Comment on "Atomic structure model of the reconstructed Si(557) surface with a triple step structure: Adatom-parallel dimer model"

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Recently, [Oh *et al.*Phys. Rev. B **77**, 155430 (2008)] reported on an atomic model for the so-called Si(557)-reconstructed surface with regular triple steps. The atomic structure model proposed was developed on the basis of high-resolution scanning tunneling microscopy (STM) images and first-principles calculations performed to match such STM images. Here we argue that the STM image presented is affected by an artifact, most likely related to a multiple tip image effect. Among other issues with the image presented, the corner holes for (7×7) reconstruction on Si(111) terraces are not visible, since a doubled image superimposed smears out such characteristic depression. The (×7) periodicity deduced for the edge facets, in contrast with previously reported STM images and electron-diffraction studies which unambiguously indicate a (×2) periodicity, arises from the same artifact. Finally, we remark that the (557) surface orientation and (112) orientation of triple steps assumed for first-principles calculations disregard the latest experimental data available, which suggests this surface has a (7 7 10) orientation and the steps in triple step do not form a well-defined plane [Surf. Sci. **600**, 4878 (2006)].

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In the recent paper of Oh *et al.*,[1] the atomic model of the silicon reconstructed surface with regular triple steps is proposed on the basis of high-resolution scanning tunneling microscopy (STM) images and on first-principles calculations. This silicon surface was initially discovered by Kirakosian *et al.*[2] and due to its highly regular structure attracted interest as substrate for formation of nanowires. In the work of Kirakosian *et al.*,[2] it was suggested that the surface with regular triple steps has a (557) orientation consisting of regularly spaced (111)-(7×7) terraces with the triple steps, having (112) orientation. The theoretically calculated period for triple steps on a surface with (557) orientation is 5.7 nm. Since then, there has been some controversy regarding the orientation of triple steps. As a way of example, in Ref. 3, it was suggested from spot profile analyzing low-energy electron-diffraction (SPA-LEED) data and its simulation in kinematic approximation that triple steps have rather (113) orientation and not (112) as initially suggested. It is interesting to note that in the fundamental paper by Baski *et al.*,[4] the (112) surface—unlike the (113) one—is not listed among the atomically flat surfaces implying that this surface is faceted.

The departure point for the study by Oh *et al.* of this silicon surface reconstruction is a high-resolution scanning tunneling microscopy image. In Fig. 1(a), we show the STM image of the surface with regular triple steps reported in Ref. 1. Clearly there are some problems in this image: first from the step edge everything is smeared to the upper right, second, and, perhaps the most obvious issue in Fig. 1(a), is the absence of the corner holes of the (7×7) surface reconstruction. Figure 1(b) shows an enlarged surface area marked by a white square in Fig. 1(a) with the dimer-adatom-stacking faults (DAS) model of (7×7) surface reconstruction by Takayanagi *et al.*[5] overlaid on the STM image. It is visible that instead of dark depressions in corner holes, there are bright spots. Another problem in Fig. 1(a) is the periodicity of (×7) along triple steps. As recognized in Ref. 1, previous LEED data show unambiguously that the periodicity along triple steps is (×2).[3,6,7] In Figs. 2(a) and 2(b) we show high-resolution STM images obtained in the same surface. These images correctly exhibit the corner holes of the (7×7) surface reconstruction and the (×2) periodicity along triple steps.

The most plausible explanation for artifacts observed in Fig. 1 is that the STM image presented was obtained with a multiple tip. Tip-related artifacts and their consequences on the resulting scanning probe microscopy images are well documented (see, for example, Ref. 8). Basically, a blunted tip can produce image(s) of surface features considerably bigger than they are in reality and eventually may smear them out completely. The multiple tip is the cause of replica images of the real feature on the surface. Note that two superimposed STM images of the surface smear out the depressions in corner holes. The periodicity of (×7) along triple steps observed in Fig. 1 is also most likely resulting from doubled image of the edge of Si(111)-(7×7) terrace. Another evidence of multiple tip used are replicated images of surface defects at the edges of (111) terraces observed in STM image, as highlighted by the arrows in Fig. 1(a). One should not get confused by the fact that some defects, such as vacancies in the 7×7 structure, away from step edges have no replica images. In fact this often happens when working with stepped/vicinal surfaces. This occurrence depends on the specific details regarding the real shape of STM tip. A given double tip can work perfectly with flat surfaces, causing the impression that a single tip is being used, while the double-tip effect can manifest itself clearly with stepped surfaces. It is easy to imagine the shape of the tip which could behave this way (Fig. 3). The STM tip would be split into two: a longer component always closer to a flat surface and a shorter tip component. When scanning flat (or slowly varying slopes) surfaces, only the lower longer tip forms the image and therefore no replica images appear. But when it

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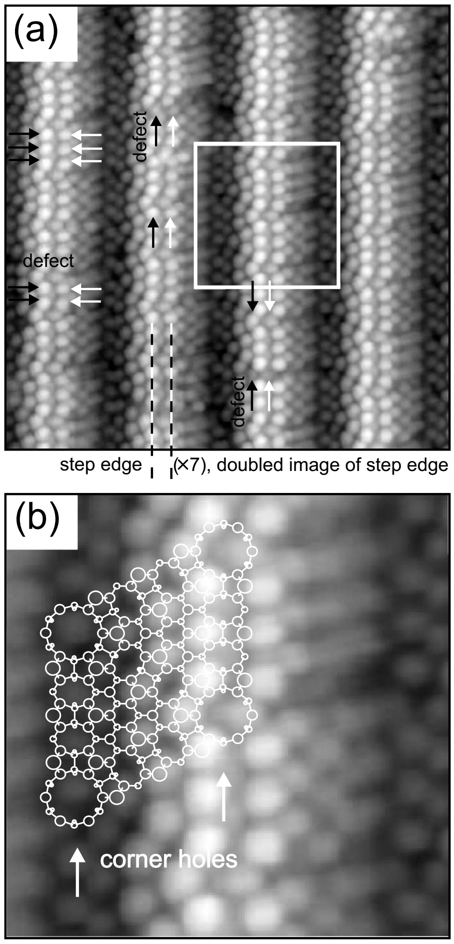

FIG. 1. (a) STM image of silicon surface with regular triple steps taken from Ref. 1. Triple steps show (×7) periodicity likely due to doubled image of step edge. Black arrows highlight real features on the surface; white arrows indicate replicated images. (b) Enlarged surface area marked by a white square in (a). The (7×7) DAS model of Takayanagi *et al.* (Ref. 5) is superimposed on the STM image. Corner holes of the (7×7) reconstruction on (111) terraces are invisible.

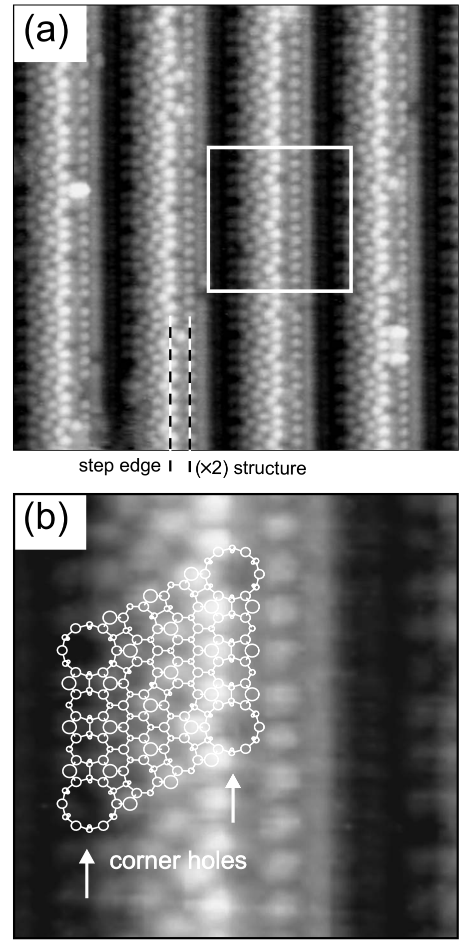

FIG. 2. (a) STM image of silicon surface with regular triple steps taken with sharp single tip. Triple steps show (×2) periodicity. (b) Enlarged surface area marked by a white square in (a). The (7×7) DAS model of Takayanagi *et al.* (Ref. 5) is also superimposed on STM image. Corner holes of the (7×7) reconstruction on (111) terraces are clearly visible.

comes to rapidly varying height relief, such as it is the case for step edges, both tips contribute to the image producing real and replica images.

Note that the replica images will be aligned horizontally with real images of artifacts only if two STM tips (of a double tip) are aligned along the scanning direction, which can only happen by fortunate coincidence. If they are not aligned, the replica image can be shifted in any arbitrary direction. The only proof of double tip would be the repetition of topographic features. If some patterns show up in the same shape and orientation then they are probably due to a bad tip. Changing the scan direction electronically will have no effect on the affected image—to verify that these features are due to the tip, one must physically rotate the sample relative to the tip and see if the artifacts have also rotated.

Finally, in Fig. 4, we present our own STM image of the silicon surface with regular triple steps taken with multiple tip. This image demonstrates basically the same features as in Fig. 1, i.e., false atomic resolution on the triple step showing (×7) periodicity and absence of corner holes of the (7×7) reconstruction. It is particularly unfortunate that this artifact was unnoticed, since two papers cited in the work of Oh *et al.* reported high-resolution STM images with the expected (×2) periodicity along the triple steps.[9]

Doubling of the STM image mislead the authors to the suggestion of structure similarity between (111)-(7×7) reconstruction and the structure of triple step. However, due to the issues discussed above, we argue that the bright spots in

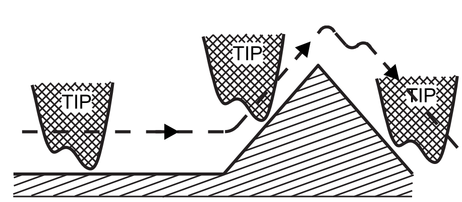

FIG. 3. Schematic view of double-tip scanning of a rough surface. The dashed line shows topography obtained during the scan. Note that the apex of triangular island in the image will be split into two due to the double tip.

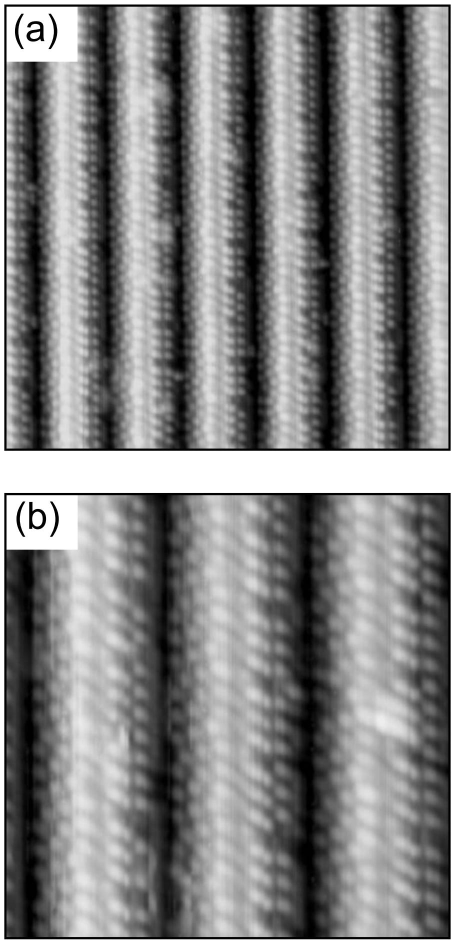

FIG. 4. (a) Large and (b) small scale STM images of silicon surface with regular triple steps taken with multiple tip in our study.

STM images in Ref. 1 do not closely represent the positions of Si atoms and cannot serve as a good starting basis for building the reconstructed surface model.

In order to build the atomic model of the surface with regular triple steps, the authors of Ref. 1 assumed, following the publication of Kirakosian *et al.*,[2] that the surface has a (557) orientation and the triple step forms a plane with (112) orientation. This assumption contradicts the latest experimental data available which suggests this surface has, in fact, a (7 7 10) orientation and the steps in triple step do not form a well-defined plane.[6] In Ref. 6 the atomic model of the surface with regular triple steps has been proposed by Teys *et al.* for the first time. This model was developed on the basis of high-resolution STM images and high-resolution LEED. In that work, a periodicity of (×2) is found along step edges, which explains streaks of 1/2 order in LEED.[3,7] It was also found that the orientation of the surface with regular triple steps is (7 7 10), which is only 0.5° off from (557) plane. Here it should be stressed that this latter result was obtained both by STM and LEED independently in separate vacuum chambers. We used samples provided by Himpsel's group,[2] who originally discovered this surface, and also homegrown samples. The preparation procedure was standard for this surface and is described in Ref. 2. High-resolution LEED systems, such as SPA-LEED, can routinely determine surface orientation with accuracy at least 0.1° or better; thus the surface orientation determined by this technique is very reliable. In STM, it is much harder to obtain similar level of precision because STM images always suffer from some level of sample thermal drift and piezocreep, making precise determination of lengths and angles more difficult. Following a procedure similar to that described by Kirakosian *et al.*[2] to reduce the influence of sample thermal drift or piezocreep and taking into account the projection of (7×7) unit cell on a sample surface plane by analyzing systematically several STM images of identical surfaces, we obtained a period of 5.17 ± 0.21 nm for the triple steps. The value obtained experimentally is more compatible with a period of 5.3 nm calculated for the triple steps on a (7 7 10) surface than the period of 5.7 nm deduced for the (557) surface.

Besides the assumption of a (557) orientation and the use of (112) plane for triple steps, which disregard the latest experimental findings, the overall modeling approach chosen by Oh *et al.*[1] is also questionable. The authors of Ref. 1 tried to model the atomic structure of triple steps, treating the (112) facet as infinite. It should be noted, however, that this plane as a part of the triple step is under mechanical stress.[10] The surface under stress can exhibit completely different reconstruction compared to the fully relaxed case.[11] One example are strained Ge films[12] or islands[9,13] grown on Si(111) surface, which show (7×7) reconstruction, not observable on Ge(111) samples. Another case is the surface with triple steps itself: while on flat Si(111) surfaces the (5×5) reconstruction is very rare and regarded as metastable, on surface with triple steps the areas with (5×5) reconstruction are relatively easy to find.[3,6] The reason for this is that under mechanical stress, the (5×5) reconstruction becomes more favorable. Therefore, due to the mutual influence between terrace and step edge, the correct way to address this problem is to account for the structural relaxation as a whole unit. Thus the role of the Si(111)-(7×7) terrace should not be neglected in the calculations.

In conclusion, we argue that the model of the surface with regular triple steps proposed by Oh *et al.*[1] is based on STM images which are affected by multiple tip artifacts. The results obtained regarding the periodicity along triple steps are also in disagreement with the latest experimental data available. Unfortunately, neither STM data presented nor *ab initio* simulations performed allow to clarify which surface orientation [(557) or (7 7 10)] is valid for such interesting Si surface reconstruction.

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