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Atomic structure of the Ge(15 3 23) surface

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We report a stable germanium surface (15 3 23), which among all known stable germanium as well as silicon surfaces is the only one inside the unit stereographic triangle and has the highest indices. On the basis of high-resolution dual-bias scanning tunneling microscope images, a detailed model has been proposed for it for further investigation. The surface does not consist of nanometer facets of any other stable surfaces while some unstable surfaces, such as (102), may facet to including {15 3 23} facets, and thus is also a major stable surface, the same as (001), (111), (113), etc.
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As a result of the enormous effort dedicated in the past to understanding silicon surfaces, the atomic structures of the Si(111) and (001) surfaces have been determined.[1–3] Since then the interest of the surface science community in this regard has naturally been shifted to high index silicon surfaces. Very recently, models of the atomic structure of Si(113) (Ref. 4) and (114) (Ref. 5) surfaces have been proposed, while the atomic structures of (112),[6] (5512),[7] and other (hhl) (Ref. 8) surfaces are of current interest.

On the other hand, germanium surfaces, including both the low and high index ones, have received much less attention than their silicon counterparts[1–3] because of their lesser importance with regard to applications. However, we believe that from a basic scientific point of view, investigation of germanium surfaces should not be neglected and a comparison of germanium surfaces with their silicon counterparts would substantially enhance our knowledge about surfaces of both silicon and germanium. Accordingly, we have been carrying out a series of investigations of germanium surfaces, in a bid to know their atomic structures.[9–13] As a continuation of these works, we report on the atomic structure of the Ge(15 3 23) surface, which is very stable, because we find that an annealed Ge(102) surface can completely facet to {15 3 23} along with (103) facets.

The experiment was carried out in the UHV system that has been used in recent studies of germanium surfaces.[9–13] Briefly, the system consists of a main chamber, where low-energy electron diffraction (LEED), Auger electron spectroscopy (AES), and a home-made scanning tunneling microscope (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. All images shown here were acquired with the ac mode, i.e., differential or local-contrast-enhanced mode. The tip was made out of W wire with electrochemical etching. The Ge(102) sample was cut from a single-crystal rod with a resistivity of 40–50 Ω cm. After several cycles of ''argon-ion bombardment plus subsequent annealing'' the surface was clean as verified by AES, but it was also completely faceted as verified by LEED and STM.

Although it was reported that the Ge(102) surface is 2×2 reconstructed and is stable,[14] we find that the surface can be completely faceted after being thoroughly annealed, thus not being really stable. A typical LEED pattern of the faceted Ge(102) surface is shown in Fig. 1(a). As always, to interpret the patterns of a completely faceted surface in term of the indices of the involved facets is not a trivial thing. Especially when facets being inside the unit stereographic triangle and having high indices are involved this may become very difficult.[14] By varying the primary beam energy of LEED it was not difficult to identify three (00) or specular reflection

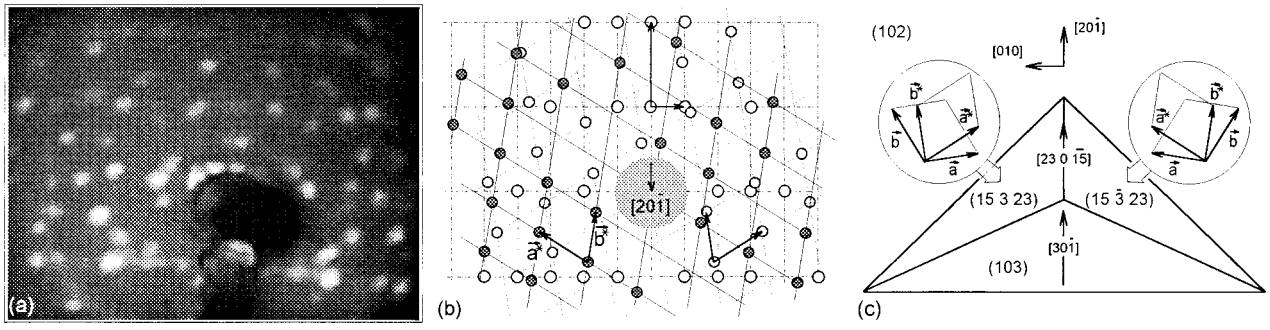

FIG. 1. (a) LEED pattern of the well-annealed and thus completely faceted Ge(102) surface. The primary beam energy is 27 eV. (b) Schematic LEED pattern (27 eV) of a Ge(102) surface consisting of (103)1×4 (open circles), (15 3 23)1×1 (heavily shaded circles), and (15 −3 23)1×1 (lightly shaded circles) facets. (c) Schematic drawing, showing the facets and their unit vectors as well as intersecting lines projected onto the (102) plane.

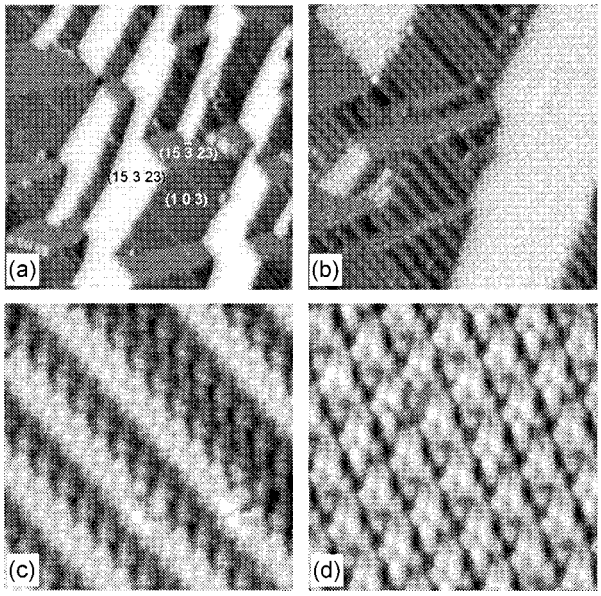

FIG. 2. STM images acquired from the completely faceted Ge(102) surface. (a) Low-resolution image (2140×2140 Å, 5.0 V, 1.0 nA), showing the general morphology of the faceted surface. (b) Medium resolution image (620×620 Å, 2.0 V, 1.0 nA). (c) High-resolution image (90×90 Å, −2.0 V, 1.0 nA) of an area of a (103)1×4 facet containing a step. (d) High-resolution image (90 ×90 Å, −1.6 V, 1.0 nA) of a (15 3 23)1×1 facet.

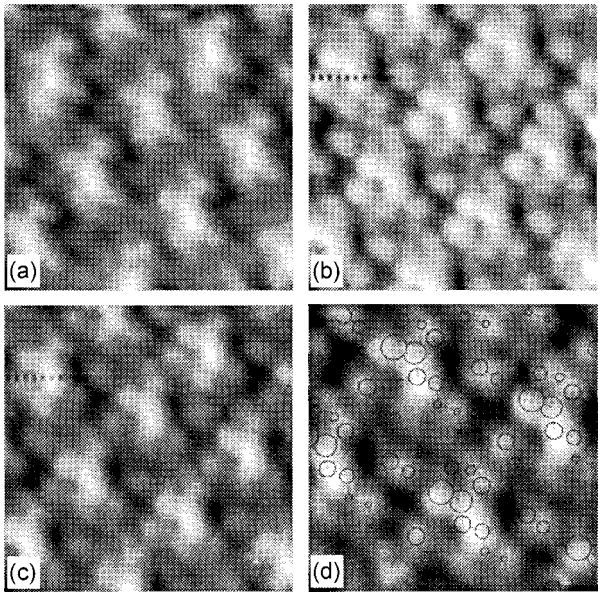

FIG. 3. A pair of high-resolution images (46×46 Å, 1.0 nA) of a (15 3 23)1×1 facet, obtained simultaneously with (a) 1.6 V (empty-state) and (b) −1.6 V (filled-state). (c) ''Atomic image''(Ref. 9) of the same area as imaged in (a) and (b), which is the average of (a) and (b). (d) Portion (32×32 Å) of (c) with the model superimposed on it.

spots in the pattern. From the measured polar and azimuthal angles of these spots, the three sets of facets were primarily identified as (103), (5 1 8), and (5 −1 8), respectively. However, this identification was not able to reproduce the LEED pattern. We then had to try other possibilities with higher indices around these planes. It turned out that the three sets of facets are (103), (15 3 23), and (15 −3 23), respectively [see Fig. 1(c)], because according to *this and only this* identification the LEED patterns [see Fig. 1(a)] can be nicely reproduced [see Fig. 1(b)].

The STM images acquired from the well-annealed Ge(102) surface further confirm that the surface completely facets to and only to (103), (15 2 23), and (15 −3 23) facets. To show this, several typical images with different magnifications are given in Fig. 2. From Fig. 2(d) we see that the unit cell of the (15 3 23)1×1 facet does have the right shape and size as well as orientation: $\mathbf{a}=14.4$ Å, $\mathbf{b}=16.6$ Å, $\alpha_{\mathbf{ab}}=112.3°$, and the angle between **b** and [23 0 −15] is 31.5° [see also fig. 1(c)] Figure 2(c) shows unambiguously that it is an image of a (103)1×4 facet.[10] Note that although the {15 3 23} facets are flat the (103) facets are not that flat. The reason for this seems to be twofold. On one hand, straight intersecting edges between (103) and {15 3 23} facets may be energetically unfavorable. On the other hand, as it has been shown very recently,[10] the Ge(103)1×4 surface consists of narrow (113)3×1 and (1 −1 3)3×1 strips in the (3 0 −1) direction and thereby may introduce many straight steps to make the (103) facets not flat only by varying the tiling sequences of the strips, and hence the stepped (103) facets would not have markedly higher specific surface free energy.

Since Ge(15 3 23) is a stable surface it would be interesting if its atomic structure can be determined. A pair of high resolution empty- and filled-state images of the surface are then given in Fig. 3. Since it has been suggested[9] and tested[10–13] that the averaged image or the so-called ''atomic'' image obtained from a pair of empty- and filled-state images resembles the surface atomic structure more than either of the original images does also given in Fig. 3 is the atomic image obtained from Figs. 3(a) and 3(b). As one can immediately see, the three images are actually quite similar to each other although there do exist some differences: some of the imaged features are more pronounced in the empty-state image while some others are just the opposite. All these images show that the surface morphology is quite rough, and this seems to be responsible for the geometry dominance and hence the similarity of these images. With these images in mind we can start to figure out the model of the surface atomic structure.

As always, to begin with we need to know the arrangement of atoms at the truncated surface, which is then schematically shown in Fig. 4(a). As one can see, this surface is already quite rough because a unit cell of it consists of four inclined short zigzag chains. As it has been shown in the case of Ge(101)$c(8\times10)$ (Ref. 11) and Ge(313)5×1,[13] long zigzag chains must be cut into short segments otherwise it would be difficult to reduce the dangling bonds in order to reduce the induced local strains. In the present case, however, the zigzag chains are already short, while it has been shown that dangling bonds of such chains may be easily reduced simply by rebonding their head atoms, putting adatoms at some places, and dimerizing some neighboring atoms.[11,13] A model has been constructed quite straightforwardly and given in Fig. 4(b). In fact, this model is not that different from the truncated surface. Comparing Figs. 4(a) and 4(b), one can easily see that in each unit cell only three atoms, i.e., atoms *A*, *B*, and *C* are added onto the truncated surface before rebonding and dimerization of some atoms.

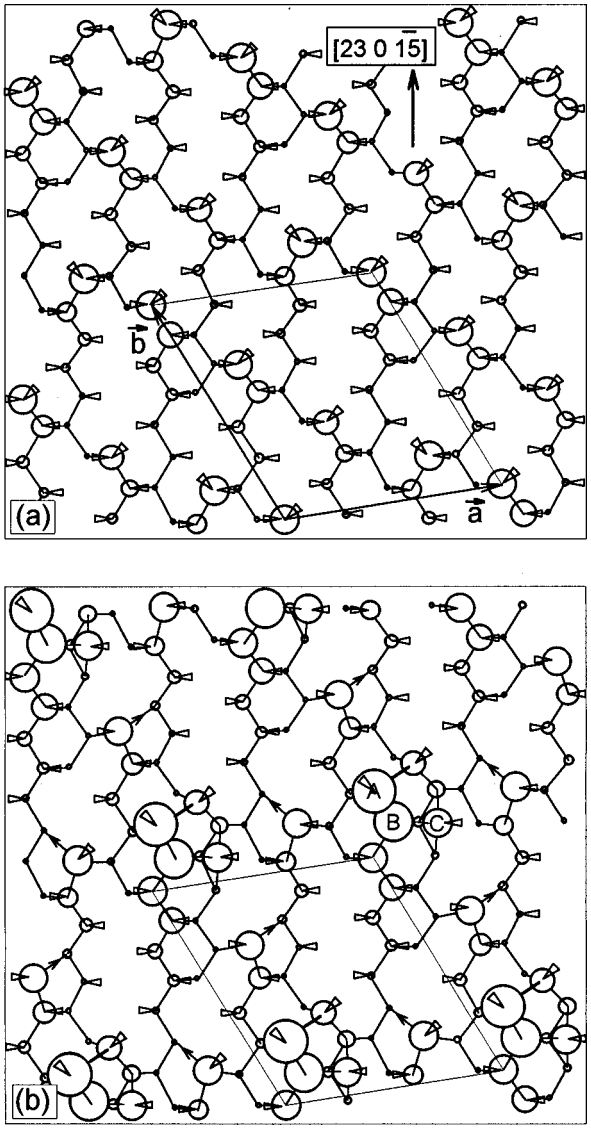

FIG. 4. (a) Schematic drawing of the truncated Ge(15 3 23) surface. The triangles represent the dangling bonds. A 1×1 unit cell is outlined with thin lines. (b) Model proposed for the real Ge(15 3 23)1×1 surface. A 1×1 unit cell is also outlined with thin lines. Atoms *A*, *B*, and *C* are those added to the truncated surface. Bonds between dimer atoms and rebonded atoms are represented by thick bars and arrows, respectively.

Atoms *A* and *B* are added to elongate the chain that consists of six atoms with one or two dangling bonds each, in order to increase the roughness of the model surface so as to match the rough morphology of the surface (see Fig. 3). Atom *C* is at the T_4 position, which is favored by silicon and germanium adatoms,[1–3] and is for dangling bond reduction.

To show that the model does account for the features seen in high-resolution STM images of the surface, it is superimposed onto the ''atomic image'' in Fig. 3(d). Obviously, the agreement between the model and the image is very nice, and thus leaves almost no room for any doubt about the correctness of the model. At this point it also becomes quite clear why the model must have atoms *A*, *B*, and *C* on it. Comparing the model with the empty- and filled-state images in Fig. 3 one finds that in both images almost the entire long chain is imaged clearly while the rest of the two- and three-

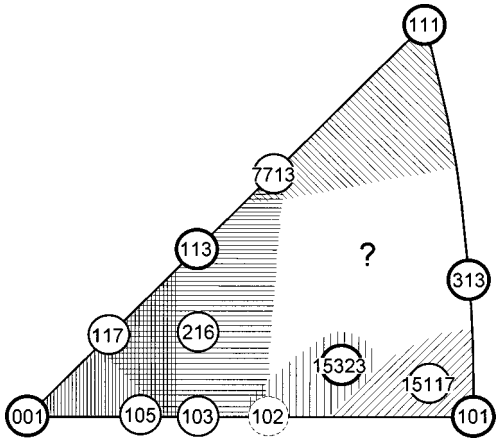

FIG. 5. Unit stereographic triangle of Ge surfaces. The major stable, minor stable, and unstable surfaces are marked with thick, thin, and dashed circles, respectively. The territories of different major stable surfaces are shaded differently.

member short chains are imaged either too bright (high) in the latter or too dark (low) in the former, indicating that the dangling bonds of these short chains are mostly filled.

The driving forces of this surface structure are also clear. In each unit cell there are only 15 dangling bonds (DB's), corresponding to a density of 0.068 DB/Å^2, which is only slightly higher than 0.063 DB/Å^2 of the Ge(001)2×1 surface as well as the Ge(313)5×1 surface.[13] As for the relief of induced local strains, without calculations it is difficult to say anything concretely. The following characteristics of the surface, however, must make relief of local strains and redistribution of dangling-bond charges not difficult: a rich variety of building entities (rebonded atoms, adatoms, dimerized atoms, and rest atoms), a rough morphology, and a low symmetry.

At this point, it seems to be worthwhile to point out that although across-zigzag-chain adatoms are often thought to be possible building entities of Si(101),[15–20] do not exist on Ge(101) (Ref. 11) nor on Ge(313).[13] Now, we have seen that they do not exist on Ge(15 3 23) either. Consequently, it seems to be reasonable to rule them out as possible building entities of germanium and very likely silicon surfaces as well.

As mentioned above, both LEED and STM show that a well-annealed Ge(102) surface facets to {15 3 23} and (103) facets. In other words, Ge(15 3 23) not only is stable but also *has its own territory* in the unit stereographic triangle, meaning unstable surfaces within which may facet to including {15 3 23} facets, and thus we say that Ge(15 3 23) is a *major* stable surface. A survey showing the territories determined so far for the currently known major stable surfaces Ge(001),[10,12] (111),[12] (113),[9,10,12] (101),[11,14] and (15 3 23) is given in Fig. 5. Ge(313) is also a major stable surface, but its territory has yet to be determined. Also shown in the figure are the minor stable surfaces, which are stable but consist of nanometer facets of one or more major stable surface.

In summary, the present LEED and STM investigations disclose that a well-annealed Ge(102) surface may completely facet to (15 3 23)1×1, (15 -3 23)1×1, and (103)1×4 facets, and hence that Ge(102) is unstable while Ge(15 3 23) is very stable. On the basis of high resolution

dual bias STM images, a detailed model has been proposed for the atomic structure of the Ge(15 3 23)1×1 surface. The surface consists of rebonded atoms, dimerized atoms, T_4 adatoms, and rest atoms at different height levels, thus being quite rough. This surface could not be further resolved into nanometer facets of other major stable surfaces, such as (001), (111), (113), (101), and (313), and thereby is also a major stable surface. Among all known stable silicon and germanium surfaces,[1–13] this one has the highest indices and is the only one located inside the unit stereographic triangle.

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