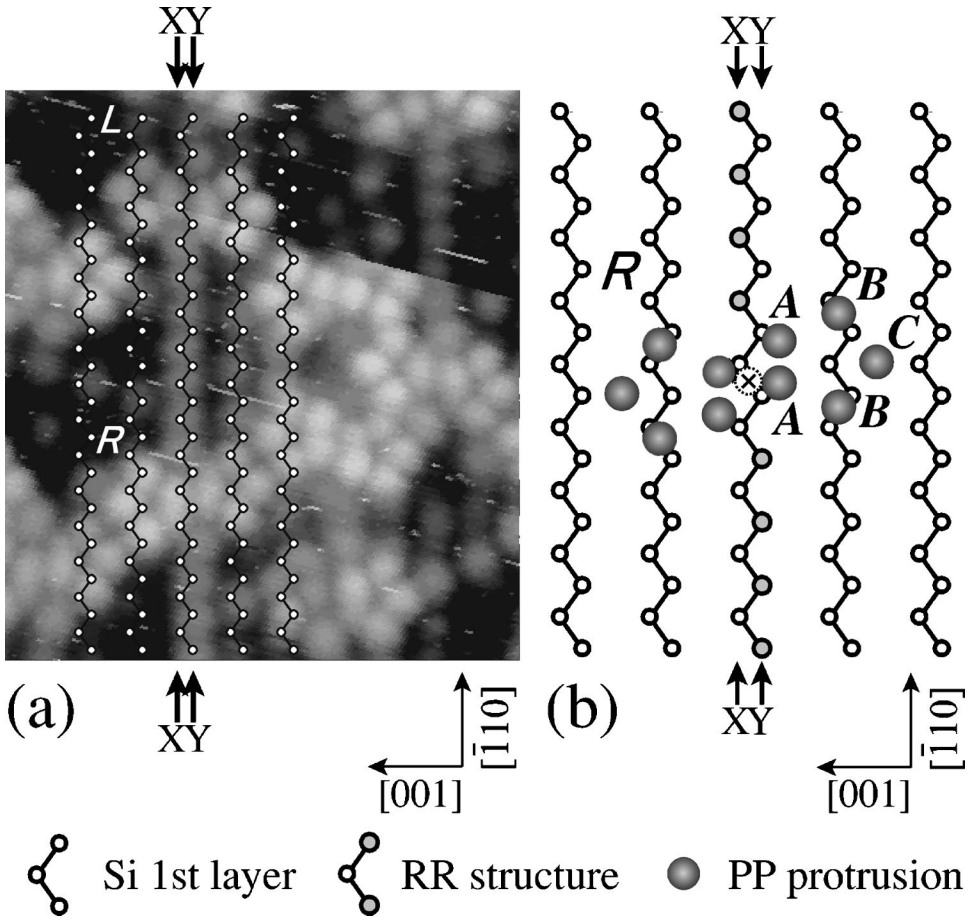

FIG. 3. (a) An STM topographic image obtained in the disordered region ($V_s=-1.6$ V, $I=0.10$ nA, 6 nm×5.5 nm). The bulk-terminated Si lattice is superimposed, supposing that a chain of atoms along the [110] direction is located between X-X and Y-Y indicated by arrows. (b) Schematics of the protrusions of the PP located on the underlying RR structure. A cross point shows the symmetric center of a pair of pentagons.

former structure the adatoms are located on the hollow site of the substrate lattice as previously proposed by Shkrebtii *et al.*[15] Two equivalent hollow sites exist between the adjacent atomic rows, which could account for the ''shift'' mentioned above. However, to realize the sequential arrangement of the adatoms along the [110] direction with **b** periodicity, each substrate atom must bond with two adatoms and totally it forms fivefold bonding coordination, which seems energetically unprobable. Moreover, we hardly observe vacancies of adatoms in the ''tube'' experimentally. On the other hand, the latter RR structure was previously proposed by Harrison[22] and Chadi[23] for the surface-relaxation structure on the clean Si(110) surface. In this model, surface atoms are buckled outward and inward alternatively by surface relaxation. To date the RR structure has not been observed on the Si(110) surfaces but is well known as a stable structure on the cleaved (110) surface of III-V semiconductors such as GaAs.[24] If we assume that the ''tube'' corresponds to the RR structure, the ''shift'' can be explained by the change in the buckled direction. Then the shift is estimated about 0.20 nm by summation of ideal distance (0.136 nm) and twice the calculated displacement[19] (2×0.035 nm), in agreement with the measured value. From the above discussion we conclude that the substrate structure corresponds to the RR structure rather than the row of adatoms, and the outward-buckled atoms in the RR structure are predominantly observed as the ''tube'' in Fig. 3(a).

Figure 3(b) shows an illustration of the observed position of the PP [''*R*'' in Fig. 3(a)] on the RR structure. Judging from the illustration as well as the STM images, the pentagons are symmetric with each other around the cross point. Therefore, we pay attention to the pentagon at the right side. Five protrusions of pentagon are classified into three kinds of protrusions, in consideration of the STM images and the locations on the substrate lattice (labeled as *A*, *B*, and *C*). The protrusions *A* and *B* are located on the row of substrate atoms and *C* is in between. The height difference between the PP and the ''tube,'' 0.1 nm, is comparable to the value of adatom on the hollow site studied theoretically by Menon, Lathiotakis, and Andriotis.[19] Then, most of protrusions of the PP are likely to correspond to adsorbed Si atoms, which is consistent with previous experimental studies.[17,18]

In consideration of the polarity dependence of bias voltage to the STM images of the pentagon (Fig. 2), adjacent *A* adatoms seem to have formed a dimer from the analogy with the Si(100)2×1 surface.[25] In addition, from Fig. 3(b) they are likely to bond with the substrate atoms located below, which could affect the buckling direction in the substrate by charge transfer. In fact, it is reported that the adatom on Si(110) loses electrons to the substrate.[19]

At the 5×1 surface, the ''tube'' was observed every second row and missing-row model was considered.[7,16] However, we sometimes observe that the pentagons are arranged with one time periodicity in the [001] direction, for instance, in the disordered region or the Sn-induced reconstructions.[14] Then, we exclude possibility of the missing row model in the present study.

Tentatively we propose four possible atomistic models of the PP based on the above discussions as shown in Fig. 4. Figure 4(a) shows the ''adatom-tetramer'' model, where *B* atoms bond with *A* atoms forming tetramer. This model is similar to the tetramer model of clean Si(114) and Si(115) surfaces,[26] although the bonding coordination of the substrate atom which bonds with both *B* atoms is fivefold, being

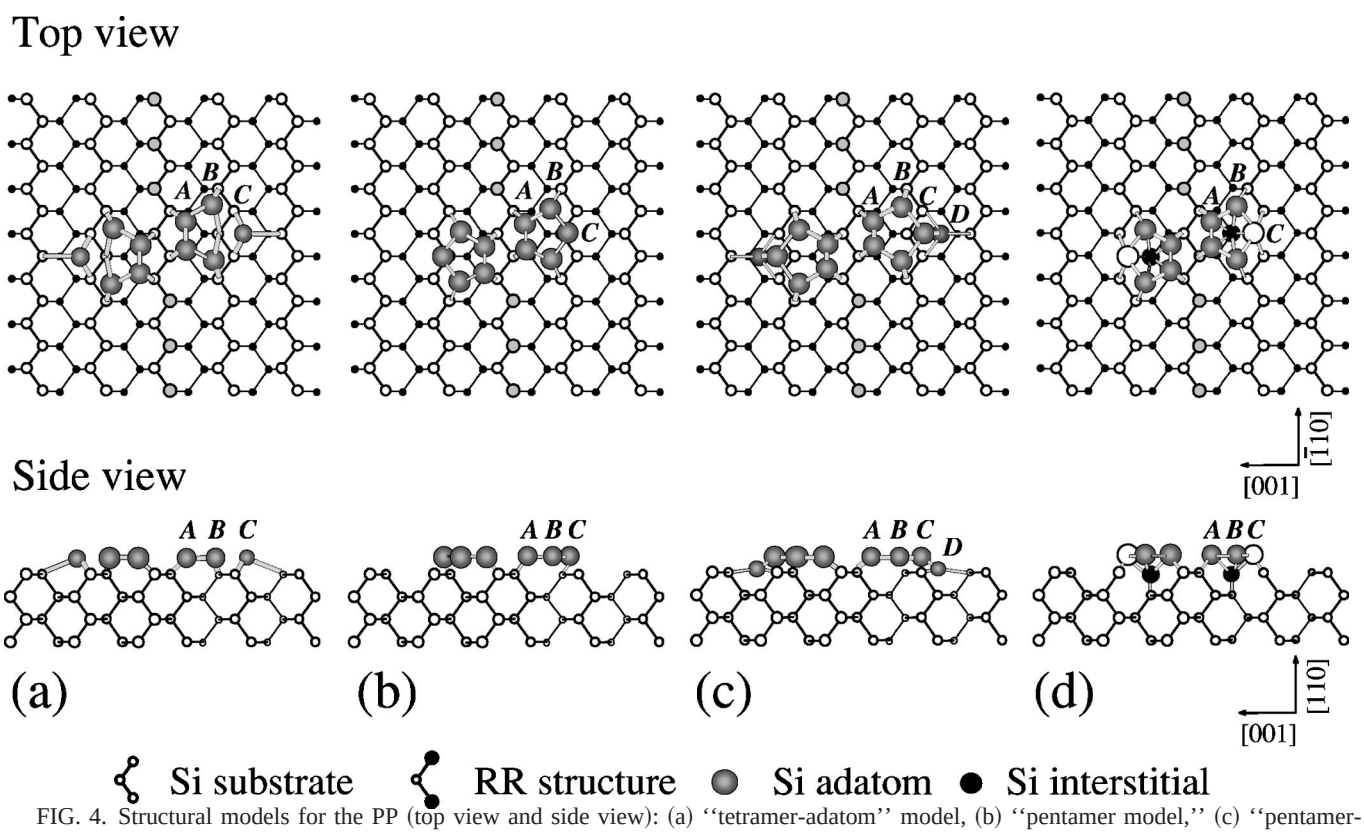

FIG. 4. Structural models for the PP (top view and side view): (a) ''tetramer-adatom'' model, (b) ''pentamer model,'' (c) ''pentamer-adatom'' model, and (d) ''tetramer-interstitial'' model. Adatoms are shown as shaded circles in each structural model and labeled as ''*A*''-''*D*.'' Surface interstitial atoms are shown as solid circles in (d).

different from the tetramer model. The outermost *C* adatom is located on the hollow site of the substrate as proposed by Shkrebtii and Menon *et al.*[15,19] In this model the tetramer (*A* and *B* adatoms) and the adatom (*C*) are separated from each other. However, experimentally they are always observed in one body, with almost same brightness.

Figure 4(b) shows the ''pentamer'' model, where five adatoms bond with each other. Though the size of the pentamer seems slightly smaller than that of the STM images, it is natural when the extension of dangling bonds of adatoms is considered. In the ''pentamer'' model the orientation of the backbond of *C* adatom is reversely inclined. Figure 4(c) shows the ''adatom-pentamer'' model, where *C* adatoms sit on additional adatoms (*D*) on the hollow site, while the network of the pentamer is retained. The configuration turns the orientation of the backbond of *C* adatom. However these models [Fig. 4(b) and (c)] seem strained.

Figure 4(d) shows the ''tetramer-interstitial'' model, where the pentamer is stabilized by the surface self interstitial. In this model the pentagon consists of a tetramer (*A* and *B* adatoms) and a substrate atom (open circle labeled as ''*C*''). The *C* atom protrudes toward the vacuum in the presence of the sixfold coordinated interstitial. This model is very similar to the structural elements of tetramer and interstitial on clean Si(113) and Ge (113)-3×1 and 3×2 surfaces[27,28] except for the bonding coordination of the *C* atom. This unusual sixfold coordinated surface self interstitial is justified by the stability of the similar [110]-split bulk interstitial defect.[27,28]

We consider that the ''tetramer-interstitial'' model [Fig. 4(d)] is most appropriate for the pentagon which we observed in Si(110). However, at present we cannot exclude the other models [Figs. 4(a)–4(c)]. Detailed theoretical study will be necessary to determine the precise atomic arrangement.

Finally, in order to show the structural relation of the PP's in the ''16×2,'' we illustrate the arrangement of the PP's using the ''tetramer-interstitial'' model in Fig. 5. The translational symmetric unit of $(5,11)\times(2,2)$ is outlined at the upper layer PP's. The PP in the lower layer is centered in the solid line. At this stage, however, we could not illustrate atomic structures at the step which would play an important role in stabilizing the ''16×2'' reconstruction. The elucidation of the step structure is now under investigation.

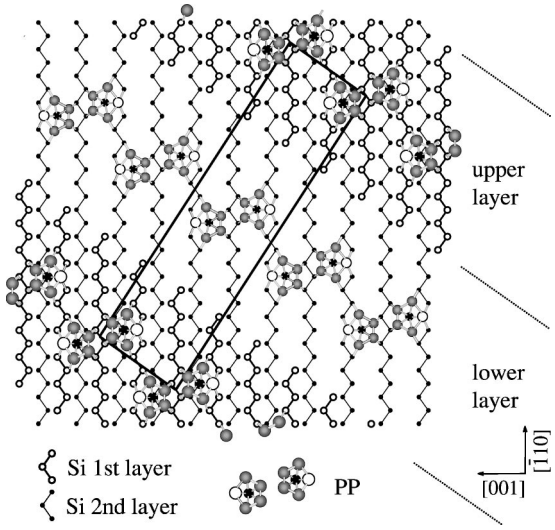

FIG. 5. The arrangement of the PP's in the ''16×2'' reconstruction using the ''tetramer-interstitial'' model. The translational symmetric unit of $(\bar{5},11)\times(2,2)$ is outlined at the upper layer PP's.

IV. CONCLUSION

We have investigated the Si(110)-''16×2'' structure by STM. High-resolution STM images have revealed that elemental unit structure in the ''16×2'' is a pair of pentagons. The surface-relaxation structure of the bulk-terminated surface was also observed, and the position of atoms in the pentagon was uniquely determined with respect to the bulk-terminated surface. Then we propose here four structural models, the ''adatom-tetramer'' model, ''pentamer'' model, ''adatom-pentamer'' model, and ''tetramer-interstitial'' model for the pair of pentagons. We consider the last model most appropriate. In order to determine which structural model is most likely, further theoretical investigation is required.

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