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TOPICAL REVIEW

Elementary structural building blocks encountered in silicon surface reconstructions

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Abstract

Driven by the reduction of dangling bonds and the minimization of surface stress, reconstruction of silicon surfaces leads to a striking diversity of outcomes. Despite this variety even very elaborate structures are generally comprised of a small number of structural building blocks. We here identify important elementary building blocks and discuss their integration into the structural models as well as their impact on the electronic structure of the surface.

(Some figures in this article are in colour only in the electronic version)

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1. Introduction

Understanding the structural and electronic properties of silicon surfaces at the atomic scale is of tremendous scientific and technological importance. It has been known since 1958 that atoms at the surface of a semiconductor assume a different structure than that of the bulk [1]. The creation of a surface results in broken chemical bonds, so-called dangling bonds, pointing towards the vacuum. Dangling bonds are energetically unfavorable causing surface atoms to

rearrange or reconstruct in order to lower the total energy of the surface, which may result in highly complex atomic architectures. The determination of the atomic structure requires the complementary role of different experimental and theoretical techniques and remains a formidable challenge. It took 26 years of combined effort to solve the atomic structure of the famous Si(111)-(7 × 7) reconstruction [2].

Surprisingly only a handful planar silicon surfaces with a stable reconstruction are known [3]. Most studies have concentrated on surfaces with a surface normal between the [100] and [110] direction including the (111) surface (see figure 1 for an overview). Only little is known about surfaces with orientations away from this plane.

Despite the high structural complexity of silicon surface reconstructions one often encounters common elementary structural building blocks (figures 1(a)–(f)). Identifying these building blocks is important not only for a better understanding of these surfaces but also as they may serve as a guide for the elaboration of new structural models. In this short review we describe the most important silicon surface reconstructions emphasizing the role of these elementary structural building blocks. First we discuss the properties of the bulk-truncated

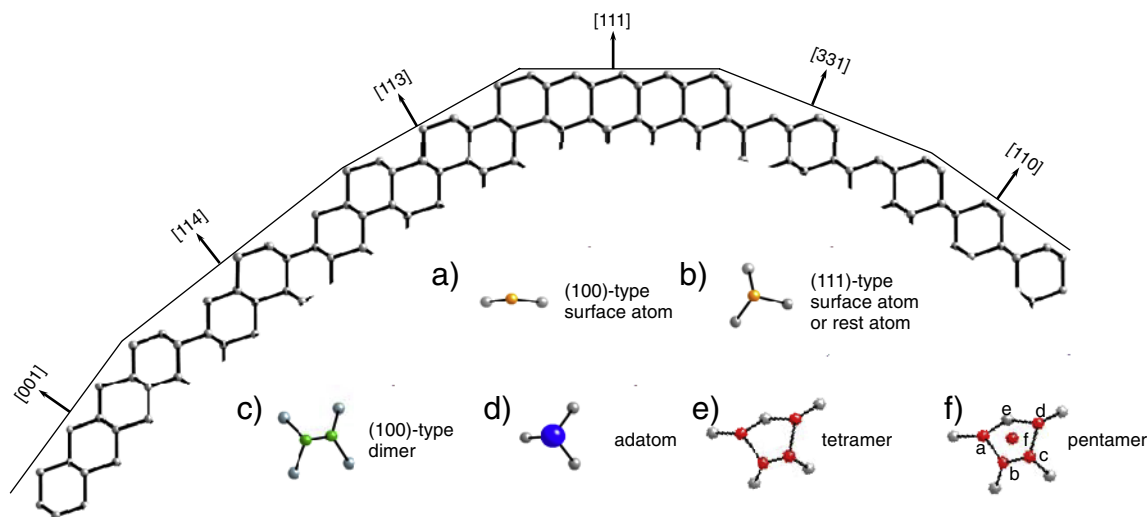


Figure 1. Side view of silicon crystal along the $[1\bar{1}0]$ direction with various surfaces indicated. An overview on the elementary structural building blocks encountered in silicon surface reconstructions is also shown.

surfaces and identify two prototypical types of surface atoms. Then we focus on the strategies adopted by the various surfaces in order to reduce the number of dangling bonds by integrating these building blocks into more complex structures. We also include a discussion on the relation between their structural and electronic properties.

2. Bulk-truncated surfaces

In bulk silicon, each of the tetrahedrally coordinated atoms forms four covalent bonds with its four nearest neighbors. Each bond contains two paired electrons. When a surface is formed, some of these bonds will be broken, leading to unsaturated orbitals, the so-called dangling bonds, containing only one unpaired electron. The lack of electron pairing makes dangling bonds unstable. The atoms in the surface region will move away from their bulk positions trying to minimize the surface energy. When this happens, the surface is said to relax or reconstruct depending on how the surface atoms seek new coordinates. Surface relaxation refers to the case when surface atoms are displaced from their bulk positions but there is no change in the surface periodicity. Surface reconstruction on the other hand refers to atomic displacements causing the symmetry parallel to the surface to be lower than that of the bulk.

At metal surfaces, the electrons are free to rearrange their distribution in space. Relaxation by adjustment of the interlayer spacing of the first few atomic planes is often sufficient to minimize the surface energy. At semiconductor surfaces, the truly directional chemical bonds between atoms lead to considerable elastic strain which increases the total energy of the surface. Stable surface reconstructions are obtained when the strain energy is compensated by the energy gain which results from the reduction of dangling bonds.

When studying the energetics of semiconductor surface reconstructions, it is important to take into account the electronic structure of the surface as well. Further lowering

of the total energy may be achieved when surface states are either empty or fully occupied by two electrons. Spontaneous symmetry breaking and the related lifting of degeneracies, opening a gap between electronic states, is often the origin of the driving force for surface reconstruction. In fact, besides a few exceptions, the bandstructure of reconstructed semiconductor surfaces tends to be semiconducting. In subsequent sections, several mechanisms leading to a gap in the electronic spectrum of the surface will be discussed.

A thorough understanding of the geometry of the non-reconstructed bulk-truncated surfaces is the starting point for the elaboration of any structural model. Figures 2(a), 3(a), 4(a), 5(a), 6(a), and 7(a) present the dangling bond configuration of the bulk-truncated Si(100), Si(111), Si(114), Si(113), Si(110), and Si(331) surfaces respectively, whose reconstructions will be discussed in the following. Yellow colored atoms represent surface atoms with dangling bonds. Two prototypical types of surface atoms may be distinguished: the (100)-type surface atoms found on the (100) bulk-truncated surface (figure 2(a)) and the (111)-type surface atoms occurring on the (111) bulk-truncated surface (figure 3(a)). (100)-type surface atoms carry two dangling bonds and have two backbonds to the substrate, while the (111)-type surface atoms carry only one dangling bond and share three backbonds. These two types of surface atoms also occur on surfaces with other orientations. On bulk-truncated Si(114) (figure 4(a)) and Si(113) (figure 5(a)) surfaces, both types of surface atoms exist simultaneously, whereas on the Si(110) (figure 6(a)) and on the Si(331) (figure 7(a)) surface only (111)-type surface atoms occur. In the following we discuss several strategies with which the silicon surfaces reduce the number of dangling bonds.

3. Strategy 1: dimers

A conceptually simple strategy to reduce the number of dangling bonds is the formation of dimers found on the Si(100)

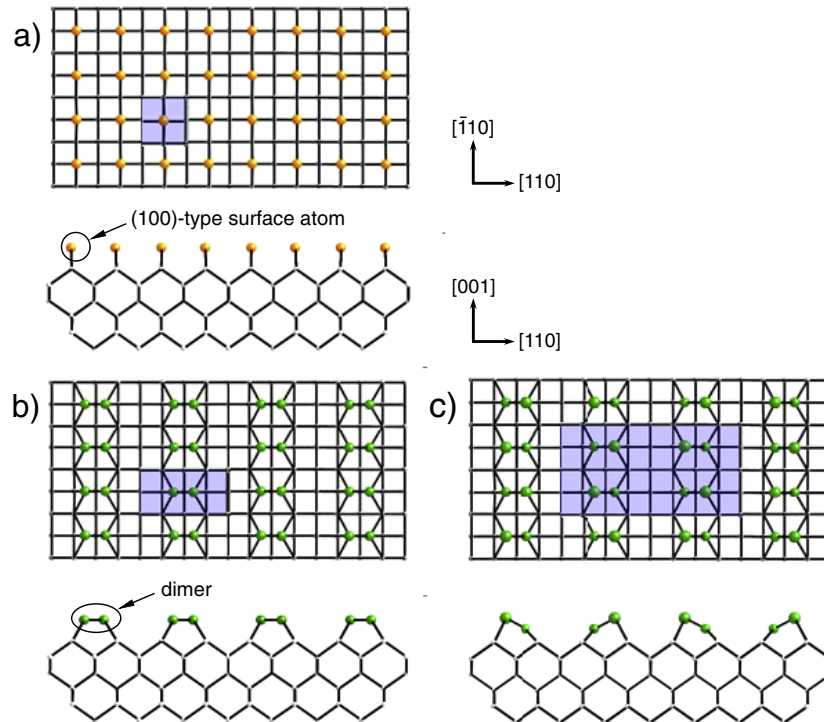


Figure 2. (a) Bulk-truncated Si(100)-(1 × 1) surface. (b) Si(100)-(2 × 1) with symmetric dimers. (c) Si(100)-c(4 × 2) with asymmetric dimers. The corresponding unit cells are also shown.

surface. In 1958 Farnsworth *et al* [1] reported that low-energy electron diffraction (LEED) of clean Si(100) produces half-integral diffraction spots indicating a (2 × 1) periodicity in real space. However, it was not until 1992, after the publication of the first low-temperature scanning tunneling microscopy (STM) images [4] that a general consensus about its detailed atomic structure emerged [5]. In order to minimize their energy, surface atoms on clean Si(100) move pairwise towards each other and form a new bond resulting in the symmetric dimers shown in figure 2(b). However, low-temperature STM images [4, 6] clearly showed that the dimers on Si(100) are buckled, i.e. the two atoms of the dimer have different heights above the surface plane (see figure 2(c)). These asymmetric dimers are also supported by LEED [7] and other techniques [5]. Asymmetric dimers prefer higher periodicities, (2 × 2) and c(4 × 2), which appear because the direction of buckling of neighboring dimers is correlated. Unless stabilized by surface defects, the correlation is partially destroyed around 200 K. Above this temperature LEED usually sees an average (2 × 1) order. At room temperature, the dimers appear symmetric in STM images, since thermal vibrations flip the buckling direction of dimers faster than can be observed by STM.

How does the formation of dimers influence the electronic structure of the surface? When two surface atoms pair up to form a dimer only one of the two dangling bonds carried by each (100)-type surface atom gets eliminated. The orbitals, associated with the electrons participating in the formation of the dimer bond, overlap resulting in a bonding σ and antibonding σ^* combination [5]. Since the overlap is large, the energy splitting between the two states is large, causing

the occupied σ state and the empty σ^* state to become broad resonances in the valence and the conduction band respectively. The remaining two dangling bonds mix into a π and π^* bond [5]. For symmetric dimers the energy splitting between these two states is small, resulting in a partial overlap, which renders the system metallic. The formation of asymmetric dimers allows a slight energy gain and opens up a gap between the π and π^* state, which renders the system semiconducting in agreement with experiment.

4. Strategy 2: adatoms and rest atoms

Prototypical adatoms in combination with rest atoms are encountered on the (111) surfaces of the elemental semiconductors. Here we first discuss the Ge(111)-c(2 × 8) reconstruction (figure 3(b)), because it is less complex than the famous Si(111)-(7 × 7) reconstruction (figure 3(c)). The Ge(111)-c(2 × 8) reconstruction was identified in 1963 [8–10] by LEED. On the bulk-truncated surface (111)-type surface atoms are arranged in a hexagonal pattern and are only second-nearest neighbors (figure 3(a)). Their nearest neighbors are three subsurface atoms, with which they share a bond. In order to reduce the number of dangling bonds on the surface, additional germanium atoms, called adatoms (blue atoms in figure 3(b)), saturate each three adjacent dangling bonds by forming three bonds, called backbonds, with the three nearest surface atoms [11]. Its fourth orbital, carrying a single electron, points towards the vacuum. An adatom thus replaces three dangling bonds by a new dangling bond.

Adatoms may occupy the two possible sites indicated in figure 3(b). These geometries are distinguished as hollow

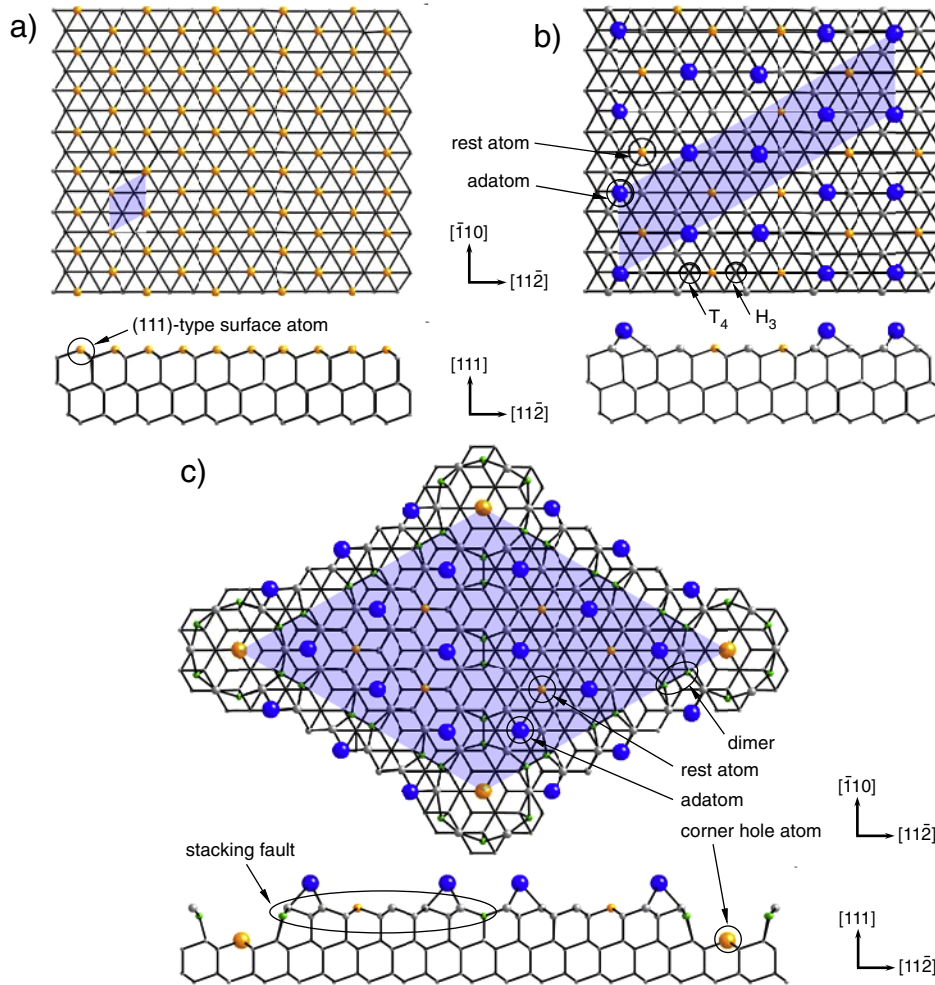


Figure 3. (a) Bulk-truncated Si(111)-(1 × 1) or Ge(111)-(1 × 1) surface. (b) Ge(111)-c(2 × 8) reconstruction. (c) Si(111)-(7 × 7) reconstruction.

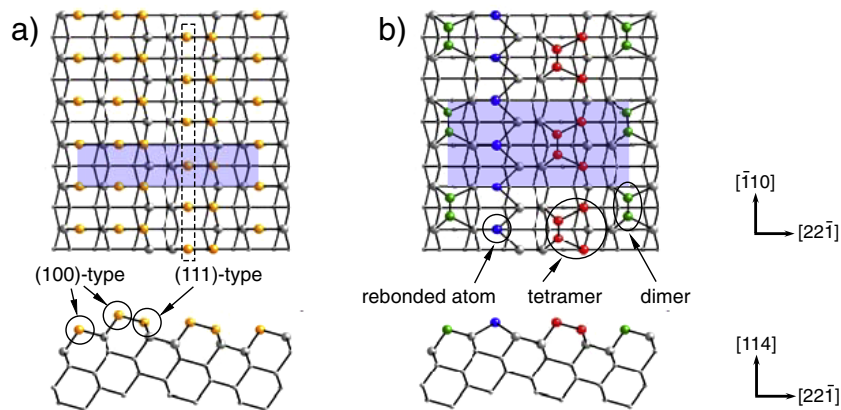


Figure 4. (a) Bulk-truncated Si(114)-(1 × 1) surface. (b) Si(114)-(2 × 1) reconstruction.

(H₃) and atop (T₄) sites depending on whether the substrate atom below the adatom is found in the fourth or second layer. In H₃ sites the adatom is three-fold coordinated, in T₄ sites the adatom is approximately four-fold coordinated due to the substrate atom directly below in the second layer. The unambiguous discrimination between adatoms in T₄ and H₃

sites was finally achieved by x-ray diffraction in 1990 [12] favoring T₄ sites.

Although each adatom reduces the number of dangling bonds, it is not favorable to saturate a surface with the maximum number of adatoms. Of the 16 dangling bonds per c(2 × 8) unit cell of the bulk-truncated Ge(111) surface,

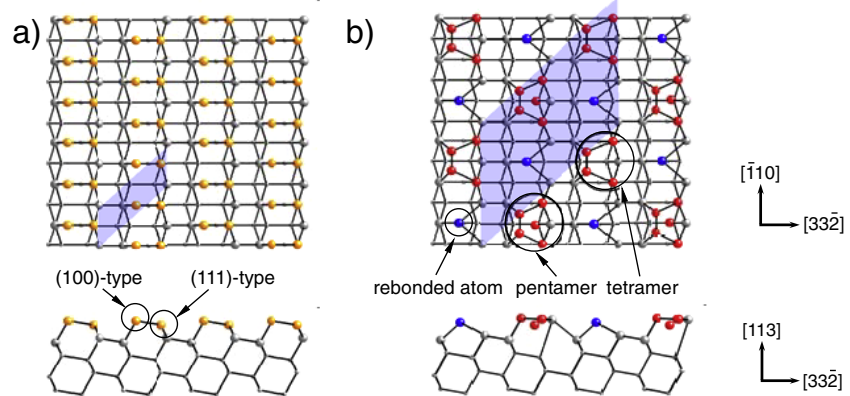


Figure 5. (a) Bulk-truncated Si(113)-(1 × 1) surface. (b) Si(113)-(3 × 2) reconstruction.

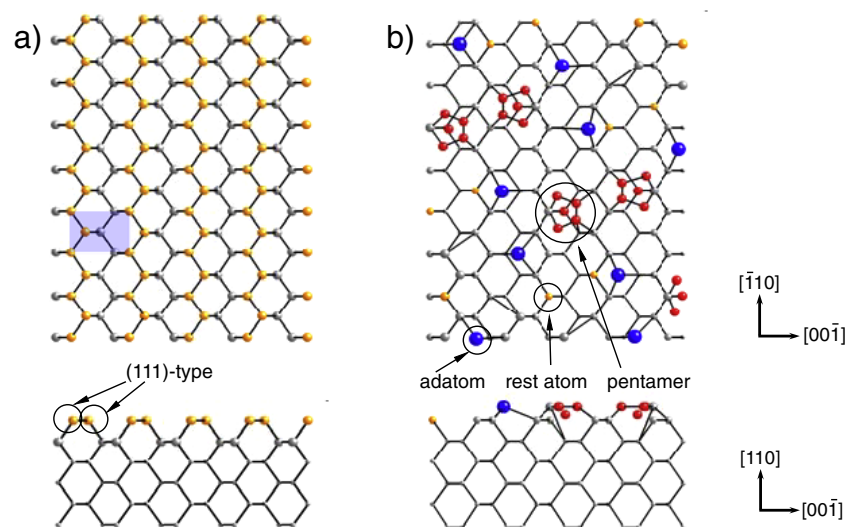


Figure 6. (a) Bulk-truncated Si(110)-(1 × 1) surface. (b) Si(110)-(16 × 2) reconstruction.

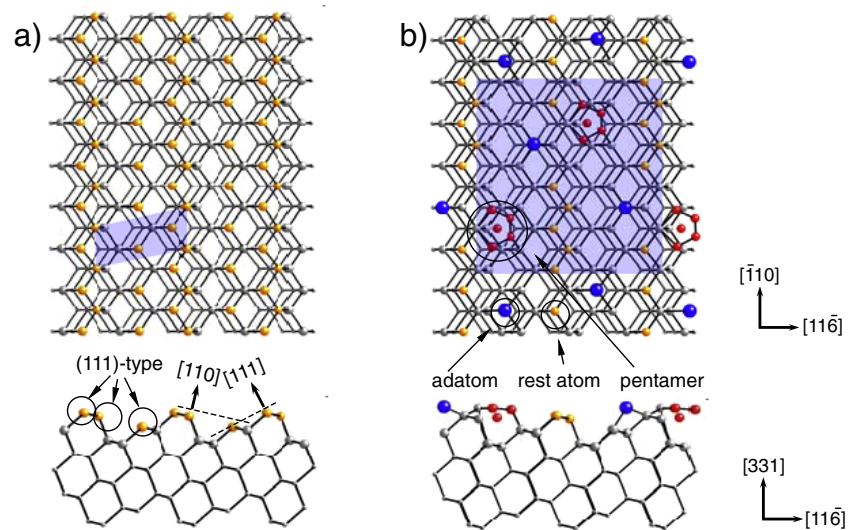


Figure 7. (a) Bulk-truncated Si(331)-(1 × 1) surface. (b) Si(331)-(12 × 1) reconstruction.

four adatoms saturate 12. Each adatom still carries one remaining dangling bond. So the number of dangling bonds per reconstructed $c(2 \times 8)$ unit cell is 8. The four surface atoms (yellow atoms in figure 3(b)), whose dangling bonds have not been saturated by adatoms are called rest atoms. The structure is further stabilized by an electronic charge transfer from the adatoms to the rest atoms [13–15] resulting in fully filled rest atom states and empty adatom states in agreement with experiment [16, 17].

The balance between the lowering in energy due to the reduction of dangling bonds and the energy increase caused by the bond distortion is very delicate [13, 18]. Compared to the Ge(111)- $c(2 \times 8)$ reconstruction, the Si(111)- (7×7) reconstruction is much more complex. Since its discovery in 1959 [19] using LEED the (7×7) reconstruction has become the prototype for studying complex reconstructions occurring at semiconductor surfaces.

A mystery for many years, the atomic structure of Si(111)- (7×7) was resolved by Takayanagi *et al* [2, 20] in 1985 on the basis of transmission electron diffraction data, assisted in part by the observation of adatoms in STM images by Binnig *et al* [21]. Their now widely accepted dimer-adatom-stacking fault (DAS) model shown in figure 3(c) consists of 12 silicon adatoms in the first layer (blue atoms), a stacking fault bilayer (second and third layer), within which 9 dimers (green atoms) in the third layer border the triangular faulted and unfaulted subunits. Note that the dimers observed on Si(111)- (7×7) are not the same as the ones observed on Si(100)- (2×1) . Whereas the two atoms of a standard (100)-type dimer each carry one remaining dangling bond, the (111)-type dimers are completely saturated. A deep vacancy, called the corner hole is located at each apex of the unit cell (on top of the large yellow atom). The 6 three-fold bonded atoms in the second layer falling in between the adatoms of each triangular subunit are rest atoms (small yellow atoms).

The DAS model reduces the number of dangling bonds from 49 for the unreconstructed (7×7) unit cell to 19 (12 dangling bonds for the adatoms, 6 dangling bonds for the rest atoms and one dangling bond for the atom below the corner hole). These 19 dangling bonds deliver 14 electrons which fill the energetically lower lying rest atoms and corner hole states, i.e. 7 electrons are transferred from the adatom states to the rest atom and corner hole states. The remaining 5 electrons remain in the adatom bands resulting in a metallic semiconductor surface in agreement with experiment [22, 23].

5. Strategy 3: tetramers and pentamers

Tetramers and pentamers are more complex schemes to eliminate dangling bonds. Tetramers are found on Si(114) and Si(113). We first discuss the conceptually simpler Si(114)- (2×1) reconstruction.

The Si(114)- (2×1) reconstruction was first reported in 1993 [24]. A structural model was proposed by Erwin *et al* in 1996 [25]. On the bulk-truncated Si(114) surface shown in figure 4(a) both (111)-like and (100)-like surface atoms are observed carrying one and two dangling bonds respectively. The (100)-like surface atoms marked by a dashed rectangle

in figure 4(a) dimerize. Due to the immediate vicinity of two neighboring (111)-like surface atoms bonding to the dimer atoms, the dimer is topologically different from the standard dimer encountered on the Si(100) surface. The resulting structure containing the dimer atoms plus the two (111)-like surface atoms is called a tetramer (red atoms in figure 4(b)). An additional standard dimer is formed by pairs of (100)-like surface atoms (green atoms). The remaining four surface atoms per unit cell are replaced by two so-called rebonded atoms (shown in blue), each having three backbonds and one dangling bond.

The reconstructed Si(114) surface unit cell exhibits a total of 8 dangling bonds: 4 on the tetramer, 2 on the two rebonded atoms and 2 on the standard (100)-like dimer. The 8 electrons coming from these 8 dangling bonds fill four surface states. Two unoccupied surface states separated by a small gap from the filled part of the spectrum have also been identified in a first-principles study [26].

We now turn to the Si(113) surface reconstruction reported in 1985 by Gibson *et al* [27]³. The (113) bulk-truncated surface consists of alternating rows of (111)- and (100)-like surface atoms. The model proposed by Dabrowski *et al* in 1994 [28] is shown in figure 5(b). It shares several building blocks with the Si(114)- (2×1) reconstruction, namely tetramers and rebonded atoms. Tetramers and rebonded atoms are arranged in a (3×1) order such that they alternate along $[\bar{1}10]$. Taking into account the dangling bond on the rebonded atom and the 4 dangling bonds on the tetramer, we end up with 5 dangling bonds per unit cell. Thus from an electron-counting point of view this structure is expected to be metallic in contrast to the semiconducting nature of the surface observed in experiments. To solve this problem, every second tetramer captures an interstitial silicon atom (atom f in figure 1(f)) leading to the (3×2) periodicity observed at room temperature [5, 28]. This interstitial atom affects the electronic structure of Si(113), changing the metallic (3×1) into a semiconducting (3×2) surface, however inducing considerable strain. The vertical component of the strain is relieved as the structure relaxes strongly towards the vacuum, elevating a pentagonal ring of atoms. This pentamer, formed by the original tetramer and the common neighbor of the two (111)-like surface atoms, is almost flat and parallel to the surface. Above 800 K, interstitial atoms hop from one tetramer to the other [29]. Due to the missing correlation between hopping interstitial atoms, the periodicity observed by LEED is (3×1) .

A structural model containing a slightly different pentamer has been proposed by An [30] to explain the pentagons observed in STM images of the (16×2) reconstruction of Si(110).⁴ Already in 1965 Jona [9] had studied the Si(110) surface by LEED and observed a structure with a periodicity of ‘possibly 16’. The bulk-truncated Si(110) surface consists of double rows of (111)-like surface atoms running along the

³ The Si(113) reconstruction has already been observed earlier by Olshansky *et al* [37]. However this study appears to be based on Ni contaminated samples, since the Si(331)- (13×1) reconstruction also reported in this paper is known to be stabilized upon Ni contamination.

⁴ The periodicity of the conventionally labeled Si(110)- (16×2) reconstruction is more correctly described in matrix notation by $\begin{pmatrix} 11 & -5 \\ 2 & 2 \end{pmatrix}$.

$\bar{1}10$ direction. Since all surface atoms of the bulk-truncated Si(110) surface are (111)-like, the original pentamer found on the Si(113) surface must be modified. In the adatom-tetramer-interstitial (ATI) model [30–32] shown partially in figure 6(b) (for the complete structural model, including the steps, see [31]), pentamers are formed by four adatoms (atoms a, b, c, and d in figure 1(f)) forming the tetramer, one surface atom (e), and the interstitial atom (f). In contrast to the pentamers encountered on the Si(113) surface, only atom e, which serves as an anchor point for the pentamer, is provided by the surface atoms. All other atoms (a, b, c, d, and f) are additional atoms which must be provided by the step which is an integral part of the unit cell. Besides the pentamers, adatoms accompanied by rest atoms are found to interlink the double rows of surface atoms in a complex way. Although we encounter rest atoms on surfaces away from the $[111]$ direction, it is important to note that rest atoms are always (111)-type surface atoms carrying only one dangling bond. Since (100)-type surface atoms carry two dangling bonds, which render them energetically highly unstable, they do not qualify as rest atoms and have not been observed.

Using STM, we have recently been able to resolve, for the first time, pentagons on the Si(331) surface [33], very similar to the ones observed on the Si(110) surface [30]. Since the discovery of the Si(331)-(12 × 1) reconstruction more than 17 years ago [34]⁵, several structural models containing dimers and adatoms have been proposed [35, 36]. However, none of these models is able to explain the pentagons observed in our STM images.

Inspired by the structural model of the Si(110)-(16 × 2) reconstruction, we have proposed a new structural model for Si(331)-(12 × 1) containing silicon pentamers as essential structural building blocks (see figure 7(b)). The arrangement of dangling bonds on the bulk-truncated surface of Si(110) and Si(331) differ. Whereas (111)-type surface atoms on the Si(110) surface occur in double rows running along the $\bar{1}10$, double rows of (111)-type surface atoms alternate with single rows on the bulk-truncated Si(331) surface. The bulk-truncated Si(331) surface can actually be viewed as consisting of small alternating (110) and (111) terraces (see figure 7(a)). In analogy with the Si(110) model the two pentamers for the Si(331) model are anchored on the double rows of surface atoms in a way such that the local bonding geometry is exactly the same as on the (110) surface. Some of the remaining dangling bonds are saturated by adatoms. Stekolnikov *et al* [31] have already noted for the Si(110) case that it is energetically more favorable to leave some rest atoms unsaturated than to introduce the maximum number of adatoms into the model. This allows further reduction of the surface energy by electron transfer from the adatom to the rest atom in analogy with Ge(111)-c(2 × 8) and Si(111)-(7 × 7).

6. Summary and conclusion

Important lessons may be learned by analyzing and comparing existing structural models for silicon surface reconstructions.

⁵ The periodicity of the conventionally labeled Si(331)-(12 × 1) reconstruction is more correctly described in matrix notation by $\begin{pmatrix} 2 & 0 \\ 1 & 6 \end{pmatrix}$.

Although each surface adopts its own strategy to reduce the number of dangling bonds, we identified elementary structural building blocks including dimers, adatoms, rest atoms, rebonded atoms, tetramers, and pentamers common to several reconstructions. We discussed their integration into the structural models and the consequences on the electronic structure.

Acknowledgments

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