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Atomic structure of the Ge(101) surface

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The atomic structure of the Ge(101)$c(8\times10)$ surface is studied in the present paper by means of scanning tunneling microscopy and low-energy electron diffraction. A detailed model of the structure has been proposed for further investigation. The surface consists of zigzag chain atoms, adatoms, dimers, rebonded atoms, and rest atoms arranged at different levels and in different orientations, and thus is even more complicated than the Si(111)7×7 surface. [S0163-1829(98)51312-4]

Among low index silicon surfaces, (101) is the only one with a surface structure still unknown, although it is a stable plane of equilibrium silicon crystals and has a surface specific free energy only slightly higher than that of the (111) plane.[1] The first investigation of the Si(101) surface was conducted early in 1965,[2] and the interest on the surface has never been reduced since then.[3–29] Through these efforts the following facts seem to have been established.

(i) A clean and well-annealed Si(101) surface reconstructs to ''16×2'' or, more precisely, to

$$\begin{pmatrix} 1 & 17 \\ 2 & 2 \end{pmatrix},$$

while only a very small amount of Ni, such as 0.007 ML can stabilize the surface to the ''5×1'' reconstruction or others.[9,13] The ''5×1'' reconstruction, though having a markedly different translational symmetry, consists of the same building blocks as those of the ''16×2'' reconstruction.[28]

(ii) The ''16×2'' reconstruction consists of equally spaced but alternately raised and lowered strips lying along the ⟨112⟩ direction, and the height difference between the two types of strips equals to the layer spacing of the surface.[10,13]

(iii) The ''16×2'' reconstructed Si(101) surface is at least as complicated as the Si(111) 7×7 surface, because its photoemission spectra,[4] angle-resolved photoemission spectra (ARUPS),[27] and high-resolution synchrotron radiation Si $2p$ core-level spectra[26] are similar to those of the Si(111)7×7 surface. This conclusion is supported by chemical titration of the ''5×1'' reconstruction of the surface with N_2O and O_2.[18] The ''16×2'' reconstruction must also contain some zigzag chains because its ARUPS are also similar with those of the Si(111)2×1 surface, which contains π-bonded chains.[8] Specifically, the ''16×2'' surface must contain some adatoms, rest atoms, and dimers,[26,27] as well as zigzag chain atoms[8] (or A atoms[18]).

On the basis of the above facts, several structural models of the surface have been proposed.[17,18,28] However, some of these models[17,18] are obviously incompatible with scanning tunneling microscopy (STM) images,[12,25,28] while others that are based on STM images do not include all structural details and are thus incomplete.[28] So, the reconstructions of the Si(101) surface are still unknown.

On the other hand, only little attention[2,3,6,30–32] has been so far paid to the Ge(101) surface, as in the case of other germanium surfaces, because they have less importance with regard to applications. Nevertheless, it has been disclosed that a clean and well-annealed Ge(101) surface is $c(8\times10)$ reconstructed,[30–32] and that the building block of this surface is similar to that of the Si(101)''16×2'' surface.[32]

It is our belief that from a basic scientific point of view investigations of germanium surfaces should not be neglected and that comparisons of germanium surfaces and interfaces with their silicon counterpart can make our knowledge about group-IV semiconductor surfaces and interfaces more systematic. Accordingly, we have been carrying out a systematic investigation of germanium surfaces[33–38] and interfaces.[39] As a result, three important common features of group-III/group-IV interfaces have been disclosed.[39] To continue the investigation of clean germanium surfaces, in the present paper, by means of STM and low-energy electron diffraction (LEED), we study the atomic structure of the Ge(101)$c(8\times10)$ surface.

The experiment was carried out in the UHV system that has been used in recent studies.[34–37] Briefly, the system consists of a main chamber, where LEED, Auger electron spectroscopy (AES), and a homemade STM are installed, and a sample preparation chamber, where ion bombardment and annealing are carried out. In STM experiments the bias voltage is applied to the sample and the tip is grounded. The constant-current mode of the STM was used throughout the work and the scanning rate was from 200 to 2000 Å/sec. Some of the images shown here were acquired with the ac mode, i.e., the differential or local-contrast-enhanced mode, as mentioned in figure captions. The tip was made out of W wire with electrochemical etching. The Ge(101) sample was cut from a single crystal rod with a resistivity of 40–50 Ωcm. After several cycles of ''argon-ion bombardment plus subsequent annealing'' a clean and well-ordered surface was obtained, as verified by Auger-electron spectroscopy (AES) and LEED.

The clean and well-annealed Ge(101) surface gives rise to nice $c(8\times10)$ LEED patterns that are the same as those reported long ago,[30] and thus not to be shown here. Since the truncated (101) surface has a glide line in the $[-1\ 0\ 1]$ direction, the reconstructed surface can have two types of domains, and hence the LEED patterns have a mirror plane

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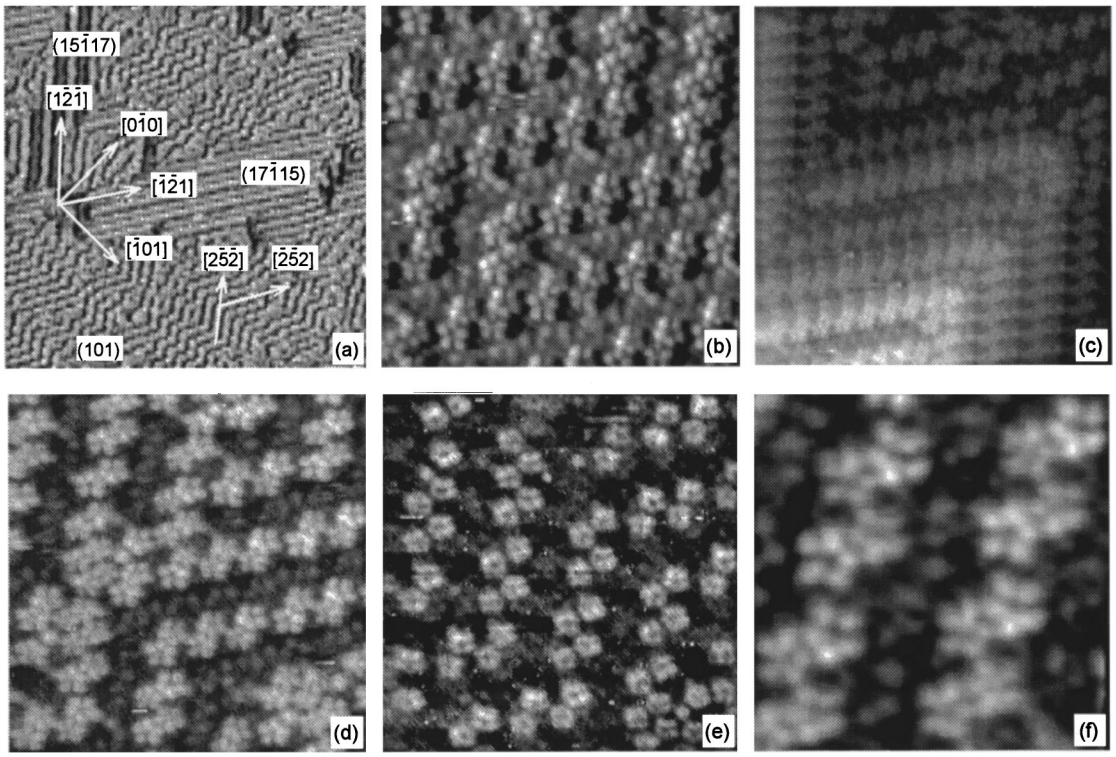

FIG. 1. STM images (empty state, unless otherwise mentioned) obtained from the clean and well-annealed Ge(101)$c(8\times10)$ surface. (a) Low magnification image (ac mode, 970×970 Å, 3.0 V, 1.0 nA), showing the general morphology of the surface. Note that this imaged area contains more facets than average so to show them clearer. (b) A pure $c(8\times10)$ area (ac mode, 130×130 Å, 1.2 V, 1.5 nA). (c) An area with the (17 −1 15) and (15 −1 17) facets coexisting with the $c(8\times10)$ reconstruction (225×225 Å, 1.2 V, 1.0 nA). (d) A $c(8\times10)$ area (130×130 Å, 1.2 V, 1.5 nA). (e) Filled-state image of a $c(8\times10)$ area (130×130 Å, −1.6 V, 0.5 nA). (f) Image of four $c(8\times10)$ unit cells (54×54 Å, 1.2 V, 1.5 nA).

parallel to the [−1 0 1] direction. This was reported previously[30] and is also confirmed by our LEED patterns.

Several typical STM images acquired from the surface are given in Fig. 1. Figure 1(a) shows the morphology of the surface, which consists of large areas of the $c(8\times10)$ reconstruction as well as facets of (15 −1 17), (17 −1 15), (15 1 17), and (17 1 15). Each $c(8\times10)$ reconstruction area consists of many small domains with their building blocks forming rows either in [2 −5 −2] or in [−2 −5 2] direction, as expected from the mirror plane of the LEED patterns. This can be seen more clearly in Fig. 1(b), and from this figure we can also see that each of the eye-catching building blocks of the $c(8\times10)$ reconstruction actually is a twin of pentagons. Figure 1(c) shows that {15 1 17} facets also consist of pentagon twins. Actually, features with a ''pentagonal shape and hollow in their middle'' were reported to have been imaged from a (101) surface of germanium very recently.[32] Looking at the features in some published STM images of the Si(101)''16×2'' and ''5×1'' reconstructions,[12,25,28] we believe that the so-called ''octets'' [25] and ''stretched hexagons'' [28] are actually pentagon twins but imaged with a lower quality. In other words, our STM observations confirm the conclusion that Ge(101) and Si(101) surfaces consist of similar building blocks.[32] With Fig. 1(d) we show that pentagon twins form rows or ridges separated by troughs and the protrusions in troughs locate one layer spacing below the pentagon twins, and hence that the surface is rough. Given in Fig. 1(e) is a filled-state image. However, the images of the pentagon twins in both figures are very similar, although slightly more vague in the latter. This fact indicates that these STM images of the $c(8\times10)$ reconstruction are dominated by its topology or geometry rather than the local charge density, very likely because of the rough morphology of the surface. This character makes interpretation of its STM images quite straightforward because it is unnecessary not only to do any image calculations but also to construct the so-called ''atomic image,'' which is defined as the average of a pair of dual bias images so as to increase the ''topology-to-charge ratio.'' [35] Given in Fig. 1(f) then is a high-resolution image directly reflecting the atomic structure of the $c(8\times10)$ reconstruction.

On the basis of Fig. 1(f) a detailed structural model of the $c(8\times10)$ reconstruction has been proposed and is given in Fig. 2. We are afraid that the model is so complicated that a guided-tour-type detailed description of it would be not only too lengthy but also helpless, and thereby we would leave readers to inspect the model entity by entity freely. First, it would be helpful to keep in mind two things: the main features of Fig. 1(f) on one side and the driving force of the reconstruction on the other. So, we briefly describe the possible driving force here. Recall that it is the balance between reduction of dangling bonds and the relief of induced local strains that determine the reconstruction of semiconductor surfaces.[40] Apparently, a flat Ge(101) surface is very unfavorable in the sense that there is no easy way which the surface can reduce its dangling bonds while simultaneously relieving the induced strains. So, whatever the concrete reconstruction is the surface must first break its long zigzag

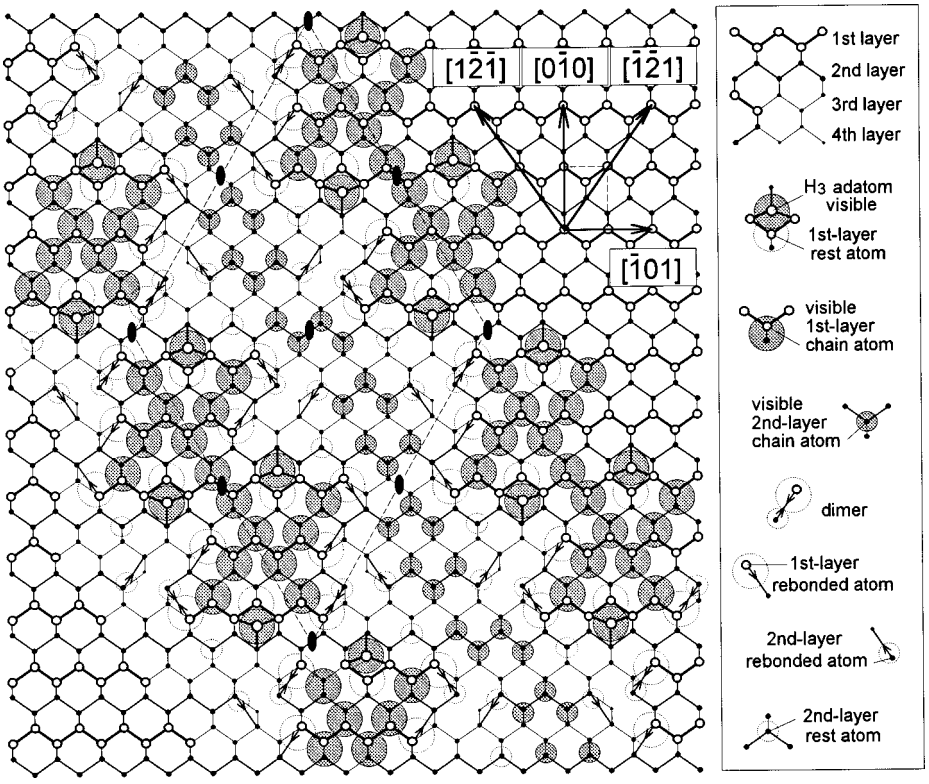

FIG. 2. Structural model of the Ge(101)$c(8\times10)$ surface, with a 1×1 and a $c(8\times10)$ unit cell outlined by dashed lines and the twofold axes represented by filled ellipses. The dotted and gray circles represent the invisible (inward relaxed or pointing inward) and visible (outward relaxed) dangling bonds, respectively. For the meanings of the other symbols see inside the box to the right of the model. Note that for comparison the upper-right and lower-left parts of the figure are left unreconstructed.

chains into short fragments by making itself rough as in Fig. 1(f). Clearly, the model satisfies this requirement. Next, through adatom formation and dimerization as well as rebonding,[18,26,27] the surface reduces its dangling bond (DB) number to 62 in a $c(8\times10)$ unit cell, equivalent to a density of 0.086 DB/Å^2, only slightly higher than the value of 0.063 DB/Å^2 for the Ge(001)2×1 surface. The rich variety of these reconstruction entities as well as some rest atoms[18,26,27] and chain atoms[8] existing at different levels and in different orientations in turn makes it not difficult to relieve the local strains induced by dangling bond reduction. Moreover, the surface can further reduce its energy through redistributing the charge of the remaining dangling bonds.[40] At this point, we suggest that those who are really interested in the details of the model take some time to go through the model.

Now we show that the model structure can indeed give rise to the features in Fig. 1(f). This is quite straightforward if among all remaining first-layer atoms and adatoms only those that carry a dangling bond represented by gray circles are higher (because of their outward relaxation) than others and thereby are more visible. Inward and outward relaxations usually are accompanied by charge transfer, and normally the dangling bond of inward relaxed atoms is *p* like and thus essentially empty, while that of outward relaxed atoms is *s* like and essentially filled.[40] Since the populations of these two kinds of atoms are not very different it is not difficult to believe this. The protruding atoms in the troughs are not imaged very clearly, but obviously they are mainly concentrated around the center. In the model the protruding second-layer atoms are also located near the center, in accordance with the image.

From the distribution of the suppressed spots (or missing spots[41]) seen in LEED patterns of the $c(8\times10)$ surface it has been concluded that a $c(8\times10)$ unit cell must mainly consist of two equal groups of atoms, and the relative shifts between neighboring groups in a row are alternatively $(2\mathbf{a}+2\mathbf{b})$ and $(2\mathbf{a}+3\mathbf{b})$, here **a** and **b** are the unit vectors of the truncated (101) surface in the $[-1\ 0\ 1]$ and $[0\ -1\ 0]$ directions, respectively.[30] The present model obviously is in accordance with this character because the pentagon twins are nearly equal and their relative shifts are correct.

As Fig. 1(c) shows, {15 1 17} facets also consist of pentagon twins. The only difference is that in {15 1 17} facets pentagon twins forming ridges in ⟨1 2 1⟩ rather than ⟨2 5 2⟩ directions. Consequently, in a ridge the relative shift between any two neighboring pentagon twins is always $(2\mathbf{a}+2\mathbf{b})$. Moreover, we believe that the major difference between Ge(101) $c(8\times10)$ and Si(101)''16×2'' and also ''5×1'' is the long-range arrangement of the very similar pentagon twins. Besides, note that in Si(101)''16×2'' both the upper strips and lower strips consist of pentagon twins, while in Ge(101)$c(8\times10)$ there are no pentagon twins in the troughs but only on the ridges.

In summary, a careful survey of the published papers concerning clean and well-annealed (101) surfaces of silicon and germanium leads to the conclusion that these surfaces consist of very similar building blocks, which in turn consist of a

variety of reconstruction entities, and thus are at least as complicated as the Si(111)7×7 surface. On the other hand, our high-resolution STM images of the Ge(101) surface reveal that the $c(8\times10)$ reconstruction as well as the coexisting {15 1 17} facets consist of same kind of pentagon twins in such a way that the pentagon twins aggregate into ridges separated by one-layer-spacing deep troughs. On the basis of all these, a detailed structural model has been proposed for the $c(8\times10)$ reconstruction for further investigation. The model consists of zigzag chain atoms, adatoms, dimers, rebonded atoms, and rest atoms arranged at different levels and in different orientations.

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