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Atomic arrangements of 16×2 and (17,15,1) 2×1 structures on a Si(110) surface

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The 16×2 structure and the (17,15,1) 2×1 structure have been found on a Si(110) surface. Scanning-tunneling-microscope (STM) observations showed that the 16×2 structure was similar to the (17,15,1) 2×1 structure and both of them had a common structural unit. In the top view, the 16×2 structure is identical to the (17,15,1) 2×1 structure, but in the side view, the 16×2 structure is on the (110) plane and the (17,15,1) 2×1 structure on the (17,15,1) vicinal plane. A unit cell of the (17,15,1) 2×1 structure is identical to the common unit cell and that of the 16×2 structure is represented by a pair of the upper and lower terraces formed by the common unit cell. A rumpling model for the 16×2 structure and the (17,15,1) 2×1 structure is proposed on the basis of STM and ultraviolet-photoelectron-spectroscopy results, where Si atoms are displaced in the direction normal to the (110) surface and the displacement oscillates along the [110] direction. The corrugation in the rumpling is 0.5 nm.

I. INTRODUCTION

A lot of structures, for example 5×4,[1-5] 1×2,[2,4] 1×5,[2-4,6-9] 16×2,[10-18] and (17,15,1) 2×1,[4,13,19] have been found on clean Si(110) surfaces. The 16×2 structure was found in 1980 by using reflection high-energy electron diffraction (RHEED).[10] In the RHEED patterns, superstructure spots divide the fundamental spots 00 and 11 or 00 and $\bar{1}\bar{1}$ into 16. Accordingly, the structure was called the 16×2, or, briefly, the 16 structure. The structure is written as $\sqrt{171}\times\sqrt{6}-R\,(32.7°,35.3°)$ in Wood's notation[20] and $(2,2)\times(\bar{1}\bar{1},5)$ in our notation.[1] Ichinokawa *et al.* reported that the 5×4, 1×2, and 1×5 structures were induced by a small amount of Ni deposition on a Si(110) surface, giving the 16×2 structure.[11] Olshanetsky and Shklyaev found the (17,15,1) 2×1 structure in 1977 by using low-energy electron diffraction (LEED).[4] Van Loenen, Dijkkamp, and Hoeven found the coexistence of the 16×2 and (17,15,1) 2×1 structures in 1988 by using the scanning tunneling microscope (STM).[13]

Ampo *et al.* made a step structure model for the 16×2 structure based on analysis of the LEED pattern.[21] Van Loenen, Dijkkamp, and Hoeven confirmed it by STM observation. In this structure, repetition of the upper and lower terraces is proposed.[13] We reported a structural model composed of Si adatoms and the repetition of the upper and lower terraces.[22]

Recently, high-temperature scanning tunneling microscopy (HTSTM) was developed to observe the dynamic behavior of surface atoms at high temperature up to 900 °C, and succeeded in analyzing the movement of surface atoms at a phase transition of a Si(111) surface.[23] The HTSTM observation showed the growth of the vicinal plane (17,15,1) at the atomic level on a Si(110) surface.[24,25] The (17,15,1) 2×1 structure was formed at the side of the hillock at 710 °C and developed on the (110) surface at 707 °C. The size of this structure was dependent on the size of the hillock. The 16×2 structure developed on flat areas at the top and bottom of the (17,15,1) 2×1 structure. HTSTM observation showed that the 16×2 structure was similar to the (17,15,1) 2×1 structure; it grew from a common structural unit and the (17,15,1) 2×1 structure was more stable than the 16×2 structure.

In this paper, the structural similarities and differences are shown from observation of the crystal growth of the 16×2 and the (17,15,1) 2×1 structures, and the atomic arrangement common to these structures is discussed with reference to ultraviolet-photoelectron-spectroscopy (UPS) results.

II. EXPERIMENTAL

A mirror-polished (110) surface of a *p*-type silicon wafer having a resistivity of 100 Ω cm was prepared. Its crystallographic orientation was determined by the Laue method of x-ray diffraction. The surface was (110) within an accuracy of 1°. Samples of $1\times7\times0.3\ \mathrm{mm}^3$ in size were cut from the wafer. They were rinsed in acetone before mounting on a tantalum sample holder in a STM apparatus. Surface cleaning was performed by annealing the sample at 600 °C for 60 h followed by several cycles of heating to 1200 °C in the STM chamber under a vacuum kept at better than 1×10^{-7} Pa. The vacuum during observation was better than 2×10^{-8} Pa at about 700 °C. The heating was done by a direct current. The sample temperature was measured by a digital infrared-radiation thermometer with a wavelength of $0.96\ \mu$m.

III. RESULTS

After heating the Si(110) surface at 1200 °C, the sample was cooled down to 710 °C. Figure 1 shows a HTSTM image at this temperature in constant-current mode. Two large hillocks are observed with sizes of about $50\times50\ \mathrm{nm}^2$ and about $25\times20\ \mathrm{nm}^2$. Eight pairs of white and dark stripes can be seen on the side of the larger hillock, where a faceted structure with seven steps is formed. Further, some steps with notched edges are seen to flow on the (110) surface and others are in contact with the hillock. When the surface was cooled down by a few degrees

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FIG. 1. HTSTM image at 710 °C in constant-current mode. Scanning area is 100×100 nm^2, sample bias voltage −0.84 V, and tunneling current 0.2 nA.

from 710 °C, the faceted structure progressed on the surface in the ⟨112⟩ direction. From measurements of the surface corrugation and the crystal orientation, the {17,15,1} vicinal plane was found to be made of the successive stacking of (110) atomic layers of 2.5 nm width and 0.19 nm thickness.

The sample was cooled down to 690 °C while observing the crystal growth. Figure 2 shows a HTSTM image at this temperature in constant-height mode, where two hillocks are confirmed. Periodic arrangements of clear white and narrow gray lines and of clear white and wide black lines represent the (17,15,1) vicinal plane and a faceted structure on the flat (110) plane, respectively. The faceted structure began to be formed at the uppermost and then at the lowermost layer of the (17,15,1) vicinal plane.

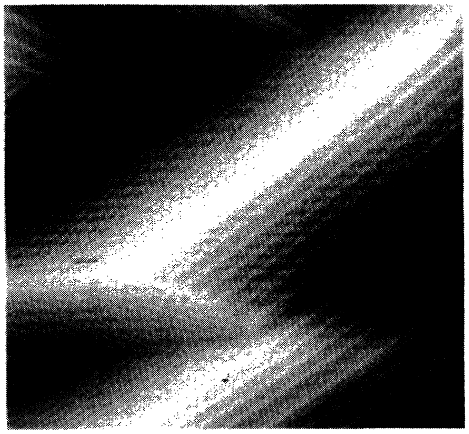

FIG. 3. HTSTM image at 655 °C in constant-current mode. Scanning area is 100×100 nm^2, sample bias voltage −0.73 V, and tunneling current 0.2 nA.

Figure 3 shows a HTSTM image at 655 °C in constant-current mode, where the (17,15,1) vicinal plane and the faceted structure are confirmed. In the figure, the vicinal plane has about 20 steps. The STM images for both structures are similar.

A STM image of an empty state of the faceted structure on the flat (110) plane is shown with constant-current mode in Fig. 4. The image was taken at room temperature. In it, the rectangle shows the unit cell of the structure with size 1.33×5 nm^2. It was determined that the faceted structure was a 16×2 structure. The letters A, B, and C represent the bright positions in the image. The bright zigzag chains are clearly seen to run parallel to each other. Furthermore, faint zigzag chains are also seen to run between them in parallel. The spheres in the chains are clearly resolved. The distance between the

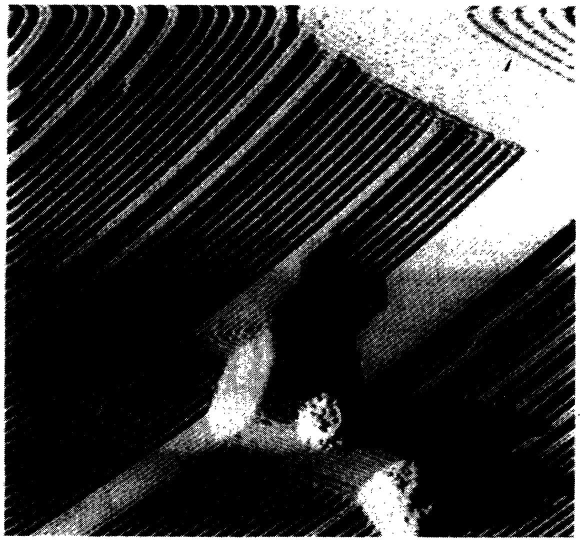

FIG. 2. HTSTM image at 690 °C in constant-height mode. Scanning area is 200×200 nm^2, sample bias voltage −1.22 V, and tunneling current 0.09 nA.

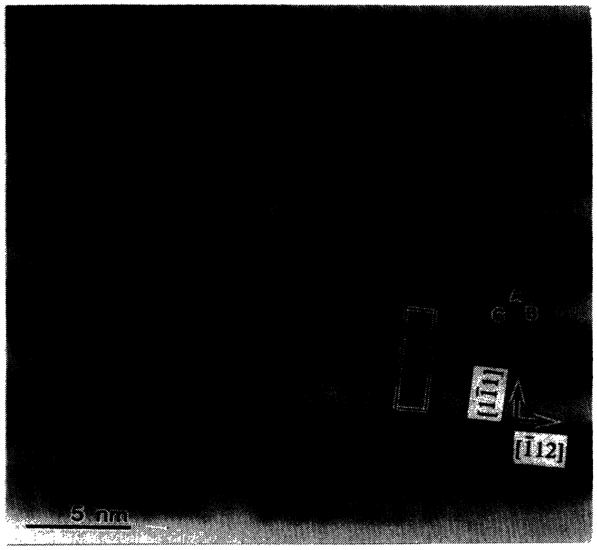

FIG. 4. STM image of the empty surface state of the 16×2 structure at room temperature. Scanning area is 28×29 nm^2, sample bias voltage 3.0 V, and tunneling current 0.3 nA.

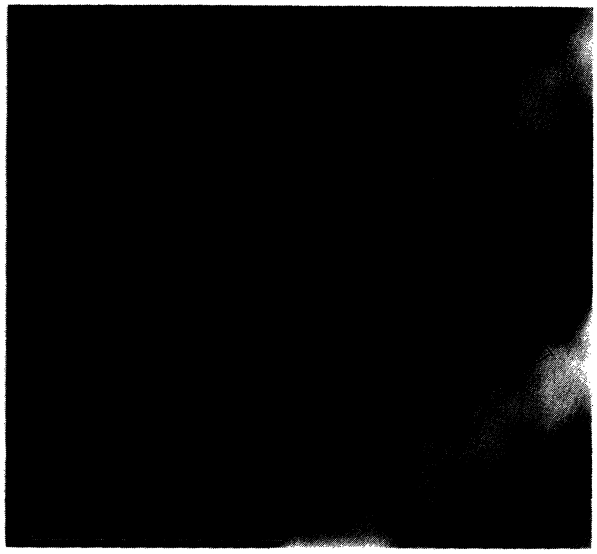

FIG. 5. STM image of a filled state of the 16×2 structure at room temperature in constant-current mode. Scanning area is 10×10 nm^2, sample bias voltage -0.74 V, and tunneling current 0.3 nA.

spheres A and B is about 1 nm, which is almost equal to three times the length of the basic translation vector on the Si(110) plane, 0.38 nm. The distance between the spheres A and C is about 0.9 nm. The distances between the respective kinds of chains are also equal at 5 nm and coincide with the length of the basic translation vector of the 16×2 structure. The height difference between the bright and faint zigzag chains is about 0.2 nm, which is almost equal to the step height of the $\{17,15,1\}$ vicinal plane.

Figure 5 shows a STM image of a filled state of the 16×2 structure at room temperature taken in constant-current mode. In it, the rectangle shows a unit cell of the 16×2 structure. The arrangement of bright spots is different from that in Fig. 4 and reflects the distribution of density of surface states.

FIG. 6. STM image of a filled state of the connection between the 16×2 and the (17,15,1) 2×1 structures at room temperature in constant-current mode. Scanning area is 10×10 nm^2, sample bias voltage -0.78 V, and tunneling current 0.3 nA.

Figure 6 shows a STM image of a filled state of the 16×2 structure and the faceted structure on the $\{17,15,1\}$ vicinal plane at room temperature taken in constant-current mode. The vicinal plane composed of three (110) terraces and two steps is confirmed in the lower part of the image. The 16×2 structure, which is shown at the upper right side, is connected with the faceted structure of the upper left side. The faceted structure has a unit cell with size 1.33×2.5 nm^2 and is the (17,15,1) 2×1 structure. The image of the (17,15,1) 2×1 structure is identical with that of the upper and lower terraces of the 16×2 structure.

In this study, the STM images, except for Fig. 4, were taken at the same surface region, varying only the temperature. Only Fig. 4 was taken at room temperature in a different region, after several repetitions of heating to 1200 °C caused the hillock of a few tens of nm to disappear from the 200×200 nm^2 area investigated.

IV. DISCUSSION

The present HTSTM observations showed that flowing steps were pinned by a hillock and a (17,15,1) 2×1 structure was formed on the vicinal plane. After the crystal growth of the (17,15,1) 2×1 structure was completed, a 16×2 structure was made on a flat area. The 16×2 and (17,15,1) 2×1 structures are reconstructed structures formed with Si atoms on a Si(110) surface and the (17,15,1) 2×1 structure is more stable than the 16×2 structure. There were a variety of hillock sizes on the Si(110) surface. In the case of Fig. 1, the hillocks might be fine particles of SiC, because the hillock was not investigated after several cycles of heating to 1200 °C The (17,15,1) 2×1 structure with a few tens of atomic steps does not exist on a clean Si(110) surface, because the (17,15,1) 2×1 structure as shown in Fig. 3 was not observed in our RHEED study.[12] The number of steps of the (17,15,1) 2×1 structure is dependent on the hillock size. If the size of the hillock is of the order of nanometers, the (17,15,1) 2×1 structure with a few atomic steps is formed. A doped element and a defect on the Si wafer can be the hillock on the nanometer scale.

Figures 7(a), 7(b), and 7(c) show the similarities and differences between the 16×2 structure and the (17,15,1) 2×1 structure, where (a) is the top view of these structures and (b) and (c) are the side views of the 16×2 structure and the (17,15,1) 2×1 structure, respectively. The rectangle in Fig. 7(a) shows a common structural unit of the 16×2 structure and the (17,15,1) 2×1 structure, where $\mathbf{a}=\frac{1}{2}[\bar{1}10]$ and $\mathbf{b}=[001]$ are the basic translation vectors on the Si(110) plane, and solid circles and gray circles represent Si atoms in the upper and lower layers of the Si(110) plane, respectively. The unit size is 1.33×2.5 nm^2. In the top view shown in Fig. 7(a), the 16×2 structure and the (17,15,1) 2×1 structure are iden-

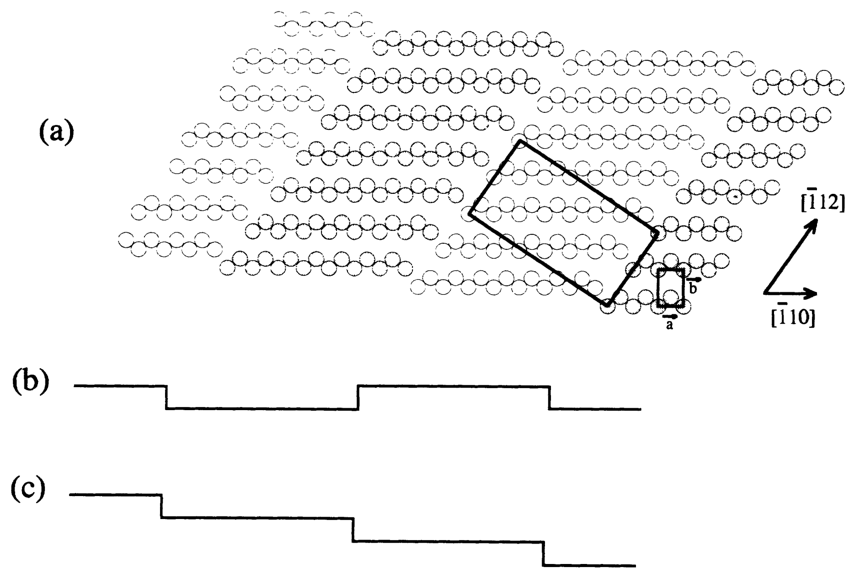

FIG. 7. Schematic diagrams of the 16×2 and the (17,15,1) 2×1 structures, where $\mathbf{a}=\frac{1}{2}[\bar{1}10]$ and $\mathbf{b}=[001]$ are the basic translation vectors on the Si(110) plane, and solid circles and gray circles represent Si atoms in the upper and lower layers of a Si(110) plane, respectively. (a) is a top view, where the rectangle represents the common structural unit. (b) is a side view of the 16×2 structure, and (c) a side view of the (17,15,1) 2×1 structure.

tical, but in the side views shown in Figs. 7(b) and 7(c), the 16×2 structure is on the (110) plane and the (17,15,1) 2×1 structure on the (17,15,1) vicinal plane. The unit cell of the (17,15,1) 2×1 structure is identical with the common structural unit and that of the 16×2 structure is represented by a pair of the upper and lower terraces formed by the common structural unit.

From the UPS results for the 16×2 structure, a surface state is found to exist at −0.8 eV below the Fermi energy,[26] which is almost identical to the sample bias voltages of Figs. 5 and 6. This state disappeared after 0.3 monolayer deposition of Sn atoms. Therefore it is considered that the state reflects the density of states of the dimers and trimers, which are made by two and three dangling bonds, respectively. The formation of the dimers and trimers reduces the number of Si dangling bonds on the (110) surface. Figure 8 shows how the dimers and trimers are formed, where the letters Y and the reverse Y represent the trimers, the solid arcs the dimers, and the broken arcs the backbond dimers. 0.3 monolayer deposition of Sn atoms in sufficient to break the dimers and trimers. It is deduced that the formations cause stress in the $[\bar{1}10]$ and $[1\bar{1}2]$ directions and this stress results in a rumpling of the $[\bar{1}10]$ atomic row. The STM image of the empty state shown in Fig. 4 can be interpreted by the rumpling model. In it, the distance from top to top of the rumpling in the $[\bar{1}10]$ direction is 1.15 nm. The displacement in the normal direction is about 0.05 nm. The origin of the rumpling is mainly the trimers, because this coordination causes an attraction along the $[\bar{1}10]$ and $[1\bar{1}2]$ directions and the attraction displaces Si atoms in the direction normal to the (110) surface. The displacement is generated near positions of higher density of trimers, where Y in Fig. 8 faces a reversed Y. The letters *A*, *B*, and *C* in Fig. 4 represent these positions.

The rumpling model for the 16×2 structure is shown in Fig. 9, where (a) is the top view and (b) the side view along the solid line in (a). A similar rumpling model can be made for the (17,15,1) 2×1 structure.

V. SUMMARY

In summary, the present HTSTM observations reveal that the vicinal plane {17, 15, 1} is formed on the wall of a hillock with size of the order of a few tens of nanometers at 710 °C and the hillock plays the role of the nucleus for Si crystal growth. The (17,15,1) 2×1 structure is formed on the vicinal plane. The 16×2 structure grows on a flat surface from the (17,15,1) 2×1 structure at the uppermost and lowermost layers of the vicinal plane. A rumpling model is proposed for the 16×2 structure and the (17,15,1) 2×1 structure on the basis of STM and UPS results, where Si atoms are displaced in the directions normal to the (110) surface. The formation of dimers and tri-

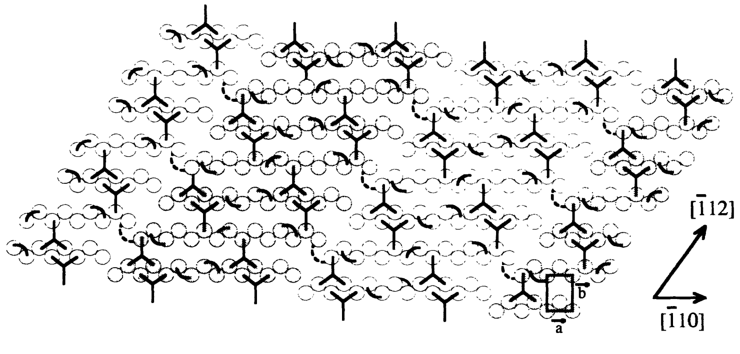

FIG. 8. Formation of the dimers and trimers of Si atoms on the (110) surface, where Y and reversed Y represent the trimers, solid arcs the dimers, and broken arcs the backbond dimers.

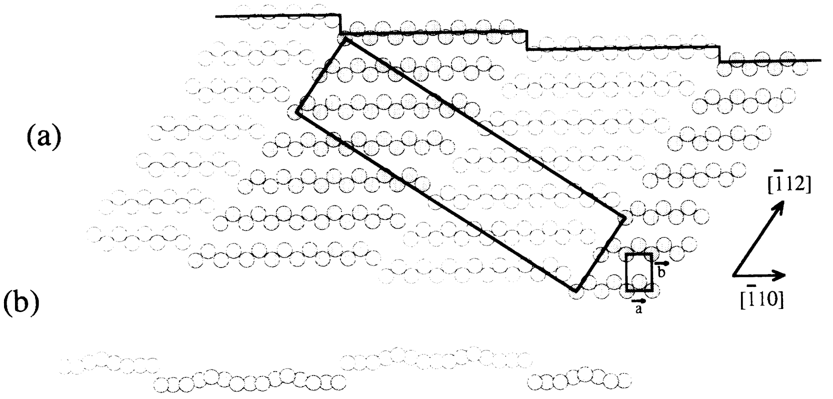

FIG. 9. Rumpling model for the 16×2 structures. (a) is a top view, where the rectangle represents the unit cell, and (b) a side view along the solid line in (a).

mers causes stress in the [$\bar{1}10$] and [$1\bar{1}2$] directions and the stress results in rumpling of the [$\bar{1}10$] atomic row. The distance from top to top of the rumpling in the [$\bar{1}10$] direction is 1.15 nm. The displacement in the normal direction is about 0.05 nm.

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[1] In order to describe the superstructures, we define the basic translation vectors on the Si(110) surface as $\mathbf{a}=\frac{1}{2}[\bar{1}10]$ and $\mathbf{b}=[001]$. Then the superstructure has the basic translation vectors $\mathbf{a}s=m\mathbf{a}+n\mathbf{b}$ and $\mathbf{b}s=k\mathbf{a}+1\mathbf{b}$, and this is named the $(m,n)\times(k,l)$ structure. When $n=k=0$, it is named the $m\times l$ structure. Here, m,n,k, and l are integers.

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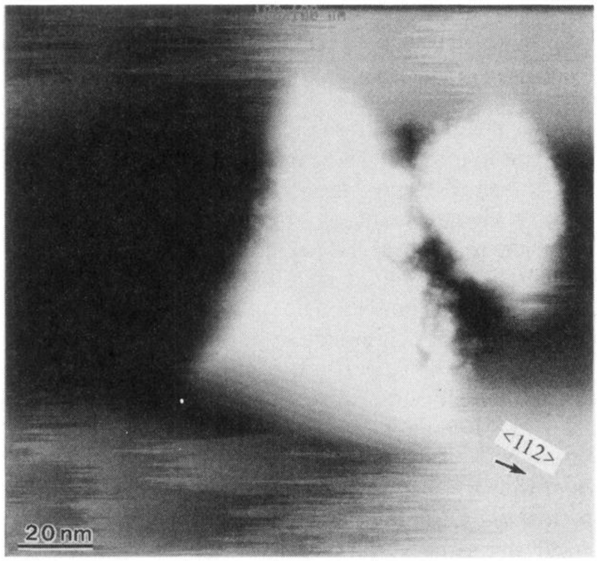
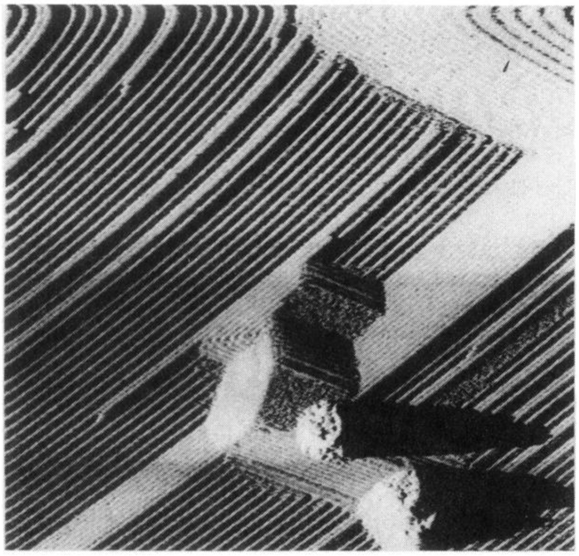


FIG. 1. HTSTM image at 710 °C in constant-current mode. Scanning area is 100×100 nm^2, sample bias voltage -0.84 V, and tunneling current 0.2 nA.



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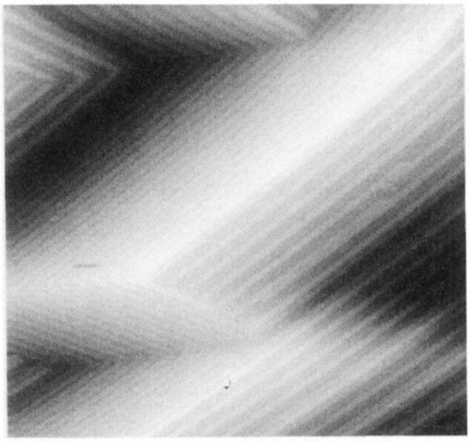

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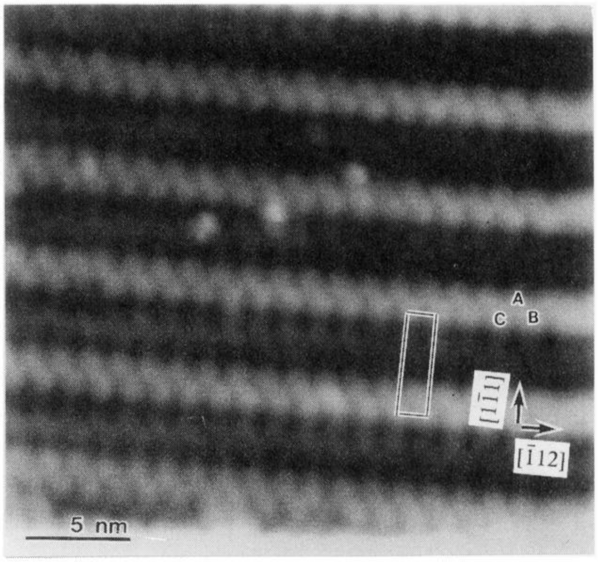

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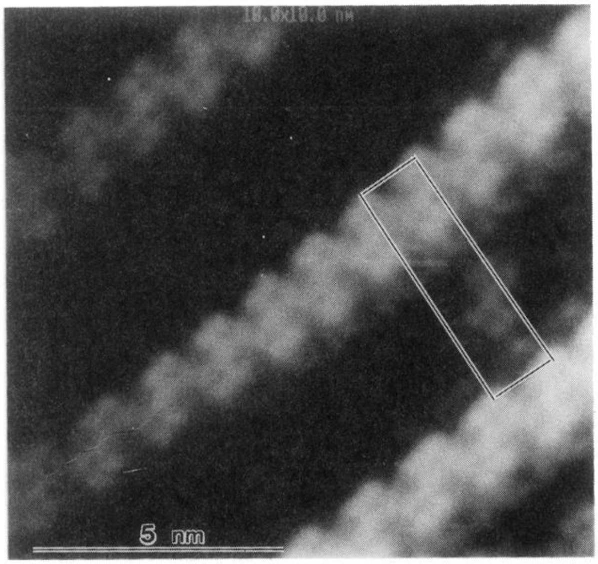
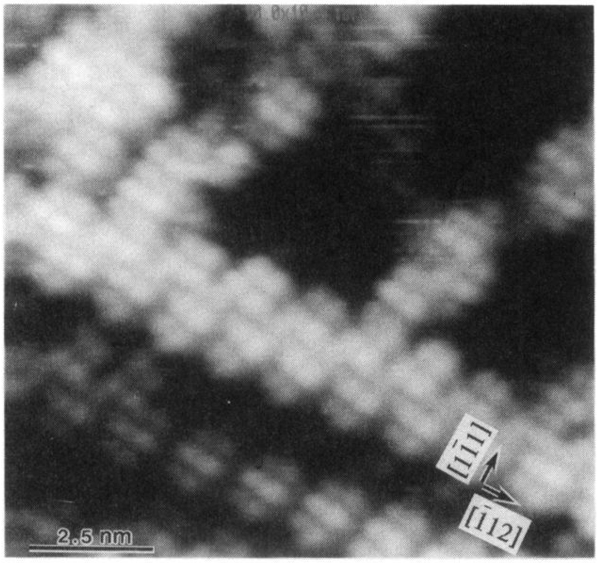


FIG. 5. STM image of a filled state of the 16×2 structure at room temperature in constant-current mode. Scanning area is 10×10 nm^2, sample bias voltage -0.74 V, and tunneling current 0.3 nA.



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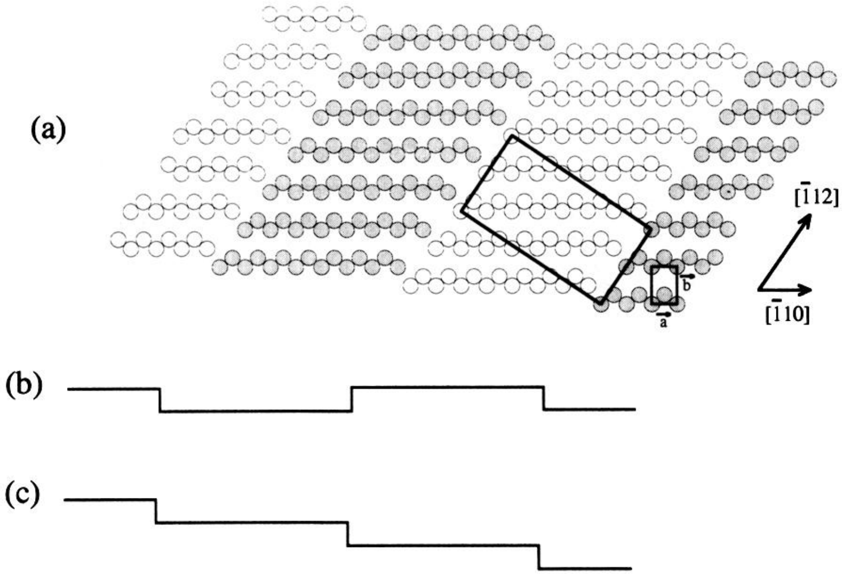
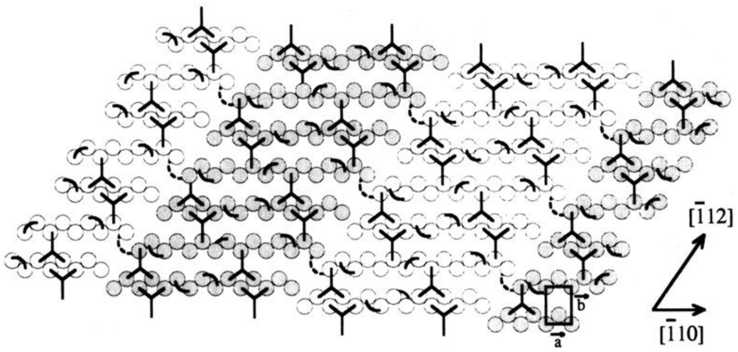


FIG. 7. Schematic diagrams of the 16×2 and the (17,15,1) 2×1 structures, where $\mathbf{a}=\frac{1}{2}[\bar{1}10]$ and $\mathbf{b}=[001]$ are the basic translation vectors on the Si(110) plane, and solid circles and gray circles represent Si atoms in the upper and lower layers of a Si(110) plane, respectively. (a) is a top view, where the rectangle represents the common structural unit. (b) is a side view of the 16×2 structure, and (c) a side view of the (17,15,1) 2×1 structure.



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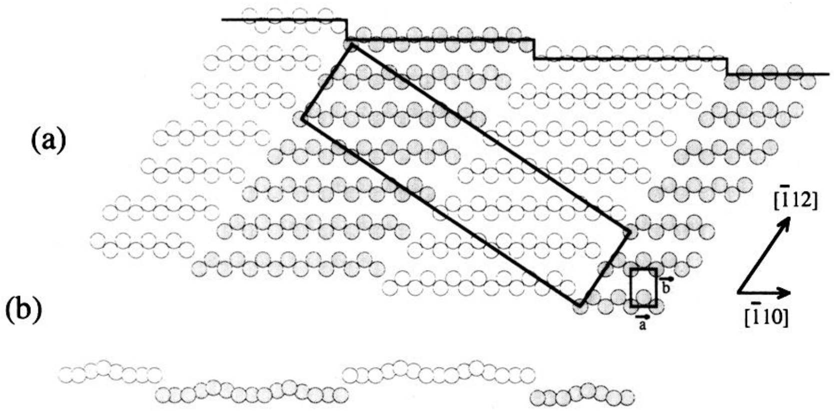

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