

**Regular step distribution of the bare Si(553) surface**

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Vicinal Si(111) surfaces are known to undergo faceting when the temperature is lowered below the  $(1 \times 1)$  to  $(7 \times 7)$  phase transition temperature. Depending on the cutoff angle value and direction with respect to the crystallographic axis, various facets, together with low Miller index terraces, are formed. Here, we report the formation of regularly distributed steps over macroscopic sample regions of the bare Si(553) surface. The surface morphology is studied with scanning tunneling microscopy and reflection high energy electron diffraction techniques. The (111) terraces of 2.88 nm in width, which are separated by double atomic height steps, reveal an unusual reconstruction. However, the electronic structure determined with angle resolved photoemission spectroscopy shows bands very similar to those observed for the Si(111)- $(7 \times 7)$  surface.

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**I. INTRODUCTION**

Vicinal silicon surfaces have continued to be increasingly interesting since the 1990's [1,2]. Among various scientific problems, such as interactions of steps or faceting, the preparation of surfaces with a uniform distribution of steps over macroscopic sample regions was one of the main goals of the investigations. Such anisotropic templates could be used for the growth of one-dimensional structures and their studies using laterally averaging techniques.

There have been many attempts to obtain a regular step distribution on vicinal surfaces, most of them performed with the Si(557) surface [3–10]. The results always show a surface which consists of (111) terraces and triple steps. However, the morphology of the steps is still under debate, with reports of the formation of (113) [4], (112) [6,10], or (223) [8] facets. There are also data suggesting that the entire surface prefers a  $(7 \times 7)$  orientation with triple height steps which do not form a well-defined plane [5,9]. In any case, the surface does not form a homogeneous system.

It must be mentioned that vicinal silicon surfaces already have been ordered either by sample annealing or by deposition of additional atoms. In 1996 it was shown that Si(114) forms a uniform reconstruction over large sample regions after a proper annealing treatment [11]. However, this surface should be categorized as a low Miller index plane with a rather flat, atomically corrugated surface. Then in 1997 it was reported that a perfect step order on high Miller index planes can be obtained by deposition of a submonolayer amount of Au on a bare vicinal surface and subsequent annealing at about 900 K [12]. Since then it has been shown that a number of silicon crystallographic planes undertake the transition to a phase with regularly distributed steps over macroscopic size areas induced by the presence of Au atoms. Among the most often investigated are Si(557)-Au, Si(335)-Au, and Si(553)-Au, to name a few [12–25].

Recently, it has also been shown that a regular distribution of steps can be obtained by adsorption of about 1.3 monolayers (ML) Pb with subsequent annealing at much lower temperatures of about 500 K [26,27]. Almost perfect order has also

been reported for a similar system of 1.3 ML Pb/Si(557) [28]. However, in that case, the Si(557) surface is split into two phases: (223) facets and wide (111) terraces. Although the wide (111) terraces cover only a small fraction of the surface, it means that the whole surface does not have a uniform morphology.

In the present paper we report a regular step distribution over a macroscopic area of a bare silicon high Miller index plane which forms a homogeneous phase without additional facets. Annealing of the Si(553) surface, without the deposition of atoms of other elements, within a narrow temperature range around 450 °C results in the formation of regularly distributed double atomic height steps running along the  $[1\bar{1}0]$  direction. The (111) terraces of equal width undergo an unusual surface reconstruction. The scanning tunneling microscopy (STM) and reflection high energy electron diffraction (RHEED) experiments reveal an  $8a_{[1\bar{1}0]}$  periodicity along the step edges and no periodic features across the terrace. The electronic structure studied with angle resolved photoemission spectroscopy (ARPES) reveals bands similar to those observed for the  $(7 \times 7)$  superstructure.

**II. EXPERIMENT**

Experiments have been performed in two separate ultrahigh vacuum (UHV) chambers consisting of variable temperature VT STM and ARPES systems with a base pressure in the middle of the  $10^{-11}$  mbar range. The photoemission experiments have been made with the He I line (21.2 eV). The energy and angular resolution of the hemispherical electron energy analyzer (Phoibos 150) were set to 50 meV and  $0.5^\circ$ , respectively. Both UHV systems are equipped with the RHEED apparatus. The STM measurements have been performed at room temperature and the ARPES and RHEED experiments at  $-150^\circ\text{C}$ . The same ARPES and RHEED results, except for the thermal broadening, have been obtained at room temperature.

The Si(553) sample with an orientation accuracy of better than  $\pm 0.05^\circ$  was cut from a B-doped ( $\sim 0.14 \Omega \text{ cm}$  at room temperature) silicon wafer. Before each experiment the sample was cleaned by several flashes up to 1500 K under UHV conditions.

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The reported results have been obtained after sample annealing for several hours at temperatures in the range of 450–600 °C by direct current passing along the step edges. The sample temperature was controlled by a K-type thermocouple attached to the sample holder. Prior to the measurements, the sample temperature was scaled in a separate experiment in which the other K-type thermocouple was attached to the Si surface. Finally, the Si sample temperature was determined with  $\pm 10^\circ\text{C}$  accuracy.

### III. RESULTS

#### A. Structural properties

Figure 1(a) shows the RHEED pattern (the 0th Laue zone) of the Si(553) surface annealed at 450 °C. The regularly distributed diffraction streaks are clearly elongated in the direction perpendicular to the macroscopic surface of the Si sample (horizontal edge of the frame), indicating a periodic distribution of steps. The distance of  $0.21 \pm 0.01 \text{ \AA}^{-1}$  between the streaks, obtained from the intensity profile [lower black line in Fig. 1(b)], corresponds to a period of  $29.9 \pm 0.4 \text{ \AA}$ . It means that the step separation on the bare Si(553) is twice as large as on the Si(553)-Au surface [18,29] [blue upper line in Fig. 1(b)]. This in turn means that the steps have to be two times higher in order to preserve the macroscopic tilt with respect to the (111) plane.

The Laue subzones visible in the RHEED pattern [Fig. 1(c)] indicate  $8a_{[1\bar{1}0]}$  periodicity along the  $[1\bar{1}0]$  direction ( $a_{[1\bar{1}0]} = 3.84 \text{ \AA}$ ). Figure 1(d) shows the corresponding intensity profile taken along the  $[1\bar{1}0]$  direction. The ticks indicate the calculated positions of the intensity maxima for  $8a_{[1\bar{1}0]}$  periodicity.

STM images corroborate the RHEED results. A long range order of Si(553) after annealing at 450 °C is shown in Fig. 2(a). The distance between periodic rows equals  $29.4 \pm 0.5 \text{ \AA}$  [Fig. 2(b)]. The large ordered regions are separated by steps with heights of  $0.67 \pm 0.15$  and  $1.35 \pm 0.15 \text{ \AA}$ . These distances correspond to the single and double steps along the Si [553] direction, respectively ( $a_{[553]} = 0.71 \text{ \AA}$ ).

The STM images reveal periodic features along the  $[1\bar{1}0]$  direction [Fig. 2(c)]. The distance of  $30.4 \pm 1.0 \text{ \AA}$  between

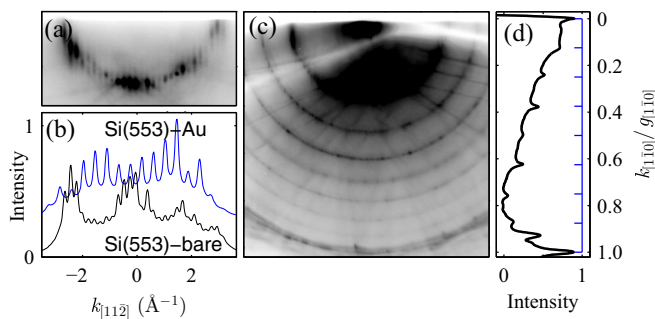


FIG. 1. (Color online) RHEED patterns of the Si(553) sample annealed at 450 °C with an electron beam along  $[1\bar{1}0]$  (a) and (c). (a) The 0th Laue zone. (b) Intensity profile (black lower line) taken from the pattern of (a) and from Si(553)-Au (blue upper line) for comparison. (d) Intensity profile taken from the diffraction pattern shown in (c).  $g_{[1\bar{1}0]} = \frac{2\pi}{3.84} \text{ \AA}^{-1}$ .

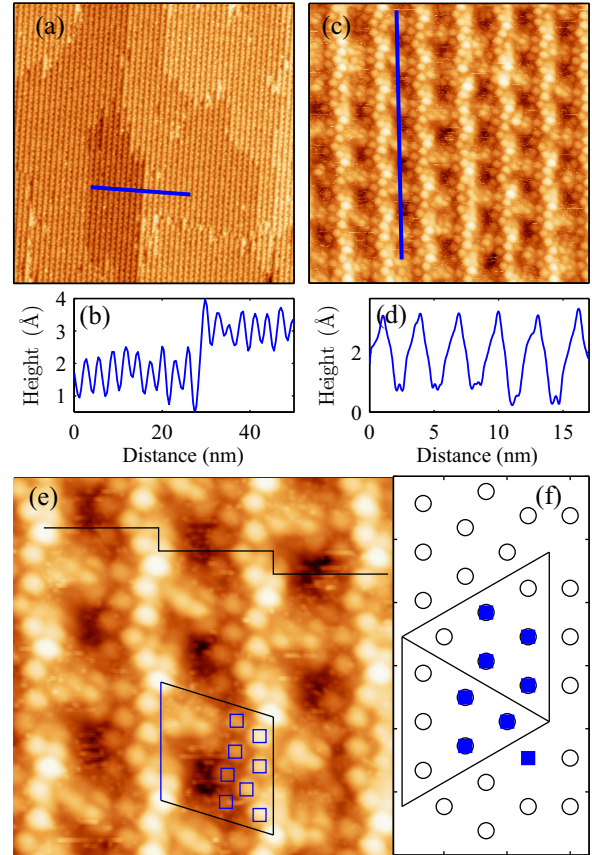


FIG. 2. (Color online) (a)  $150 \text{ nm} \times 150 \text{ nm}$  ( $U = -1.5 \text{ V}$ ,  $I = 0.20 \text{ nA}$ ) and (c)  $20 \text{ nm} \times 20 \text{ nm}$  ( $U = 1.0 \text{ V}$ ,  $I = 0.15 \text{ nA}$ ) STM images of Si(553) annealed at 450 °C. (b) and (d) profiles taken along the lines shown in (a) and (c), respectively. (e)  $10 \text{ nm} \times 10 \text{ nm}$  ( $U = 0.5 \text{ V}$ ) STM image with a marked step direction and outlined surface unit cell. (f) Sketch of the  $(7 \times 7)$  reconstruction with circles indicating adatoms. Blue squares in (e) indicate adatoms with similar locations as in (f).

the features [Fig. 2(d)] indicates  $8a_{[1\bar{1}0]}$  periodicity along the step edges ( $30.4 \text{ \AA}/a_{[1\bar{1}0]} = 7.92$ ) and is consistent with the RHEED results.

Figure 2(e) presents the high resolution STM image of the unoccupied states with the outlined unit cell of  $8a_{[1\bar{1}0]} \times 8\frac{2}{3}a_{[11\bar{2}]}$ . Although the perfect terrace width distribution is obvious, some differences between adatom locations on terraces can be found. The outlined cell is an often seen unit, however, there are also other cells (with the same length along  $[1\bar{1}0]$ ) which show slightly different positions of the adatoms. It suggests that the observed reconstruction is not energetically very stable. At first glance the location of the Si adatoms within the unit cell is quite different from the known  $(7 \times 7)$  reconstruction. There are, however, similarities to the dimer adatom stacking (DAS) model of  $(7 \times 7)$  [30]. Several Si adatoms, marked by the squares, are located at similar relative positions as in the  $(7 \times 7)$  unit cell [Fig. 2(f)]. Moreover, the adatoms are separated from each other by two lattice constants in the  $\langle 1\bar{1}0 \rangle$  ( $7.47 \pm 0.5 \text{ \AA}$ ) and  $\langle 11\bar{2} \rangle$  ( $6.43 \pm 0.5 \text{ \AA}$ ) directions.

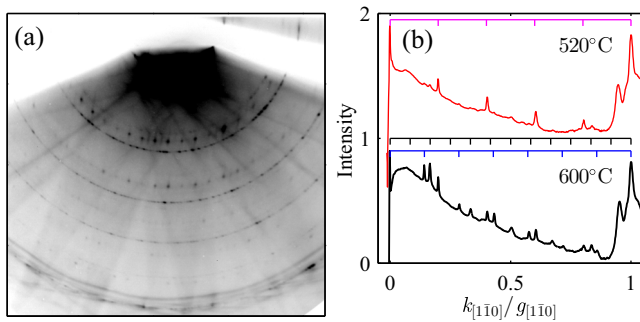


FIG. 3. (Color online) (a) RHEED pattern of Si(553) annealed at 600 °C with the electron beam along  $[1\bar{1}0]$ . (b) RHEED intensity profiles taken along the  $[1\bar{1}0]$  direction for Si(553) annealed at 520 and 600 °C.  $g_{[1\bar{1}0]} = \frac{2\pi}{3.84} \text{ \AA}^{-1}$ .

Annealing the sample at higher temperatures, 520 and 600 °C, causes surface faceting. Figure 3(a) shows the RHEED pattern of Si(553) annealed at 600 °C. Two sets of different streaks can be distinguished. The streaks of the one group are perpendicular to the (111) plane. They reveal periods of  $5a_{[1\bar{1}0]}$  and  $7a_{[1\bar{1}0]}$  and indicate the existence of  $(5 \times 5)$  and  $(7 \times 7)$  reconstructions on the wide (111) terraces [Fig. 3(b)]. The streaks from the other group are tilted by  $23.5^\circ \pm 2.0^\circ$  with respect to the first ones. It suggests that they are perpendicular to the (331) plane. The (331) facet is tilted by  $22^\circ$  with respect to the (111) plane and has been reported to be a stable facet of Si vicinal surfaces cut toward the  $[11\bar{2}]$  direction [31]. Moreover, the distance between the streaks perpendicular to the (331) plane equals  $0.78 \pm 0.01 \text{ \AA}^{-1}$  and corresponds to  $8.1 \pm 0.4 \text{ \AA}$ , which is very close to the distance between the steps of the ideal (331) plane ( $7.76 \text{ \AA}$ ).

Figure 3(b) shows the intensity profiles taken from the RHEED patterns along the  $[1\bar{1}0]$  direction for samples annealed at 520 and 600 °C. In both cases the  $5a_{[1\bar{1}0]}$  and  $7a_{[1\bar{1}0]}$  periodicity appears in the RHEED patterns. It is interesting to note that after annealing at 520 °C the  $5a_{[1\bar{1}0]}$  period is much stronger than the  $7a_{[1\bar{1}0]}$  one. Annealing at 600 °C results in the appearance of intense diffraction streaks due to the  $7a_{[1\bar{1}0]}$  periodicity. The  $5a_{[1\bar{1}0]}$  period is still present and, in addition, a different period of  $12a_{[1\bar{1}0]}$  appears. It can be attributed to the  $(12 \times 1)$  reconstruction of the (331) facets [31].

### B. Electronic structure

Figure 4 presents photoemission intensity maps of the Si(553) surface along the  $[11\bar{2}]$  [Fig. 4(a)] and  $[1\bar{1}0]$  [Fig. 4(c)] directions, respectively, and of the Si(553)-Au for comparison [Fig. 4(b)]. The Si bulk band with its apex located at about 1.5 eV below the Fermi level is visible in Figs. 4(a) and 4(b). The band is repeated with a period of  $0.21 \text{ \AA}^{-1}$  [Fig. 4(a)] compared to  $0.42 \text{ \AA}^{-1}$  for Si(553)-Au [Fig. 4(b)]. It is due to the diffraction of photoelectrons on a surface with regularly distributed structures, as previously observed [32]. Beside these bands, there are three almost nondispersive bands. They are also visible in the perpendicular direction, along the step edges, over the whole Brillouin zone [Fig. 4(c)]. These bands resemble weakly dispersive bands associated with the  $(7 \times 7)$  reconstruction of the Si(111) surface which come from the

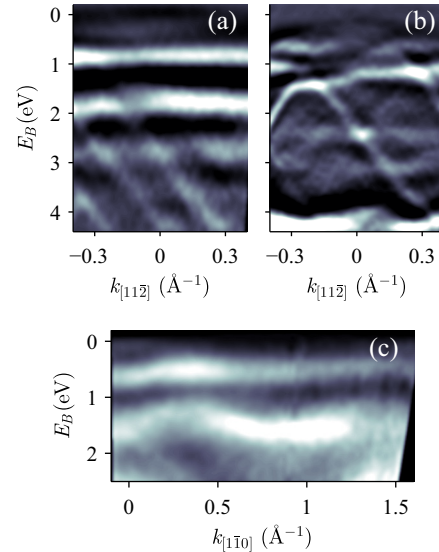


FIG. 4. (Color online) Photoemission intensity maps (second derivative) of Si(553) annealed at (a), (c) 450 °C and (b) Si(553)-Au. Zero binding energy denotes the Fermi level position.

dangling bonds of adatoms (at the Fermi level) and of the rest atoms (located at about 0.8 eV) and back bonds (at about 1.8 eV) [33–35].

## IV. DISCUSSION

There are two important findings reported in the present paper: first, the formation of regularly distributed steps over macroscopic regions of a high Miller index plane of silicon without deposition of additional atoms, and, second, the formation of a different superstructure on the (111) terraces.

The stability of the Si(553) surface has been suggested by Men *et al.* [36]. The authors studied vicinal Si(111) surfaces with various miscut angles. They noticed that after annealing at 950 °C all surfaces developed facets which consist of (111) terraces 28 Å in width separated by 6.3 Å high steps ( $2a_{[111]} = 6.27 \text{ \AA}$ , where  $a_{[111]} = 3.135 \text{ \AA}$  is the distance between two double layers of Si along  $[111]$ ). The obtained terrace width, together with the double step height, suggest a (553) plane. It is important to note that the authors of Ref. [36] obtained the same facet [the same tilt angle with respect to the (111) plane] for a number of vicinal surfaces with miscut angles ranging from  $0.3^\circ$  to  $6^\circ$ .

Similarly, stable Si(553) facets have been reported by Bruns *et al.* [37]. The authors studied faceting of the highly B-doped Si(111) surface tilted by  $0.35^\circ$  off the (111) plane in the  $[11\bar{2}]$  direction. They found that the only stable facet consists of bi-atomic height steps and (111) terraces of 2.86 nm. These values fit very well to the Si(553) plane. The authors concluded that the facet is apparently stabilized by the  $(\sqrt{3} \times \sqrt{3})R30^\circ$  reconstruction induced by the segregation of B atoms at the surface.

On the other hand, studies of bare Si(553) have shown that the surface undergoes faceting and does not form uniformly distributed steps [38]. It consists of the (331) facets and wide (111) terraces with  $(7 \times 7)$  and  $(5 \times 5)$  reconstructions. However, the authors of Ref. [38] annealed the sample at



800 °C, which is much higher than the temperature used in our experiments (450 °C).

Our results obtained at higher annealing temperatures (above 500 °C) remain in very good agreement with the reported data. There are (331) facets with  $(12 \times 1)$  and wide (111) terraces with  $(7 \times 7)$  and  $(5 \times 5)$  reconstructions. The observed differences in the surface morphology are obtained after annealing of Si(553) at 450 °C. Moreover, our sample is not highly B doped ( $0.14 \Omega \text{ cm}$  compared to  $0.001 \Omega \text{ cm}$  as in Ref. [37]) and we observe neither a  $(\sqrt{3} \times \sqrt{3})R30^\circ$  reconstruction in RHEED nor a boron signal in Auger electron spectroscopy. It is worth noticing that in our experiments, already after a high temperature flash, the RHEED patterns show short range order appearing as a precursor of the final arrangement of the surface. We conclude that in this case long range order is not associated with massive mass transport and can be reached at a much lower annealing temperature (450 °C).

It is interesting that the terrace width and step height are twice as large as in the case of the (553) surface with Au- or Pb-induced order [18,26,29]. The Au adsorption causes the appearance of a very characteristic row of honeycomb structures at the step edges which are common for most of the Au-ordered vicinal Si surfaces [29,39–41]. These structures, together with two atomic chains of Au which are incorporated into the Si lattice, stabilize the surface and make a uniform distribution of steps. The situation is different in the case of Pb-induced order. The Pb layer covers the surface, leaving the Si atoms underneath in their bulk positions. Simultaneously, Pb saturates the dangling bonds of the Si atoms while itself remaining strongly metallic and thus not forming different dangling bonds [26]. This prevents the appearance of stress which could build up on a vicinal surface due to the reduction of the number of dangling bonds and the formation of dimers or other surface reconstructions. For large enough terraces this stress can be relieved, but for narrow ones it can induce a strong interaction between the steps, causing faceting. Apparently, the terraces with a width of about 3 nm separated by biatomic height steps are wide enough for stress to be relieved.

The observed reconstruction of the (111) terraces is not of known Si(111) reconstructions:  $(7 \times 7)$  and  $(5 \times 5)$  or other  $(n \times n)$  (with  $n = 9-13$ ) which are sometimes observed on flat and vicinal surfaces [42]. It is also known that low Miller index vicinal surfaces such as (113), (331), or (114) undergo different reconstructions, but they form atomically corrugated surfaces rather than terraces separated by steps. In the present study the (111) terraces reveal another type of reconstruction with a period of  $8a_{[1\bar{1}0]}$  along the step edges.

It is known that the presence of steps significantly influences the charge distribution within the  $(7 \times 7)$  unit cell [43]. However, these changes influence the density of states at the Si adatoms and therefore their intensity in the STM images [43], but do not influence their location, as reported in the present study. The charge redistribution also does not explain the observed  $8a_{[1\bar{1}0]}$  periodicity along the step edges.

Interestingly, the electronic structure of such a reconstructed surface resembles that of the Si(111)- $(7 \times 7)$  surface. It is not surprising because the observed reconstruction consists of many Si adatoms. Similarly, as in the DAS model of the  $(7 \times 7)$  superstructure, they deliver dangling and back bonds which contribute to the observed weakly dispersive bands in the electronic structure. In addition, as shown in Figs. 2(e) and 2(f), the relative location of some of the adatoms is similar to the positions of the Si adatoms in the  $(7 \times 7)$  unit cell. Apparently, the reconstructed (111) terraces consist of the building blocks of the  $(7 \times 7)$  superstructure, however, the unit cell is significantly distorted in order to fit the terrace width. Thus the observed reconstruction can be regarded as a modification of the  $(7 \times 7)$  reconstruction. The double Si(111) terrace of the Si(553) surface is wide enough to develop a full  $(7 \times 7)$  unit cell, but due to the presence of double atomic steps in its vicinity, it forms an energetically favorable superstructure with  $8a_{[1\bar{1}0]}$  periodicity.

## V. SUMMARY

It is shown that the Si(553) surface can be ordered by a proper thermal treatment only without the deposition of additional atoms. (111) terraces of 2.88 nm width are separated by double atomic height steps. The regular distribution of biatomic steps is apparently stabilized by the formation of a different type reconstruction of the (111) terraces. The electronic structure of the ordered Si(553) surface is very similar to that of Si(111)- $(7 \times 7)$ , with three characteristic weakly dispersive bands running along the whole Brillouin zone. The bands are very likely associated with the Si adatoms clearly resolved in the STM images. The obtained results indicate that between the (111) and (110) silicon planes beside (331), the (553) surface is also thermodynamically stable against faceting.

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