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Si(110)-16×2 and Si(110)-5×1 surface reconstructions: Stretched-hexagon face-centered adatom model

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Scanning tunneling microscopy data are reported for the reconstructed Si(110)-''16×2'' and Si(110)-''5×1'' surfaces. Models of both surface reconstructions are proposed, based on a single building block, a face-centered stretched hexagon of adatoms. The models successfully explain the major experimental facts about both structures. [S0163-1829(97)04819-4]

I. INTRODUCTION

Although the relaxation and reconstruction of semiconductor surfaces has been an area of active research for years, few surface crystal structures have been conclusively solved. Even Si, whose (100)-2×1, (111)-7×7, and cleaved (111)-2×1 surface structures were among the first few to be determined,[1–3] still has a (110) surface whose structure is currently controversial, having two primary reconstructions,[4] ''16×2'' and ''5×1,'' neither of which is described by a consensus model. Moreover, neither the 16×2 nor the 5×1 structure actually exhibits genuine 16×2 or 5×1 symmetry—they merely produce low-energy electron diffraction (LEED) patterns that are *almost* 16×2 and 5×1.[5,6] The purpose of this paper is to propose that both the 16×2 and the 5×1 Si(110) surfaces can be constructed from the same building block—a stretched hexagon of Si adatoms, topped by a face-centered Si adatom. [Core-level spectra[7] strongly suggest that a correct model involves Si adatoms similar to those found on Si(111)-7×7.] With this building block, we are able to describe a large body of data for both surfaces.

Because vertically smooth sidewalls can be etched into the Si(110) surface, this surface is technologically important for the fabrication of micromachines, such as high-aspect-ratio actuators.[8] Therefore, our goal is to understand the main crystal structures of this surface, as a first step toward understanding the microscopic physics of etching on the surface. Our approach is to first obtain atomic-resolution scanning tunneling microscopy (STM) images of both Si(110)-16×2 and Si(110)-5×1,[9] and to then propose two geometrical models, based on the same building block, that are consistent with our observations.

The fact that the 16×2 and 5×1 reconstructions are the most commonly observed on the clean Si(110) surface suggests that the free energies of the two reconstructions are not very different. Some authors claim that the 5×1 structure is impurity stabilized, but the concentration of impurities purportedly required to stabilize it is so small that currently we can neither confirm nor deny that viewpoint.[6,10] However, if the 16×2 and 5×1 structures are indeed nearly degenerate, then one might suspect that there exists a common building block for both surfaces. This feature is absent from all current models, which claim to describe either the 16×2 or 5×1 structure, but not both.

II. STATEMENT OF THE PROBLEM

Figures 1 and 2 are typical STM images of the 16×2 and 5×1 structures of the Si(110) surface. A successful understanding of these two reconstructions must explain the following 23 facts contained in those and related figures. (To facilitate the presentation, we shall refer to those facts by Arabic numerals, both in the text and in the figures.)

A. Si(110)-16×2 structure

(1) The most striking fact of the 16×2 structure (Fig. 3) is the stripes and chevron structure. (2) The bright stripes are measured to be one atomic step height (1.92 Å) higher above the surface than the dark stripes, and that is why they yield bright STM images. We term the higher stripes up-stripes

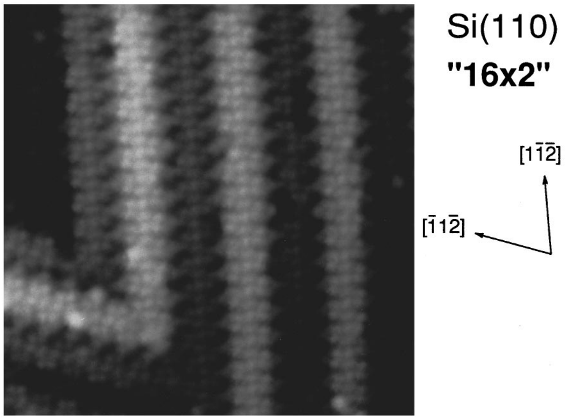

FIG. 1. STM image of the Si(110)-16×2 surface reconstruction. The image is ≈210 Å wide. The directions are indicated to the right of the figure. The bias voltage (of the sample with respect to the tip) was −2.0 V (an image of filled states), and the current was 1 nA. Note the nearly vertical white stripes which run in the [1,1,2] direction, separated by dark stripes which are one-atomic-height lower (1.9 Å). The spacing between adjacent white stripes is 50.2 Å. Also note the white stripe in the lower left of the figure, running along the [1,1,2] direction, which forms a chevron with another nearly vertical stripe.

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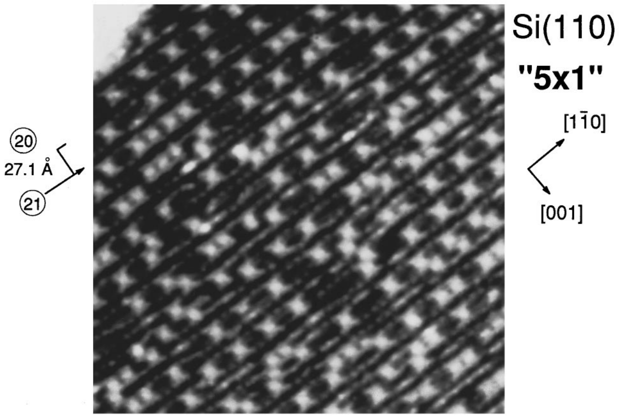

FIG. 2. STM image of the Si(110)-5×1 surface structure. The bias voltage was positive 1.2 V (empty states image), and the current was 1.3 nA. Facts (20) and (21) are indicated to the left of the figure: (20) the 27.1 Å$=5a$ periodicity, and (21) the dark lines in the $[1,\bar{1},0]$ direction. The width of the figure is ≈370 Å. The bright spots correspond to stretched-hexagons unevenly spaced in the $[1,\bar{1},0]$ direction.

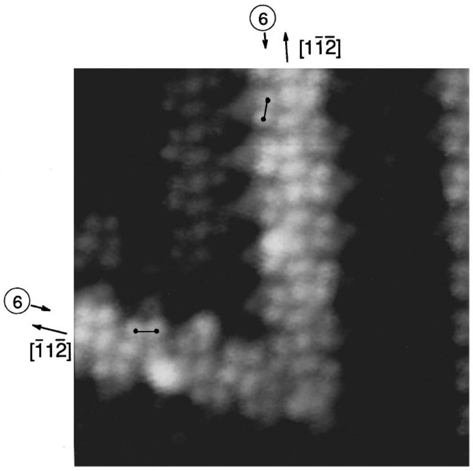

FIG. 4. STM image of Si(110)-16×2 structure. The directions of the up-stripes are depicted on the figure. Note that the $[1,\bar{1},\bar{2}]$ up-stripe has a different handedness from the $[\bar{1},1,\bar{2}]$ up-stripe [fact (6)], as can be seen by recognizing that the two lines drawn on the stripes have slopes with respect to their stripe axes of different signs. The bias is −2.0 V (filled states), with a current of 1 nA.

and the darker ones down-stripes. (3) The majority of the up-stripes in Fig. 3 are oriented along the $[1,\bar{1},\bar{2}]$ direction. (4) The chevron in this picture corresponds to two up-stripes oriented in different directions, meeting to form the chevron pattern, with a 70.5° angle. (5) The second kind of up-stripe in Fig. 3 is oriented along $[\bar{1},1,\bar{2}]$. (6) The up-stripes along $[1,\bar{1},\bar{2}]$ and the up-stripes along $[\bar{1},1,\bar{2}]$ have slightly different topological structures which we term different handedness (Fig. 4). (7) The distance between two up-stripes (or two down-stripes) is 50.2 Å (Ref. 11) (Fig. 3). (8) Viewed one way, there is a zigzag pattern on the up-stripes (Fig. 3). (9) A similar pattern is observed on down-stripes (Fig. 3). (10) The repeat distance of the zigzag pattern is 13.3 Å (Ref. 11) along the stripe (Fig. 3). (11) Viewed a different way, the stripes are stacks of stretched hexagons (Fig. 3). (12) The zigzag array of atoms is attached to the underlying bulk Si lattice. (13) The surface unit cell lattice vectors a' and b' for the next cell in this reconstruction are derived from the primitive cell's basis vectors **a** and **b** by the transformation

$$\mathbf{a}'=17\mathbf{b}-\mathbf{a},\quad \mathbf{b}'=2(\mathbf{b}-\mathbf{a})$$

instead of

$$\mathbf{a}'=16\mathbf{b},\quad \mathbf{b}'=2\mathbf{a},$$

as might be expected for a true 16×2 surface.[6] That is why we use the quotation marks: the 16×2 surface is not literally a 16×2 structure, but is actually a

$$\begin{bmatrix}-1 & 17\\ -2 & 2\end{bmatrix},$$

structure,[12] where the matrix transforms the pair $(\mathbf{a},\mathbf{b})$ into $(\mathbf{a}',\mathbf{b}')$. (14) The stretched hexagons of $[1,\bar{1},\bar{2}]$ down-stripes are displaced by a vector $(\mathbf{r}'/2)-\mathbf{c}$ from the adjacent up-stripe hexagons (Fig. 5). We shall see that $\mathbf{r}'=3\mathbf{a}+13\mathbf{b}$.[13,14] (15) The up-stripes have scalloped edges. [See the light triangle to the right of number (15) in Fig. 3.] (16) The down-stripes have holes. [See the dark area to the right of number (16) in Fig. 3, and between any two light triangular scalloped edges.] (17) The energetically favorable nature of the 16×2 structure implies that the number of dangling bonds has been reduced below that of the abruptly termi-

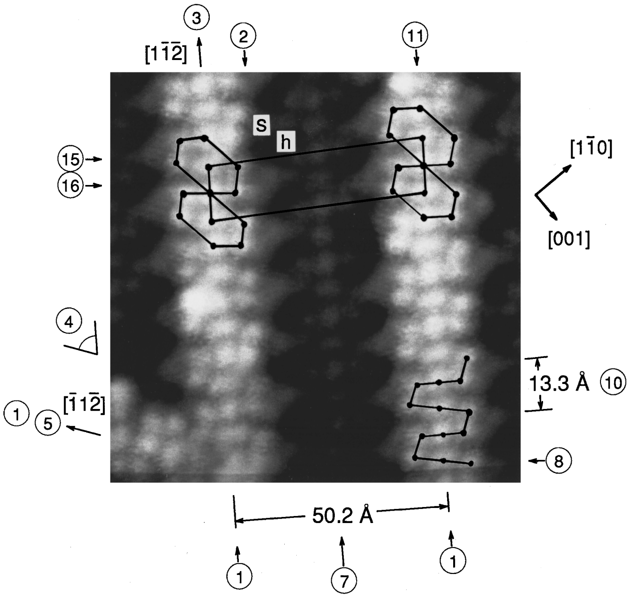

FIG. 3. STM image of the Si(110)-16×2 surface. Features visible in the image are denoted by the same fact-numbers as in the text: [fact (1)] stripes and chevron structure; [fact (2)] one atomic step-height boundary between bright up-stripes and dark down-stripes; [fact (3)] up-stripes in the $[1,\bar{1},\bar{2}]$ direction; [fact (4)] chevron with an angle of 70.5°; [fact (5)] second kind of up-stripe along $[\bar{1},1,\bar{2}]$; [fact (7)] 50.2 Å separation between up-stripes; [fact (8)] zigzag pattern of up-stripes; [fact (10)] 13.3-Å repeat distance of the zigzag pattern; [fact (11)] stacks of stretched hexagons; [fact (15)] light scalloped edges (s) of up-stripes; [fact (16)] dark holes (h) associated with down-stripes. The bias was −2.0 V, with a tunneling current of 1 nA, giving a filled-states image.

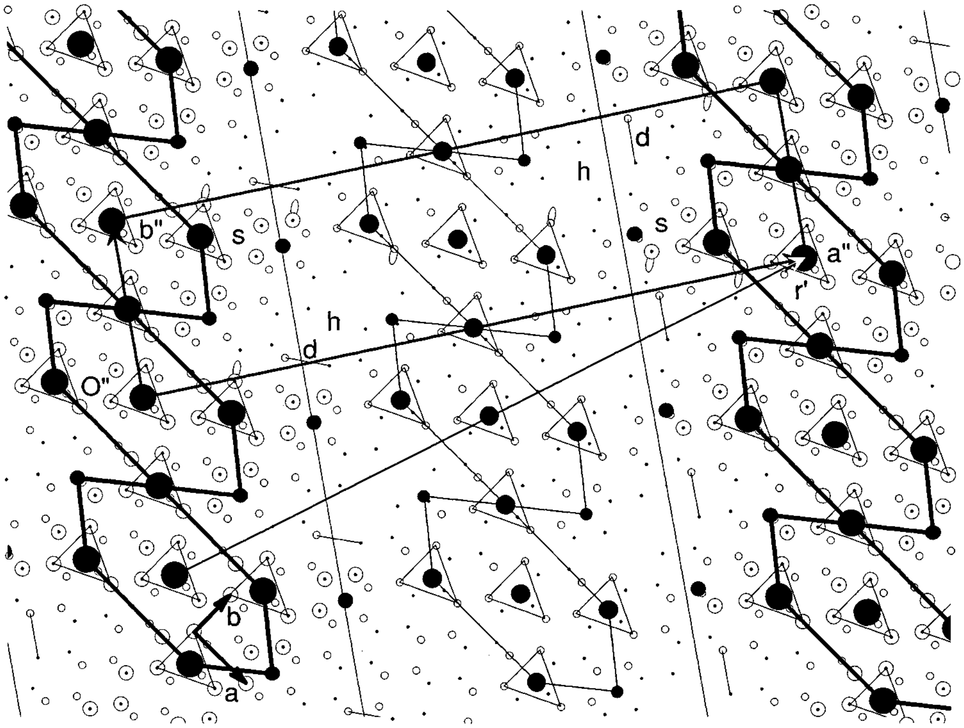

FIG. 5. Diagram depicting the stacking of stretched hexagons on the Si(110) surface to produce the 16×2 structure. Circles denote atoms, and decrease in radius as the atom lies farther from the surface, into the bulk. The adatoms are large solid circles. The triangles are bases of tetrahedra whose vertices contain Si atoms bonded to an adatom. Dimers at step edges are denoted *d*. Dangling bonds are denoted by loops. The vector $\mathbf{r}'$ is the vector from the center of an up-stripe hexagon to the center of the up-stripe hexagon in the next unit cell for the 16×2 structure proposed here; $(\mathbf{r}'/2)-\mathbf{c}$ is the center of a down-stripe hexagon. The hole regions are denoted *h* and correspond to the dark regions in Fig. 3 [fact (16)]. The scalloped regions are denoted *s* and correspond to the light scallops of Fig. 3 [fact (15)]. The parallel lines running in the [1,1,2] direction are aids to the eye, for locating adjacent step edges.

nated unrelaxed perfect Si(110) surface. (18) If the sequence of stripes is up-down-down, instead of the normal up-down-up, then [15,17,1] facets (or equivalently [17,15,1], [17,15,1], or [15,17,1] facets) are formed.

B. Si(110)-5×1 structures

(19) A primary theoretical challenge is to produce the 5×1 structure of Fig. 2 using the same hexagonal building block as for the 16×2 structure (Fig. 1)—despite the fact that, at first glance, the two structures appear to be completely unrelated. (20) This 5×1 structure must have the observed 27.1 Å$=5a$ periodicity,[11] where a is the lattice constant. (Fig. 2) (21) The STM images of empty states (positive bias with respect to the sample) yield dark lines in the [1,1,0] direction (Fig. 2). (22) The STM images of filled states, under negative bias exhibit hexagonal structures (Fig. 6). (23) The 5×1 appellation is not correct either. What is observed in low-energy electron diffraction is a structure with a repeat distance of $5a$ in the [0,0,1] direction. The repeat distance in the perpendicular ($\mathbf{b}$ or [1,1,0]) direction is not well defined.

III. BUILDING THE SURFACE FROM STRETCHED HEXAGONS

A. Stretched hexagon with face-centered adatom

The basic building block that we propose is given in Fig. 7, where we show the surface with two missing rows of atoms, with the stripe between these rows straddled by a stretched hexagon of adatoms plus one at the face center of the hexagon.[15] The five atoms labeled *B* are each directly above a surface plane (first layer) triangle of Si atoms, and bonded to those triangular lattice sites on the (1,1,0) plane of

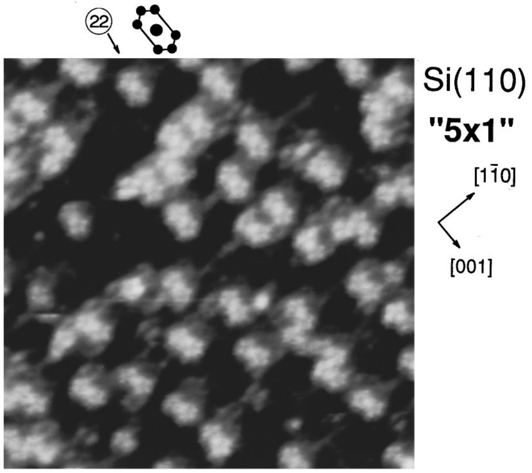

FIG. 6. STM image of the Si(110)-5×1 structure. The image is of filled states, taken under a bias voltage of −0.6 V with a current of 1 nA, and shows stretched hexagons similar to those of Fig. 7. Fact (22) of the text is visible here: hexagonal structures. The scale of this figure is 220×220 Å. The drawn hexagonal structure is enlarged.

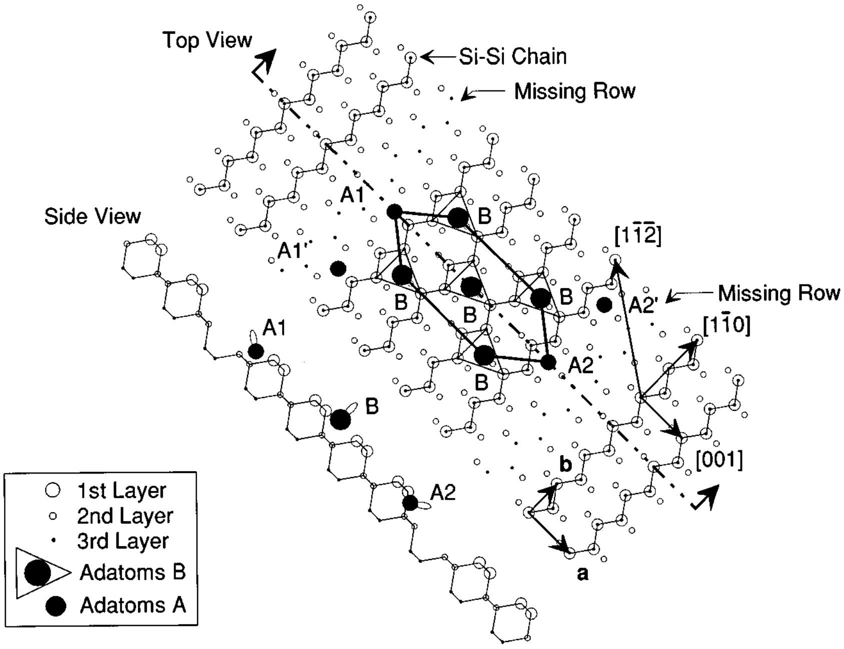

FIG. 7. Schematic depiction of the Si(110) surface with a single stretched hexagon added to it. Large-radius circles represent Si atoms farther from the bulk. The solid circles are adatoms. Each stretched hexagon is composed of (i) five above-surface adatoms B, (ii) one adatom $A1$ [bonded to one surface (first-layer) Si atom and two (second-layer) atoms below the surface, which were exposed by the removal of the missing row to the left of the hexagon], and (iii) one adatom $A2$, which is bonded to two first-layer Si atoms and one second-layer atom, which was exposed by the creation of the missing row to the right of the hexagon. The five adatoms B are bonded to triangular arrays of first-layer Si atoms. The adatoms $A1'$ and $A2'$ have identical local environments to $A1$ and $A2$, but are not part of the stretched hexagon; they are needed when stacking stretched hexagons to form our 16×2 structure. Missing rows are indicated on the figure, which also presents a side view (depicting dangling bonds).

the surface. The two extremal major-axis atoms are $A1$ and $A2$, both of which are on step edges. $A1$ is bonded to one atom on the surface (the first layer), and to two atoms below (the second layer), while $A2$ is bonded to two atoms on the surface and to one atom below.[16] The bonding to the step edges is depicted in the side view of Fig. 7. (When the hexagons are stacked into up-stripes of the 16×2 structure, but not in the 5×1 structure, the additional adatoms $A1'$ and $A2'$ are needed to complete the stripes, where $A1'$ and $A2'$ have the same local environments as $A1$ and $A2$, respectively. Although these $A1'$ and $A2'$ adatoms are required in the 16×2 reconstruction, they are not needed for the model of the 5×1 structure—but the model does not rule out occupation of some $A1'$ and $A2'$ sites.)

B. 16×2 structure

Our stretched-hexagon model *does explain* the 18 main facts about the 16×2 surface structure in terms of stacks of such hexagons: Fig. 8 shows how the model reproduces the up- and down-stripes and the resulting chevron structure, as observed in Figs. 1 and 3 [fact (1)]. The stripes are obtained by attaching stacks of stretched hexagons *commensurately* to an unreconstructed, ideal Si(110) surface. Figure 9 illustrates how "up"- and "down"-stripes alternate with one another, with a one-atom-high (1.92 Å) step in between, as observed in Figs. 1 and 3 [fact (2)]. The orientation of the [1,1,2] and [1,1,2] stripes, and the 70.5° angle of the chevron, are consequences of the stacking sequences shown in Fig. 8, and agree with the observations of Figs. 1, 3, and 4 [facts (3), (4), and (5)]. The difference in topological structures of the stripes is apparent in Fig. 8, where the different handedness of the zigzag chains seen in Fig. 4 is apparent [fact (6)]. (In Fig. 8, note the orientation of the $A1$-$B2$ line in comparison with the orientation of the the $A1$-$B1$ line. The [1,1,2] stripe is not obtained from a [1,1,2] stripe by a proper rotation, but by a reflection in a vertical mirror plane that passes through the minimum of the chevron's V in Fig. 8. This difference in handedness occurs in the STM image Fig. 4, and is a consequence of the different bonding by the $A1$ and $A2$ adatoms from the bonding of the B adatoms.) The separation of stripes in the model, Fig. 9, is indeed 50.2 Å,[11] as determined experimentally, Fig. 3 [fact (7)]. The zigzag patterns observed in Fig. 3 are apparent in the model, as shown in Fig. 8 for the up-stripes and in Fig. 9 for the down-stripes [facts (8) and (9)]. The 13.3-Å (Ref. 11) experimental distance between hexagons along a stripe (Fig. 3) is the same for [1,1,2] and [1,1,2] stripes, and is also present in the model of Fig. 8, where it arises naturally from the topology of the stacking sequence [fact (10)]. The equivalence of the stacks of stretched hexagons and the zigzag chains (as determined experimentally in Fig. 3) is displayed in Fig. 8 (see also Fig. 9), as is the fact that the adatoms fit naturally on the underlying Si [facts (11) and (12)]. The true nature of the 16×2 surface unit cell, which has two common representations, is visible in Fig. 9, where the upper unit-cell representation is spanned by $\mathbf{a}'=16\mathbf{b}+(\mathbf{b}-\mathbf{a})$ and $\mathbf{b}'=2(\mathbf{b}-\mathbf{a})$. For a true 16×2 reconstruction, we would have $\mathbf{a}'=16\mathbf{b}$, different by $\mathbf{b}-\mathbf{a}$; our model correctly accounts for this difference [fact (13)]. The other common representation of the 16×2 surface unit

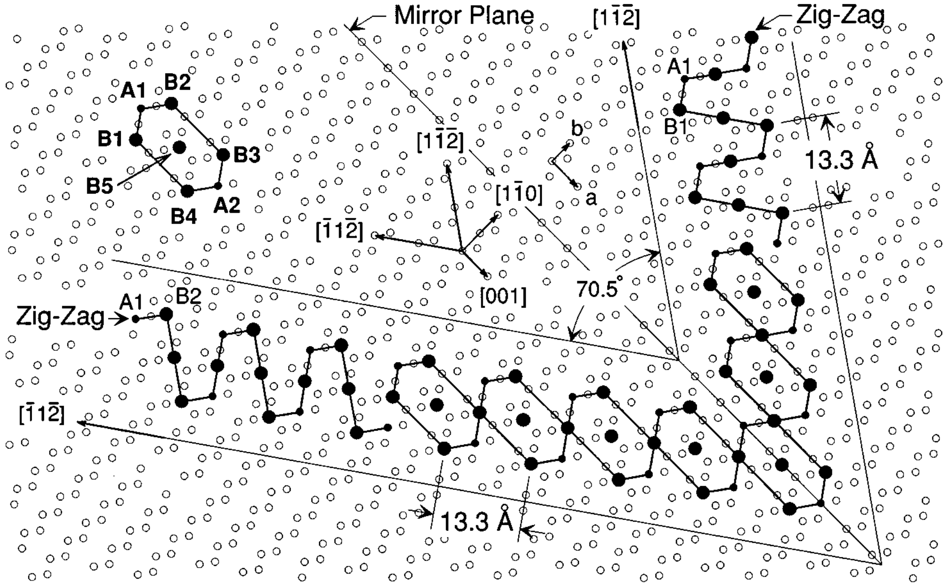

FIG. 8. Illustration of how the up-stripes of different handedness, and the 70.5° chevron are formed by stacking hexagons on the Si(110) surface. Open circles are first-layer surface Si atoms. Filled circles are adatoms. For reference, in the upper left we have numbered the B adatoms of the stretched-hexagon: $B1-B5$. We use this notation to label atoms in the chains of the two types of up-stripes in order to compare handedness of the stripes. See also Fig. 4. Note that the zigzag chains and the stretched hexagons are merely different ways of viewing the same structure. To simplify the presentation, we have not indicated the missing rows associated with the stretched hexagons; only the first-layer atoms are shown, and the major axes of the hexagons have been shortened slightly from the length in Fig. 7.

cell, shown in the lower portion of Fig. 9, is spanned by $\mathbf{a}'' = 5\mathbf{a} + 11\mathbf{b}$ and $\mathbf{b}'' = 2(\mathbf{b} - \mathbf{a})$. Also shown in that figure is the vector $\mathbf{r}' = \mathbf{a}'' + \mathbf{b}'' = 3\mathbf{a} + 13\mathbf{b}$, which passes diagonally through this cell, originating at the center of an up-stripe hexagon, passing over the center of a down-stripe hexagon, and terminating at the center of an up-stripe hexagon. The displacement of a down-stripe hexagon from an up-stripe hexagon is clearly $(\mathbf{r}'/2) - \mathbf{c}$ [fact (14)]. The scalloped edges in the 16×2 images of Fig. 3 correspond to the regions labeled s near the dimers[17,18] in Fig. 5, containing $A1'$ and

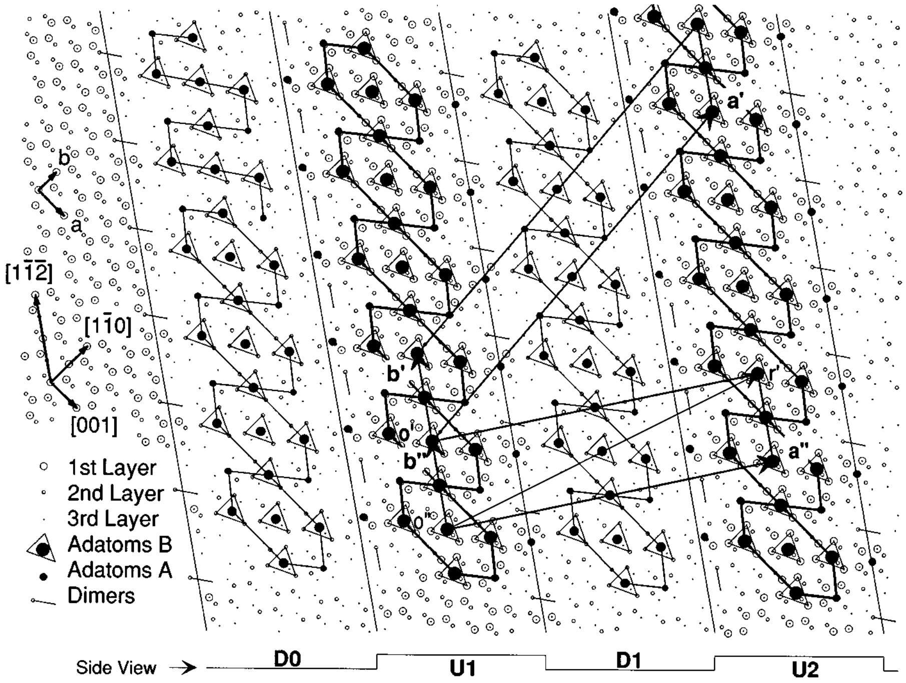

FIG. 9. Illustration of a Si(110)-16×2 structure with up-stripes $U1$ and $U2$, alternating with down-stripes $D0$ and $D1$. Two parallelepiped fundamental surface unit cells are depicted: (i) one spanned by $\mathbf{a}'$ and $\mathbf{b}'$ originating from the same point $\mathbf{O}'$, and (ii) the other spanned by $\mathbf{a}''$ and $\mathbf{b}''$ (originating from $\mathbf{O}''$). The vector $\mathbf{r}'$ is also given: $\mathbf{r}'$ is from the center of one up-stripe hexagon to the center of another (Refs. 13 and 14). We use the same representation here as in Fig. 5.

TABLE I. Effects of elements in the stretched-hexagon 16×2 structure on the number of dangling bonds, which is 64 per 16×2 surface unit cell for the unreconstructed Si(110)-16×2 surface.

Element	Number per cell	Bonds saturated per element	Reduction in dangling bonds per 16×2 unit cell
B adatoms	8	2	16
$A1$ adatoms	2	2	4
$A2$ adatoms	2	2	4
$A1'$ adatoms	1	2	2
$A2'$ adatoms	1	2	2
Dimers	2	2	4
Dangling bonds due to steps	4	-1	-4
Second-layer missing rows on either side of down-stripe hexagon	2	-2	-4
TOTAL			24 (of 64)

$A2'$ adatoms [fact (15)]. The dark hole regions seen in Fig. 3 are labeled h in Fig. 5, and are due to second-layer missing rows (on either side of the down-stripe hexagon), which are adjacent to the $A1$ and $A2$ adatoms [fact (16)]. Examination of the surface unit cell of Fig. 5 reveals that the stretched hexagon significantly reduces the number of dangling bonds at the surface (Table I), thereby reducing the surface free energy [fact (17)]. Finally, an examination of the crystal structure when the sequence of stripes is up-down-down instead of up-down-up reveals [15,17,1] facets [fact (18)].[19]

Therefore the stretched-hexagon model with a face-centered adatom successfully explains the 18 major facts about the 16×2 structure. The 16×2 structure, to our knowledge, is the largest surface reconstruction for which there is now a suitable model.

C. 5×1 structure

The 5×1 structure results from sequences of the same stretched-hexagon building blocks (without $A1'$ or $A2'$ adatoms) arrayed in the $2\mathbf{b}=[1,1,0]$ direction [fact (19)]. If the hexagons were stacked adjacent to one another in the $\mathbf{b}$ direction with their long edges coincident, the structure would be 5×2, not 5×1. The LEED data reported a 5×1 symmetry doubtless because there is considerable disorder in the $\mathbf{b}$ direction,[20–22] associated with different separations between hexagons (Figs. 2 and 6), and such disorder washes out any prominent diffraction spots associated with the $\mathbf{b}$ direction. Between the $A1$ atom of one hexagon and the $A1$ atom of another, in the $\mathbf{a}=[0,0,1]$ direction, is a missing row of surface Si atoms running in the $\mathbf{b}$ direction.

This 5×1 building block has the observed 27.1 Å$=5a$ periodicity[11] [Fig. 2, fact (20)]. The empty-state STM images reveal dark lines associated with the model's missing rows in the [1,1,0] direction [Figs. 2 and 7, fact (21)]. Also, the model's stretched hexagons of adatoms account for the observed filled-state STM images of hexagons on the 5×1 surface [Fig. 6, fact (22)]. Thus the main experimental facts for the 5×1 reconstruction are accounted for by this model. Moreover the 5×1 building block is also the building block for the 16×2 surface, making it easy to understand why both reconstructions occur on the Si(110) surface.[10]

Of the models of the 5×1 reconstruction,[23] perhaps the most widely discussed is the one proposed by Keim, Wormeester, and van Silfhout,[24] which is displayed in Fig. 10. This model has *two* adatoms near the center of a stretched-hexagon, vs one in our model, and simply cannot account for the 16×2 structure at all. Our images indicate only one face-centered adatom on each hexagon. Furthermore, in order to have two face-centered adatoms per hexagon, there would have to be two missing rows perpendicular to the long axes of the hexagons. However, Fig. 2 shows dark bands spaced $5a$ apart, which coincide with missing rows of our model. In contrast, the Keim model of Ref. 24 has missing rows $2a$ apart, not $5a$, and the rows $5a$ apart are Si-Si chains, which are expected to produce bright images, not dark ones.

Note that in the Keim model, the distance (in the $\mathbf{b}$ direction) between B adatoms on opposite sides of a hexagon is $2.5b$, vs $2b$ in our model. We believe that the distance between B adatoms is $2|\mathbf{b}|$, not $2.5|\mathbf{b}|$—but the confidence with which we can state this conclusion is not terribly high, about 75%.

The stretched hexagons of our model can be stacked so that they form the prominent [1,1,2] and [1,1,2] stripes of the 16×2 structure—but the hexagons of the Keim model are unable to reproduce either the observed stripe directions or the 16×2 structure, using any stacking sequence.

In fairness, we do note that Becker, Swartzentruber, and Vickers[22] reported seeing hexagons with two adatoms near the center, and we would not disagree with a claim that the two-face-centered-adatom hexagon structure coexists with our stretched hexagon. We would, however, insist that our stretched hexagon is more common on those surfaces that we have observed.[25]

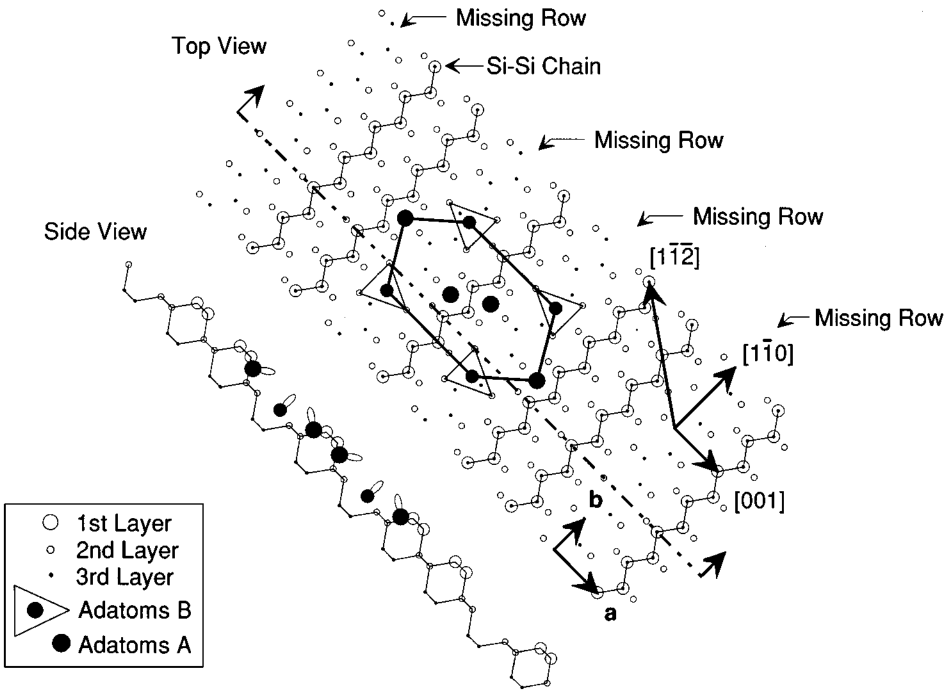

FIG. 10. The elementary building block of the Keim model (Ref. 24), in the same notation as Fig. 7.

The 5×1 surface is clearly disordered, with the bright spots of Fig. 2 corresponding to hexagons unevenly spaced in the [1,1,0] direction, reflecting the somewhat amorphous structure of the two-dimensional array of stretched hexagons. This disorder in the **b** direction washes out any nonintegral diffraction spots associated with the **b** direction, and is responsible for the erroneous notation 5×1. We also see in Fig. 6 some dislocations of the [1,1,0]-aligned surface missing rows (displaced roughly half of the hexagon major axis), and such dislocations further indicate that the surface is disordered, actually favoring our model, which can account for them by abruptly shifting [1,1,0]-aligned rows by 2**a** or 3**a**. Therefore we conclude that the stretched-hexagon model accounts for the main facts concerning the disordered Si(110)-5×1 structure.

IV. ENERGETICS

When the adatoms of the stretched hexagon bond to the (110) surface, they each bind to three dangling bonds of the unreconstructed surface, saturating them. They also each leave one of their own four bonds dangling above the hexagon, and so they each account for a reduction of two dangling bonds at the surface, thereby reducing the free energy of the surface. Normally, the bonding energy is the main contribution to the free energy at low to moderate temperatures, with elastic energies associated with bond bending and bond stretching normally being smaller. (In our stretched-hexagon model, no bond is altered from the unstretched Si-Si bond length of 2.35 Å by more than ≈6%.[26,27]) Therefore, if we make the very crude approximation that the surface gains the same energy each time an adatom saturates a bond,[10] then we expect that the favored reconstruction will be the one that leaves the surface with the fewest dangling bonds per atom. We must not be too strict in applying this rule, however, because bond-stretching and bond-bending energies can be significant, and because it is naive to think that every event of adatom binding to the surface yields the same gain in energy.[27]

With regard to the 16×2 reconstruction, Table I lists the various adatoms, dimerized surface atoms, and dangling bonds that arise when the 16×2 structure is created from the perfect unreconstructed Si(110) surface. The 16×2 structure annihilates or saturates 24 of the 64 dangling bonds per surface unit cell, leaving behind 0.625 dangling bonds per surface atom. This is to be compared with 1.0 dangling bonds per atom at the GaAs(110) surface and at the unreconstructed Si(110) surface—and indicates that the Si(110)-16×2 reconstruction is a very stable surface (see Table II).

With regard to the 5×1 surface, the present stretched-hexagon model describes that surface when the hexagons are stacked in the **b** direction with various uneven spacings between hexagons. The smallest such spacing allowed in principle (but not in fact) has the edges of adjacent hexagons coinciding in a close-packed geometry as in a 5×2 periodic structure of the present model, with 0.50 dangling bonds per surface atom, or in a 5×5 structure of the Keim model, with 0.52 dangling bonds per atom—indicating that the present model, with its fewer dangling bonds per atom, is energetically slightly preferred over the Keim model (see Table II). These two reconstructions are the close-packed ones, with coincident hexagon edges. If the hexagon edges are not permitted to coincide, but kept 1.5|**b**| apart (the next-closest packing), then both periodic structures, the Keim, 5×4 model and the present 5×7 model, have 0.6 dangling bonds per atom, and are comparably stable. The STM images (Figs. 2 and 6) indicate that the closest-packing realized in nature has the hexagon sides >1.5|**b**| apart, corresponding to a

TABLE II. Various models of the Si(110) surface, with corresponding model surface unit cells. Indicated are the number of atoms per model surface unit cell, the number of adatoms, the number of dangling bonds saturated per adatom, the total number of dangling bonds saturated per model cell, and the number of dangling bonds remaining per surface atom. For the models of the 5×1 structure, we indicate in parentheses after each model the distance in units of $|\mathbf{b}|$ between the sides of adjacent hexagons. When this distance is half-integral, the sequence of A atoms in the $\mathbf{b}$ direction on one side of the hexagons alternates: $A1$, $A2$, $A1$, $A2$, etc. When it is integral, there is no alternation: $A1$, $A1$, $A1$, etc. or $A2$, $A2$, $A2$, etc. The Keim 5×5 model features hexagons closely packed with coincident edges, while the Keim 5×4 model has a row between hexagon edges. The present 5×2 model features closely packed hexagons, with coincident edges. The 5×7 model has 1.5 rows between hexagons. The 5×4 model has 2.0 rows between hexagons, while the 5×9 and 5×5 models feature 2.5 and 3.0 rows between adjacent hexagons. Using the qualitative notion that the most stable surface model leaves the fewest unsaturated dangling bonds per atom at the surface, we find that the present model of the 16×2 reconstruction is more stable than the GaAs(110) surface, and more stable than our 5×4 model of the 5×1 reconstruction.

Model	Atoms per model cell	Adatoms per model cell	Bonds saturated per adatom	Reduction in dangling bonds per model unit cell	Net dangling bonds per atom
Si(110)-16×2 reconstruction					
Present 16×2	64	14	2	24	0.625
GaAs(110)-1×1 reconstruction					
GaAs(110)-1×1	2	0	0	0	1.00
Si(110)-5×1 reconstruction					
Present 5×2 (0.0)	20	5	2	10	0.50
Keim 5×5 (0.0)	50	12	2	24	0.52
Present 5×7 (1.5)	70	14	2	28	0.60
Keim 5×4 (1.5)	40	8	2	16	0.60
Present 5×4 (2.0)	40	7	2	14	0.65
Keim 5×5 (2.5)	50	8	2	16	0.68
Present 5×9 (2.5)	90	14	2	28	0.69
Present 5×5 (3.0)	50	7	2	14	0.72

5×4 structure in the present model (0.65 dangling bonds per atom) or a 5×5 structure with a 2.5$|\mathbf{b}|$ hexagon spacing in the Keim model (0.68 dangling bonds per atom). The present model is slightly more stable than the Keim model in this case also (Table II).

The stability of our 16×2 model should be compared with that of our 5×1 model. Here we concentrate on the observed fact that there is always a distance $>1.5|\mathbf{b}|$ between hexagon edges on the 5×1 surface (Fig. 6), and so the closest approach of two hexagons with two rows in between corresponds to a 5×4 model—with more distant pairs of hexagons yielding more dangling bonds per atom. We find for the 5×4 structure 0.65 dangling bonds per atom, just slightly more than 0.625 for the 16×2 structure. This indicates that the 5×1 structure, with the closest-approach 5×4 structure in particular, and, more generally, with any allowed ($>1.5|\mathbf{b}|$) juxtaposition of hexagons, will have more dangling bonds per atom than the 16×2 structure, and hence also explains why the 16×2 structure is the preferred reconstruction. The small difference between the number of dangling bonds per atom for the 16×2 structure, and for the 5×4 structure with the closest packing consistent with the 5×1 observations, indicates that the two reconstructions, 16×2 and 5×1, are nearly degenerate energetically.

V. SUMMARY

The same stretched-hexagon building block can account for the 23 major facts about the 16×2 and 5×1 reconstructions of the Si(110) surface, in such a way that it is easy to understand why both reconstructions are found, with the 16×2 being slightly more prevalent. This provides a very nice picture of the reconstructions, and one that hopefully will assist in the interpretation of future experiments.

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[9] The observations were conducted at room temperature with a STM in ultrahigh vacuum (UHV) at $\sim 10^{-11}$ torr. Surfaces were prepared by Ohmic heating to ≈ 1150 to 1200 °C, in several second increments.

[10] Since small impurity concentrations are thought to help stabilize the 5×1 reconstruction, it may be too crude an approximation to compare energies of two reconstructions on the basis of the number of saturated bonds alone (as we do here) without including either the impurity contributions to the energies, or the effects of bond bending and bond stretching. Some authors believe that as little as ~ 0.007 ML of Ni on the surface can prevent the 16×2 surface from forming and instead promote the formation of the 5×1 structure. Moreover, the disorder in the STM images of the 5×1 structure has been cited by some authors as evidence that the 5×1 surface is impurity stabilized. This entire question of whether the 5×1 surface is impurity stabilized leaves a number of other questions unanswered even today—not the least of which is why the 16×2 structure forms preferentially to the close-packed 5×2 structure on a Si(110) surface that is supposedly clean.

[11] Our images are calibrated against LEED data for the distance of 50.2 Å between two stripes, from which a 13.3-Å zigzag period is determined. The lattice constant a is taken to be 5.43 Å. See, for example, S. Miura, K. Kato, T. Ide, and T. Ichinokawa, Surf. Sci. **191**, 259 (1987) and Ref. 6. These calibrated values are fully consistent with the STM data. The magnitude of the uncertainty in lengths determined *exclusively* by STM is typically $<10\%$.

[12] The other 16-structure domain on this surface, the one associated with stripes along [1,1,2] can be represented in matrix notation (see Ref. 6) as

$$\begin{bmatrix} 1 & 17 \\ 2 & 2 \end{bmatrix}.$$

[13] Here we have $\mathbf{r}' = 3\mathbf{a} + 13\mathbf{b}$, where $|\mathbf{c}| = 1.92$ Å and the direction of $\mathbf{c}$ is parallel to $\mathbf{a}\times\mathbf{b}$ (perpendicular to the surface, that is, perpendicular to the [1,1,0] direction).

[14] The traditional surface unit cell for the 16×2 reconstruction is spanned by $\mathbf{a}' = (\mathbf{b} - \mathbf{a}) + 16\mathbf{b}$ and $\mathbf{b}' = 2(\mathbf{b} - \mathbf{a})$, where $\mathbf{a}$ and $\mathbf{b}$ are shown in Fig. 9. Note that $\mathbf{a}'$ is not parallel to $\mathbf{b}$, and that for an ideal 16×2 structure $\mathbf{a}'$ would be equal to $16\mathbf{b}$. An equivalent, more convenient, choice of the surface unit cell is spanned by $\mathbf{a}'' = 5\mathbf{a} + 11\mathbf{b}$; $\mathbf{b}'' = 2(\mathbf{b} - \mathbf{a})$. Both surface unit cells have the same area of $32|\mathbf{a}||\mathbf{b}|$.

[15] Y. Yamamoto, Phys. Rev. B **50**, 8534 (1994) has proposed another 16×2 model, which features trimers of Si, dimerization of adjacent atoms along a chain, rumpling of the surface, and no adatoms. Our data (Fig. 1) are inconsistent with his model.

[16] $A1$ sites are top sites and have an atom underneath the adatom, while $A2$ sites are hollow sites with no atom underneath.

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[25] A close examination of Fig. 6 reveals some disorder in the orientation of the long axes of the hexagons with respect to the [0,0,1] directions. Note that the entire hexagon reorients, not just the long axis. This feature is consistent with a defective version of our model in which each adatom of the B-$A2$-B vertex is displaced laterally by $\approx \pm 0.5\mathbf{b} + 0.17\mathbf{a}$, or the B-$A2$-B atoms are displaced by $\pm\mathbf{b}$, with the face-centered adatom displaced $\approx \pm 0.5\mathbf{b} + 0.17\mathbf{a}$. The data are inconsistent with the Keim model, because they show that the entire hexagon reorients, not just the long axis.

[26] Total energy calculations for the fictitious Si(111)-2×2 reconstruction show that its adatoms all have bond lengths within 5% of the natural Si-Si bond-length. See Ref. 27.

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