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$Si(313)12\times1$: Another metallic stable surface of silicon having a complex reconstructed layer

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By means of scanning tunneling microscopy, the Si(313)12×1 surface has been found to be, after Si(111)7×7, another stable elemental semiconductor surface with a metallic nature. On the basis of the details revealed by the high resolution STM images, an atomically rough model consisting of trenches and a variety of building entities has been proposed for the surface structure for further investigation. The common features of major stable silicon surfaces as well as the similarities and differences between these surfaces and their germanium counterparts are discussed in the context of the driving forces behind the reconstruction of elemental semiconductor surfaces.

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I. INTRODUCTION

High-index elemental semiconductor surfaces have become increasingly important in the semiconductor science and technology field because nanostructures, such as quantum dots and quantum wires, are often made up of stable high-index facets.[1] On the other hand, heterogeneous nanostructures can grow as well on high-index substrates, such as Si(313),[2] as on low-index substrates. Ever since the early investigation of Si(313) by Olshanetsky and Mashanov[3] continuous effort has been made in the last two decades in order to understand the surface.[4–12] It turns out that Si(313) is quite special because it is 22.0° from (111) and there are no other stable surfaces between it and (111).[6,7] The fact that surfaces as far as 18° away from it can still facet to (313) facets[6] indicates that it must have a very low surface-specific free energy.[13] Wei *et al.* found that a clean and well-annealed Si(313) surface is (12×1) reconstructed,[5] whereas the 13×1 reconstruction reported by Olshanetsky and Mashanov[3] was a result of Ni contamination.[5,8] The 12×1 reconstruction is almost as stable as the 7×7 reconstruction of the Si(111) surface, as it persists until 810 °C when the surface disorders via a first-order phase transition[5,11] (or becomes rough),[10] although the surface undergoes a continuous phase transition at lower temperatures before that.[11] Unfortunately, despite that several attempts were made recently,[9,12] there is still no consensus on the atomic structure of the 12×1 reconstruction. Nevertheless, on the basis of scanning tunneling microscopy (STM) observations, many have been disclosed about this surface reconstruction. (i) A 12×1 unit cell is imaged in lower magnification STM images as two identical (or very similar) mounds arranged such that the surface looks like zigzag chains of mounds separated by trenches (or ditches) in the [-1 6 -1] direction.[6,11] (ii) A mound is so stable that it does not break into atomic fragments even at domain boundaries[6] and behaves as a unit in high-temperature step fluctuation or domain boundary fluctuation,[11] and thereby was called as a ‘‘super adatom.’’[6] (iii) In high resolution STM images a super adatom consists of some four protrusions, which are at nearly the same positions in the empty- and filled-state images.[6] Of course, we have also noticed some discrepancies. For instance, the trenches are not clearly visible and the differences between the empty- and filled-state images are more significant in the STM images given by Olshanetsky *et al.*[12] On the basis of those images they proposed a detailed model for the 12×1 reconstruction but, as to be discussed later, the model does not seem to account even for the images given by themselves.[12] On the other hand, although Tanaka *et al.* have disclosed many features of the surface they did not propose any detailed model other than pointing out correctly the relative positions of the two super adatoms in the 12×1 unit cell.[6]

In the present paper we report the results of our STM investigation on the Si(313)12×1 surface. We have found that the surface is, surprisingly, metallic in nature just like the Si(111)7×7 surface and we have proposed a detailed model for the atomic structure of the surface, which has a thick and complex reconstructed layer, similar to the DAS model.

II. EXPERIMENT

The experiment was carried out in a UHV system that is equipped with STM, low-energy electron diffraction (LEED), and Auger-electron spectroscopy (AES) and was reported recently.[14,15] The STM tip was made out of a {111} W single-crystal wire with electrochemical etching and then cleaned with field emission *in situ* prior to being used. The bias voltage was applied to the sample and the tip was grounded. The constant current mode was used throughout the work and the scanning rate was set around 2500 Å/sec. The sample was cut with a precision of ±1° from a silicon single-crystal rod (p-doped, 6–8 Ω cm) and was subjected to several cycles of ‘‘argon-ion bombardment plus subsequent annealing at 1000 °C’’ followed by slow cooling (about 2 °C/sec) prior to LEED and STM observations. Several measures were carefully taken as always to assure the Si(313) surface to be metal-contamination-free, especially to be Ni-free.[14]

III. OBSERVATIONS

Our experiment shows that a clean and well-annealed Si(313) surface is indeed 12×1 reconstructed, as reported

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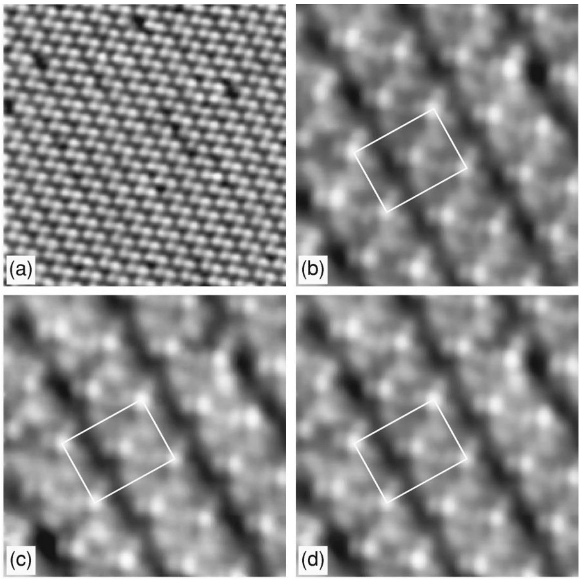

FIG. 1. STM images obtained from the clean and well-annealed Si(313) 12×1 surface. (a) Medium resolution image (290×290 Å^2, -2 V, 10 pA). (b) High resolution filled-state image (72×72 Å^2, -400 mV, 50 pA). (c) Empty-state image acquired simultaneously with (a) (72×72 Å^2, 400 mV, 50 pA). (d) Combined image (72×72 Å^2), i.e., the average of the images in (b) and (c). A 12×1 unit cell is outlined in (b)–(d), and to understand this unit cell see the caption of Fig. 2(a).

previously.[5] Typical STM images obtained from the surface are given in Fig. 1. The medium resolution STM images we obtained, such as the one given in Fig. 1(a), actually are very similar to those obtained by others, that is, the surface consists of similar mounds arranged into zigzag chains separated by trenches.[6,11] The difference is when the imaged area was reduced we were able to obtain better high resolution images [see Figs. 1(b) and 1(c)]. From these images one can clearly see that each mound actually consists of five protrusions rather than four.[6,12] The heights and shapes or sizes of these protrusions are quite different; however, in a pair of filled- and empty-state images the corresponding protrusions are essentially identical. Obviously, this is a strong indication of the dominance of the surface geometry in STM imaging. One can also clearly see that the trenches are deep compaired with the interior atomic corrugations of the mounds. Interestingly, the positions of the brightest four protrusions match very well with those marked out by Tanaka *et al.* in their Fig. 5.[6] Besides, we have noticed that a mound, though consisting of five protrusions, still does not have a mirror plane,[6] and hence the surface does not have a glide line symmetry parallel to the trenches. However, the most surprising finding is that the surface can be imaged with a dual bias of ±50 mV or even lower while the obtained filled- and empty-state images are still essentially identical. This fact indicates that the surface is *metallic* in nature. As far as we know, apart from the Si(111)7×7 surface, this is the only such surface among all elemental semiconductor surfaces studied so far. We find that varying the bias voltage from higher than ±1 V to lower than ±50 mV did not make the imaged features very different from those in Fig. 1. This means that the highest surface atoms, if not all, have metallic surface states. Later on we shall come back to this again.

IV. DISCUSSION

A. About the Olshanetsky model

Because a detailed model has been proposed for the Si(313)12×1 reconstruction by Olshanetsky *et al.*[12] we consider that model first, which then is reproduced in Fig. 2(b) to facilitate the discussion. We find that the model has some serious problems as follows. Firstly, among the three types of adatoms only the *M*-type adatoms, i.e., H_3 adatoms are possible because such adatoms exist in the Si(111)7×7 surface,[16] whereas the *K*- and *L*-types can hardly become realistic because the separation between two neighboring zigzag chains is just too large for an adatom. Specifically, even if the three back bonds of an adatom are sp^2-like or, in other words, the adatom is coplanar with the three atoms to which it is bound [see the side view of Fig. 2(b)] the three back bonds still have to be stretched by 5.9%, and this would result in very high *tensile* stresses. Moreover, the dangling bond of this adatom must be *p*-like and hence empty, and its charge has to be transferred to its neighboring atom(s). To be able to accept this charge the neighboring surface atom(s) must have an *s*-like dangling bond and accordingly must have the three back bonds to be *p*-like, and this in turn would induce *tensile* stresses again. This means that the tensile stresses around a *K*- or *L*-type adatom could not be balanced against the redistribution of the surface dangling-bond charge density, and therefore such adatoms are energetically too costly to become realistic.[17] Although such adatoms were considered as building blocks to construct models for the Si(101)''16×2'' structure,[18,19] it has been shown recently that both Ge(101)$c(8\times10)$ and Si(101) ''16×2'' consist of the unique ''pentagon twins'' and they consist of zigzag chain atoms, dimers, rebonded atoms, rest atoms, and H_3 adatoms, but not of *K*- and *L*-type adatoms.[20] The second problem with the Olshanetsky model is that it does not account for the major features in the STM images. Actually, in defense of their model they made an assumption, which is ''apparently'' the adatoms and only the adatoms of the surface can be imaged as protrusions or are visible under STM. Looking at Fig. 2(b), we have difficulties believing that the *K*- and *L*-type adatoms in the model could be more visible than the rest atoms, especially the higher ones. Besides, the model obviously does not account for the trenches either, which, as mentioned above, were reported previously and now have been confirmed by our observation as being significantly deeper compared to the interior atomic corrugations of the mounds or ''super adatoms.''[6,11] Furthermore, the model has a glide line in the [-1 6 -1] direction [see Fig. 2(b)] that the STM images do not have.[6,12] Finally, even if the model were correct, it is still hard to explain how the adatoms could form units of four, which can be stable even during domain boundary or step edge fluctuations at high temperatures, like the mounds or super adatoms in the real Si(313)12×1 surface.[6,11]

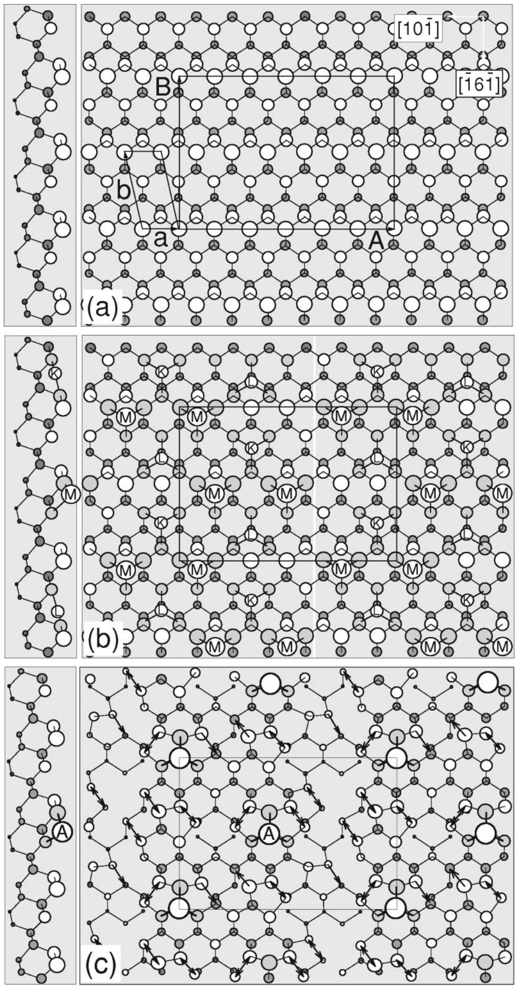

FIG. 2. (a) Side view (left) and top view (right) of the truncated Si(313) surface, with the smaller circles representing the atoms at lower positions and with the open and shaded circles representing atoms with and without a dangling bond, respectively. A 1×1 and a 12×1 unit cell along with their unit vectors **a**, **b**, **A** (23.0 Å), and **B** (17.0 Å) are shown. Note that here **A**=6**a** and **B**=**a**+2**b**, as pointed out by Olshanetsky *et al.* (Ref. 12), this unit cell is equivalent to a 12×1 unit cell but much easier to understand. (b) The model proposed by Olshanetsky *et al.* (Ref. 12). Note the three types of adatoms, namely, *K*, *L*, and *M*. The *K*- and *L*-type adatoms span across two neighboring zigzag chains of surface atoms, which are in the [1 0 -1] direction, whereas *M*-type adatoms are at typical H_3 sites. The white line represets the glide line of the model. (c) The present model of the Si(313)12×1 reconstruction. The two atoms of each dimer are connected with a double-headed arrow, while the arrow carried by rebonded atoms points to the atom they are rebonded to. Note that the lowest surface atoms are at the fifth-layer (counted from the top) zigzag chains, and chains above the fifth-layer are all cut into longer or shorter segments. Note also the trench in the [-1 6 -1] direction. The vertical distance between the highest surface atoms (adatoms) and the lowest is about 5.5 Å. In each unit cell there are eight dimers, three rebonded atoms, two adatoms, nine rest atoms, and 30 dangling bonds (0.077 dangling bonds per Å^2).

B. The present model

On the basis of the details revealed in the high resolution STM images and summarized above, a model has been proposed for the Si(313)12×1 surface and shown in Fig. 2(c). Briefly, the model was constructed by sculpting the truncated surface [see Fig. 2(a)] to match the mound-and-trench morphology of the surface and then modifying it with adatoms, dimerization, and rebonding. The entire process was under the guidance of the few general physical and chemical principles that have emerged from computational total-energy studies.[17] Before addressing the justifications of the model, we show first that it is compatible with the STM images. At this point we recall that it is the surface local density of states (LDOS), instead of the surface geometry, that directly determines the STM features, especially for semiconductor surfaces.[21] However, in the case of the present model, which has very large atomic corrugations (about 5.5 Å from the adatom level down to the bottom of trenches), it is not difficult to believe that it must be the surface geometry rather than the LDOS that dominates the STM features, especially after seeing that a pair of filled- and empty-state images acquired simultaneously are essentially identical. In spite of this, we still prefer to use the averaged image of a pair of filled- and empty-state images acquired simultaneously as the experimental image, because it has been shown that such averaged images resemble the surface geometry more than either of the original images does[22] and this idea has been successfully used afterwards.[23] To show the agreement of the model with the experimental STM images, we have to calculate the simulated image from the model and, in turn, have to know the atomic coordinates of the model. For this purpose, we use the Keating-type strain energy minimization scheme that was used with satisfaction for predicting atomic relaxations.[24] In view of that the experimental images are determined mainly by the surface geometry, as we have just discussed, to calculate the simulated image from the model we simply calculate the convolution of the surface with the STM tip, instead of the surface LDOS contours.[21] Moreover, as the bias voltage was very low and thus the STM sees only the atoms carrying a dangling bond, we need to calculate the convolution of the tip with only such atoms. The simulated image is given in Fig. 3 along with the experimental image. The overall agreement between the two images is quite good albeit not perfect, indicating that the model has, at least, caught the major features of the surface. Actually, with the long historical process of understanding the Si(111)7×7 surface in mind, for similarly complicated surfaces like the present one we do not expect to get the model completely right with one technique at once. Nevertheless, the model provides a necessary and valuable starting point for further experimental and theoretical investigations, such as LEED surface crystallography and *ab initio* molecular-dynamics calculations.

Looking at this model one may wonder why the surface prefers such a complex reconstruction. As the same question remains to be not completely answered even for the DAS model of the Si(111)7×7 surface,[16,17] we compare first the two models or the two surfaces to see if we can understand

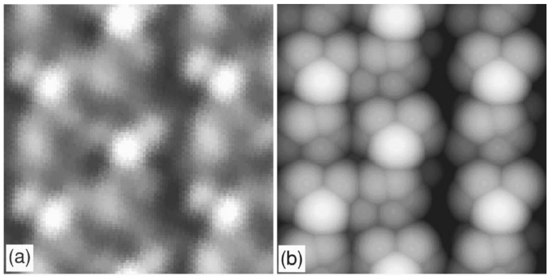

FIG. 3. (a) Real STM image ($35\times35\,\text{Å}^2$) of the Si(313)12×1 surface, which is a portion of the combined STM image in Fig. 1(d). (b) Simulated image ($35\times35\text{Å}^2$), which is simply the convolution of the tip with the relaxed model surface obtained through a Keating-type strain energy minimization scheme. The tip radius was set to 4 Å to optimize the agreement of the simulated image with the real STM image.

some. Immediately, we find that the two surfaces have many important characters in common. (i) Both are a *major stable surface*, that is, their unit cell has its own structure rather than consisting of nanofacets of any other stable surfaces.[23] (ii) Both are *atomically rough* as both have ditches and/or holes: dimer-row domain walls and corner holes in the DAS model and trenches in the present model. For both the vertical distance between the highest surface atoms (adatoms) and the lowest is about 5.5 Å.[25] (iii) Both consist of *a variety of building entities*: adatoms, rest atoms, dimers, and stacking faults in the former whereas there are dimers, rebonded atoms, adatoms, and rest atoms in the latter. (iv) Both have a very large family territory in the unit stereographic triangle,[23] meaning that surfaces far from them in the triangle may facet to facets or nanofacets of them, indicating that both have *a low specific surface free energy*.[13] (v) Both have a high *thermal stability* as the former persists until 860 °C (Ref. 26) while the latter persists until 810 °C.[5,11] (vi) On the Si(313)12×1 surface the super adatoms always appear as a unit at domain boundaries and steps even when they are fluctuating at high temperatures.[9,11] Similarly, in the case of Si(111), it has also been known that the (7×7) unit cell tends to appear as a unit along steps.[27] These common characters must be closely related to each other, instead of coming along accidentally. On the basis of these common characters of the two surfaces, we believe that a variety of neighboring building entities lying in different orientations and at different levels may conspire to satisfy simultaneously the requirements of dangling-bond reduction, local stress relief, and charge transferring among dangling bonds, and this very likely is responsible for the extremely high stability of the mounds and the very low surface-specific free energy of the surface.[17] This idea finds strong support from the fact that Si(20 4 23), which has been found very recently to be a major stable surface,[28] as well as all stable high-index surfaces of germanium are all atomically rough.[23] Actually, Phillips has pointed out in the early 1980s that for semiconductor surfaces ‘‘the weight of recent experimental evidence favors entirely new and much less obvious microfaceted models containing superlattices of islands, troughs, and steps.’’[29] Unfortunately, the history of the long process of understanding the Si(111)7×7 surface seems to have shown that people for some reason like to see surfaces be smooth and hence tend to try smooth models first.[30]

Knowing the general advantages of atomically rough surfaces does not directly answer why the Si(313) surface is reconstructed as it is. With this question in mind, we reviewed the STM images of the following major stable surfaces of silicon and germanium, that is, Ge(101),[20] (313),[31] Si(20 4 23),[28] and (101),[19] as well as the present surface Si(313), because the corresponding truncated surfaces all consist of zigzag chains of surface atoms, similar to those in Fig. 2(a). Immediately, we find an eye-catching common feature of these surfaces: they consist of trenches and mounds. Furthermore, we find that although the trenches may be either straight or not, varying from one surface to another, they always cross the zigzag chains of surface atoms or cut them into short segments. This means, we believe, that except for cutting the zigzag chains into short segments and thereby making the surface morphology trench-and-mound or atomically rough there are no easy ways, such as adding adatoms as Olshanetsky did to their model,[12] to eliminate such chains.

C. Comparison of Si surfaces with their Ge counterparts

Now, we address a different but closely related issue, that is, the systematic differences between the structures of silicon surfaces and their germanium counterparts. A comparison of the present Si(313)12×1 model with the Ge(313)5×1 model, which does not have trenches and has its adatoms at a lower level,[31] finds that the reconstruction in the silicon surface extends to deeper layers. A similar difference exists in the case of Si(101)‘‘16×2’’ (Ref. 32) versus Ge(101)$c(8\times10)$ (Ref. 20) and Si(113)3×2 versus Ge(113)3×2.[33,22] If the well-known difference between Si(111)7×7 and Ge(111)$c(2\times8)$ is also counted,[17,30] then we have encountered four times the same difference: the reconstruction is thicker or more corrugated in the silicon surface than in its germanium counterpart. Because the difference is now a systematic one, we suggest that it is simply a result of the general difference between germanium and silicon, that is, germanium is softer than silicon.[34]

D. Metallic nature of the surface

Semiconductor surfaces with a metallic nature, such as Si(111)7×7, are so rare that their existence has been thought to conflict the reconstruction principles or ‘‘there is obviously some ‘‘principle’’ that we have overlooked that allows the stabilization of metallic surfaces in specific instances.’’[17] Now we have seen that Si(313)12×1 is another metallic surface that also has a very low specific-surface free energy. Consequently, we should see this only as a warning that *the importance for surfaces of semiconductors to have a semiconducting nature might have been overestimated*,[17,35] rather than something abnormal, because only in systems with extended electronic wave functions do metallic ground states not occur in one dimension (1D) and in certain circumstances also do not occur in two dimensions (2D).[36] In other words, pairing up all of the electrons and creating an insulating or semiconducting surface may often lower the surface energy but it is *not a necessary condition*.

As for which surface atoms may have metallic surface states, as mentioned above, if not all of them, at least the highest ones seem to have. Among them are the adatoms, dimers, rebonded atoms, and rest atoms. As it has been known that in the Si(111)7×7 surface the adatoms do have metallic surface states or tails,[37] one should not be surprised to see the adatoms in the present surface having such states. Concerning the dimers, note that the reason the Si(001) surface could not have metallic surface states is not because it consists of dimers but because its dimers form 1D rows.[36] In the Si(313) surface, however, the dimers do not form 1D rows [see Fig. 2(c)] and therefore are allowed to have metallic surface states.

V. SUMMARY

In summary, our STM observations confirm that a clean and well-annealed Si(313) surface is indeed 12×1 reconstructed and that the surface consists of zigzag chains of mounds separated by deep trenches. We find that the mounds actually consist of five protrusions and that in a pair of filled- and empty-state images the corresponding protrusions are essentially identical, indicating the dominace of geometry in imaging. We also find that the surface can be imaged with a bias voltage as low as ±50 mV and that metallic surface states exist on almost all surface atoms.

On the basis of high-resolution STM images of the Si(313)12×1 surface we have proposed a model for its atomic structure for further investigation. The model consists of adatoms, dimers, rebonded atoms, and rest atoms, and these building entities are stacked into mounds and trenches so that the surface is atomically rough, similar to the DAS model of the Si(111)7×7 surface.

We suggest that a variety of neighboring building entities lying in different orientations and at different levels may conspire to satisfy simultaneously the requirements of dangling-bond reduction, local stress relief, and charge transferring among dangling bonds, and this very likely is responsible for the high stability of the mound they form and in turn is responsible for the low surface-specific free energy of Si(313)12×1, as well as some other major stable surfaces of silicon and germanium, such as Si(20 4 23), (101), Ge(313), and (101). Moreover, we also suggest that the reason the reconstructed layers of Si(111), (313), and (101) is thicker than that of their germanium counterpart very likely is that silicon is harder than germanium.

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