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Correlations between one-dimensional structures at the Si(557):Au surface

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The quasi-one-dimensional structures at the Si(557):Au surface are examined by scanning tunneling microscopy at room temperature and at low temperatures (77 K). A short-range structural correlation between adjacent chain and row structures—attributed to Si adatoms and Si step edges, respectively—located on the same terrace is found. This correlation is absent between chains and rows located on adjacent terraces, demonstrating the decisive role of the step edge preventing correlations perpendicular to the chains. In addition, the temperature-dependent variation of the image contrast does not yield evidence for an increase of the structural unit cell of the one-dimensional structure as would be expected for a Peierls transition.

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I. INTRODUCTION

In one-dimensional (1D) electronic systems, the electron-phonon and electron-electron interactions play important roles. The former gives rise to a Peierls instability yielding a charge-density-wave ground state, as observed in many inorganic and organic linear chain compounds[1,2] and on solid surfaces.[3,4] The latter can lead to a breakdown of the Fermi-liquid state and the formation of a Luttinger liquid as reported for carbon nanotubes.[5] In an ideal 1D system, a Peierls (second-order) phase transition cannot occur at finite temperatures $T>0$ due to large fluctuations of the order parameter in one dimension.[1,2] In this case, only short-range correlations exist for $T>0$, which give rise to the formation of a pseudo-energy-gap in the electronic density of states. However, in real quasi-1D systems, deviations from the ideal case, for instance, due to interchain electron tunneling or due to coupling to or via a substrate, allow a quasi-1D system to undergo a Peierls transition at a finite temperature T_c. Hence, the issue of residual correlations is of importance.

Periodic structures obtained by self-organization of metallic species on vicinal single-crystalline semiconductor surfaces are examples of 1D systems that appear to be particularly well suited because these structures consist of monoatomic chains of atoms.[6] Among the 1D reconstructions of metals on single-crystalline semiconductor surfaces, the Si(557):Au surface has attracted considerable interest due to its unusual electronic properties found by angular resolved photoemission spectroscopy (ARPES). While first experiments resolved two slightly separated bands with vanishing intensity at the Fermi level E_F as an indication of spin-charge separation in a Luttinger liquid,[7] a later ARPES study reported two similarly close bands crossing the Fermi level with finite intensity, putting the Luttinger-liquid scenario for Si(557):Au into question.[8] A further study[9] showed that the position of the upper band shifted from E_F at room temperature (RT) to ≈ 40 meV below E_F at 77 K. This gap formation was accompanied by an apparent change of the height modulation along Si chains forming the step edge observed by scanning tunneling microscopy (STM). It was interpreted as a Peierls-like instability with a mean-field transition temperature $T_c \approx 260$ K.[10] Alternatively, in a first-principles calculation, the temperature dependence of the structure observed in STM images[9] has been explained by fluctuations of atoms forming the step edge at RT which are frozen out at 77 K.[11] This model can explain the observed geometric changes in the STM images but is not able to account for the gap formation. Another model considers two coupled chains of Au and Si atoms which are observed by STM without taking into account the presence of Si adatoms nor the step edge.[12]

As mentioned above, a Peierls transition can only occur at finite temperatures in the presence of (albeit weak) additional correlations between the 1D structures. It is therefore mandatory to search for indications of such correlations on an atomic scale. For this purpose, we have re-examined the Si(557):Au surface by STM with high lateral and vertical (height) resolutions at $T=300$ and 77 K.

We interpret the observed images on the basis of the widely accepted structure model proposed for this surface,[13,11] where Si adatoms and step edges show a 1D atomic arrangement. We find strong short-range structural correlations between these 1D structures located on the same terrace by studying their response to phase-shifting defects. This suggests that the step edge is important for the electronic as well as for the structural properties of this surface inhibiting, or at least weakening, long-range structural correlations. While correlations between 1D structures are a prerequisite for a Peierls transition at $T>0$, we further demonstrate the absence of such a transition by showing that the periodicity (i.e., spatial frequency) of the chains is not changed by temperature.

II. EXPERIMENTAL METHODS

The Si(557):Au surface was prepared in ultrahigh vacuum by flash annealing a vicinal Si(111) substrate with an intentional miscut of 10° ±0.5° toward $[\bar{1}\bar{1}2]$.[14,15] The amount equivalent to 0.2 atomic layer of gold was deposited by electron-beam evaporation at a substrate temperature of 770–870 K followed by annealing to 1070 K. Special care was taken to move the sample as fast as possible from the preparation chamber (pressure after sample preparation of 5×10^{-10}–5×10^{-9} mbar) into the STM chamber (base pressure below $\approx 3\times10^{-11}$ mbar). In our studies, the uninter-

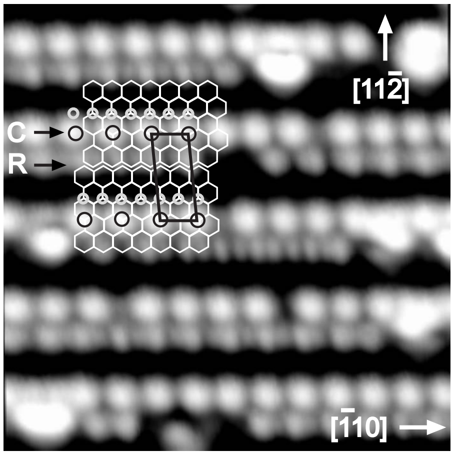

FIG. 1. (a) STM image (10×10 nm^2) of Si(557):Au taken with a sample voltage $U=+1$ V (tunneling current $I=0.1$ nA) at $T=77$ K. The terrace steps R of the vicinal surface are descending from the bottom to the top of the image. The Si lattice of two atomic terraces is indicated by honeycombs. Open circles indicate the Si adatoms on C, and gray circles the Au-atom positions according to the structure model (Refs. 11 and 13).

rupted adatom chain length mainly depended on the time the sample spent in the preparation chamber, whereas a small variation of the annealing temperature had little influence. We performed extensive STM and scanning tunneling spectroscopy measurements in a low-temperature STM (Omicron Nanotechnology, Germany) at $T=300$ and 77 K on freshly prepared samples. STM images were recorded both by scanning the tip parallel to the chain direction in order to obtain the highest spatial resolution and by scanning perpendicularly to the chain direction in order to obtain an essentially drift-free measurement of the height differences and interchain correlations. A representative selection of the data is presented in this paper. The results of the scanning tunneling spectroscopy measurements will be reported elsewhere.[16] The results were reproducible when using different STM tips.

III. RESULTS AND DISCUSSION

An overview of the surface structure is given in Fig. 1. A typical STM image of the unoccupied electronic states, measured for positive sample voltage $U=+1$ V at $T=77$ K, shows the characteristic surface structure of Si(557):Au with two adjacent chains of atoms per terrace. Randomly distributed larger protrusions are often observed on this surface and have been attributed to excess Si.[17] We denote the monoatomic structures as C (for "chain" of localized protrusions) and R (for "row").[15] If the Si-Si distance along $[\bar{1}10]$, i.e., along the chains, is denoted as $a_{[\bar{1}10]}=0.384$ nm, the distance between the protrusions on C is $2a_{[\bar{1}10]}$ and the separation between two neighboring C (or R) is $b=5\frac{2}{3}a_{[11\bar{2}]}=1.92$ nm. According to the structure model of the Si(557):Au surface, derived from previous x-ray scattering experiments[13] and previously used for *ab initio* calculations,[11] R is attributed to the step edge and C is attributed to Si adatoms on the terrace. Our, as well as previous,[7,18] low-energy electron diffraction measurements have not shown long-range correlations between the different chains C. The large number of defects along the chains leads to various phase shifts of the atomic positions and the destruction of long-range order. However, the STM images do show a strong short-range correlation between protrusions localized on C and R located on the same terrace as will be discussed now.

Figure 2(a) (top panel) shows an STM image at 77 K with two adjacent chains C belonging to the upper ($\mathrm{C_U}$) and lower ($\mathrm{C_L}$) terraces. $\mathrm{C_U}$ shows a defect that appears as a topographic minimum causing a phase shift of the Si adatoms composing the chain with respect to the Si substrate. Away from the defect, the height profile taken along R has the same period as the profile along $\mathrm{C_L}$ and $\mathrm{C_U}$, but the shape of each maximum on R shows an additional soft shoulder due to the two adjacent elliptical features of alternating heights observed on R in the STM image. This height modulation is attributed to the static buckling of the Si step edge with an almost fully occupied "up" atom and an almost unoccupied "down" atom as proposed in the first-principles calculation.[11] In order to emphasize the most intense features along R in the empty-state image, i.e., the almost unoccupied "down" atom of the buckled step edge, the image is additionally shown in color. The phase relationship between $\mathrm{C_U}$ and R as well as between R and $\mathrm{C_L}$ is indicated by white lines. On both sides of the defect, this phase relationship is in agreement with the structure model either in its original or in its mirror reflected form.[11,13] The defect-induced phase shift by $a_{[\bar{1}10]}$ on $\mathrm{C_U}$ of the upper terrace affects the periodic arrangement at R located $3\frac{2}{3}$ Si rows away [Fig. 2(a)] such that a phase shift is observed at R, too. Hence, the structural correlation between adatoms on $\mathrm{C_U}$ and the atoms of the descending step edge (R) of the *same* terrace is maintained even in the presence of the defect. The chain $\mathrm{C_L}$ on the adjacent lower terrace, on the other hand, is not affected, i.e., no phase shift is observed. This gives rise to a local mirror symmetry of the structure on terrace U that extends to $\mathrm{C_L}$ (cf. vertical dotted lines in Fig. 2).

In contrast, the periodic arrangement of protrusions on R is not affected when a phase-shifting defect is located on $\mathrm{C_L}$, i.e., on the *next* terrace. This is shown in Fig. 2(b), where two phase-shifting defects are observed on $\mathrm{C_L}$.[19] In contrast to Fig. 2(a), the periodic arrangement on R is maintained and strictly follows the (undisturbed) arrangement on $\mathrm{C_U}$ due to the strong correlation between $\mathrm{C_U}$ and R. Hence, we do not observe a correlation between R and $\mathrm{C_L}$ which are located on two adjacent terraces. It is important to note that the periodicity in R is maintained, although $\mathrm{C_L}$ is much closer to R than $\mathrm{C_U}$. We emphasize that these characteristics have been confirmed on a large number of images where single phase-shifting defects surrounded by well-ordered chains were found. We have observed such correlations at RT, too, albeit with a weaker contrast on R. Similar characteristics can also be inferred from previously reported images, see, for example, Fig. 3(c) in Ref. 10.

The correlation between R and $\mathrm{C_U}$ supports the proposed structure model[11,13] which suggests that R and $\mathrm{C_U}$ are located on the same terrace, in contrast to a recent proposal of two

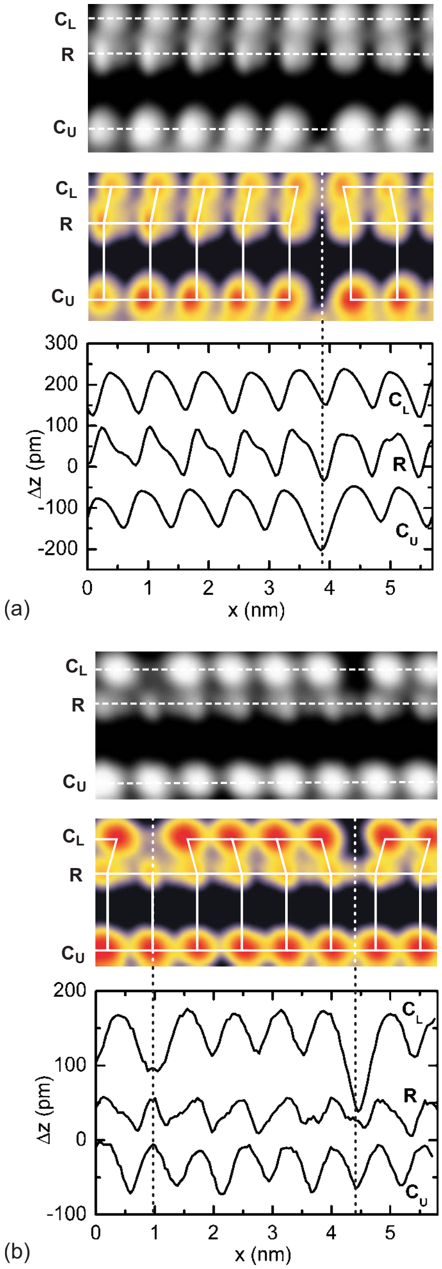

FIG. 2. (Color online) (a) STM image ($T=77$ K, $U=+1$ V, and $I=0.05$ nA; top) showing a step edge R and the adjacent adatom chains located on the lower (C_L) and upper (C_U) terraces containing a defect on R and C_U. Horizontal dashed lines indicate traces of the height profile scans $\Delta z(x)$ (bottom). White lines in the colored image (middle) indicate the correlation between atoms on C_U and the upper atoms of the buckled step edge (R). This correlation is disturbed near the phase-shifting defect. Vertical dotted lines indicate a local mirror symmetry between the two configurations. (b) STM image ($T=77$ K, $U=+1$ V, and $I=0.1$ nA; top) showing a step edge R and the adjacent adatom chains C_U and C_L with two phase-shifting defects on C_L. These do not affect the strong correlation between R and C_U.

adjacent rows comprised of Si and Au atoms, respectively.[12] Within the first structure model, the cutting off of the correlations is naturally attributed to the step edge. More importantly, the observed correlation points to the presence of a strong interaction between chains C and rows R. The correlation is stronger between C_U and R separated by $3\frac{2}{3}$ Si nearest-neighbor (nn) distances compared to C_L and R separated by only two Si nn distances. Hence, possible correlations between the 1D structures located on different terraces are disturbed by the presence of the step edge. Although we investigate the structural correlations only, we consider this to be an indication that similar limitations apply to the electronic correlations. This is in agreement with our recent local scanning tunneling spectroscopy measurements[14–16] that show little differences between C and R except for states far away from the Fermi level.

So far, we have focused on phase-shifting defects. In addition, other types of defects are present on this surface. The correlations between the bright white protrusions caused by excess Si (cf. Fig. 1) have been analyzed previously for the Si (5×2)-Au surface.[17] It has been shown that these protrusions form a lattice fluid with a small repulsive interaction of ≈ 12 meV of unknown origin between interchain nearest neighbors. Studying the response of the chains and rows to these defects is difficult, mainly because these defects strongly disturb their environment. It is, however, conceivable that the structural correlation between R and C_U constrains the step edge from fluctuating between the different step-edge configurations and therefore prevents an optimal accommodation of the lattice fluid.

For the remainder of this section, we will discuss the issue of a possible Peierls transition. As mentioned in the Introduction, a coupling between 1D structures is a necessary—but not a sufficient—condition for a Peierls transition at finite temperature. In our case, we observe strong short-range structural correlations between R and C on the same terrace. However, we cannot exclude a small residual electronic coupling across the step edge or to the substrate that may suffice for a finite-T Peierls transition of Si(557):Au. Under these circumstances, it is necessary to recur to experiments. As mentioned above, previous STM experiments were interpreted in terms of a finite-T Peierls transition. However, as already discussed, our well-resolved STM images, see Fig. 3(a), clearly indicate that the height modulation for $T=77$ K along R has the same periodicity as along C. While in many RT-STM studies R is imaged as a diffuse stripe and the height modulation is below the experimental sensitivity, a careful analysis of our STM images reveals that this height modulation is still observed at RT [Fig. 3(b)]. This indicates a remaining buckling amplitude along the step edge at RT. A residual height modulation on R at RT had, in fact, been previously reported[9,10] but was claimed to occur only in the presence of defects. Hence, the different appearance of STM images at RT compared to $T=77$ K was interpreted as a hallmark for the occurrence of a Peierls transition because the height modulation was suggested to be absent at RT.[9,10] In contrast, in our RT-STM images, the modulation is well resolved on long wires even at positions far away from defects. We attribute the splitting of the features on R observed at $T=77$ K [Figs. 1, 2, and 3(a)] to a better spatial resolution compared to RT without a change of the spatial frequency. In contrast, a Peierls transition would be accompanied by an increase in size of the structural unit cell, i.e., by a decrease of the spatial frequency at low temperatures compared to RT.

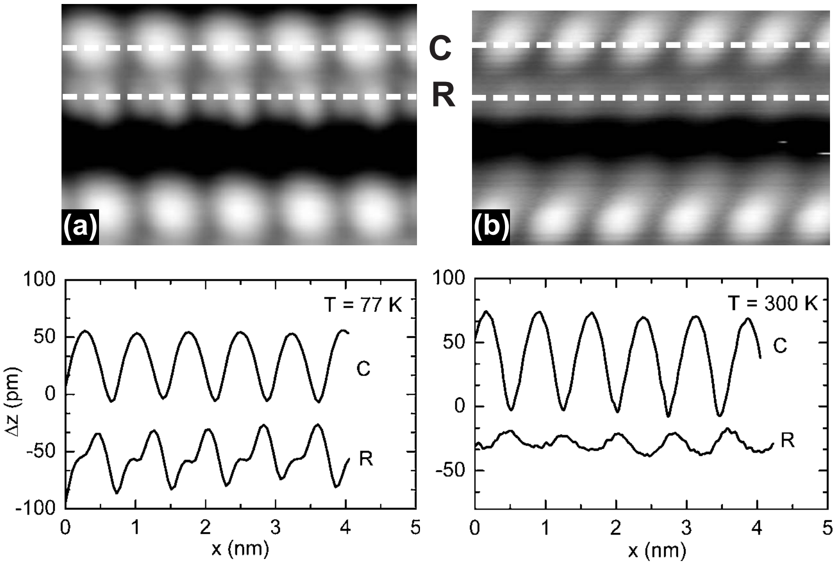

FIG. 3. Height profiles along R and C as indicated in the enlarged STM images at (a) $T=77$ K and at (b) room temperature. For both images, $U=+1$ V. The tunneling current was (a) $I=0.5$ nA and (b) $I=0.05$ nA.

In the simplest case of a commensurate transition, the structural unit cell doubles in size. Moreover, the splitting of each protrusion into two adjacent features of alternating heights at $T=77$ K compared to RT can only be described by higher harmonics of the spatial frequency signaling an incipient halving of the structural unit cell. Hence, the temperature-dependent variation of the image contrast cannot be taken as an indication of the existence of a Peierls transition.

Finally, we briefly discuss the double feature, i.e., the "peak-dip-hump" structure, in the height profile observed at 77 K only on R with increasing x upon approaching the mirror plane at $x=3.9$ nm but not on C_U or C_L [cf. Figs. 2(a)]. This feature on R to the left of the phase-shifting defect on C_U in Fig. 2(a) is roughly mirror symmetric, i.e., becomes a "hump-dip-peak" structure to the right of the phase-shifting defect [cf. also Fig. 2(b)]. This feature bears resemblance to a soliton as observed, for instance, in one-dimensional polyacetylene chains.[1] In our case, however, the soliton arises from a localized structural defect away from R, i.e., at C_U, and is therefore immobilized by that defect.

IV. CONCLUSIONS

We have shown that structural correlations between the monoatomic chains on the Si(557):Au surface are restricted to one atomic terrace. We point out that the short-range structural correlations reported here support the proposed structure model[11,13] where, in contrast to a recently proposed alternative,[12] the cutoff of the correlations is attributed to the step edge. However, apart from the decisive role of the step edge, our results are largely independent of the applied structure model and should be taken into account when proposing alternative models for the Si(557):Au surface. Concerning a possible Peierls transition, we cannot exclude a small residual coupling between 1D structures on different terraces or to the substrate which would be necessary for a finite-T transition. Experimentally, however, we see no evidence for a Peierls transition: When lowering the temperature, a lattice distortion leading to an increase of the structural unit does not occur. We therefore conclude that in our well-resolved STM images, there is no indication of a Peierls transition on Si(557):Au.

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[19] Note that the two defects shift the phase of C_L by the same amount in opposite directions and could therefore annihilate if they were sufficiently mobile and if a vacancy has lower energy than the two phase-shifting defects.