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Atomic seesaws

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Abstract
The dynamics of two types of atomic seesaws are studied by open feedback loop scanning tunneling microscopy. The first type of atomic seesaw is a regular Ge dimer of the dimer reconstructed Ge(001) surface and the second type of atomic seesaw is a dimer located on the ridges of Au induced nanowires on a Ge(001) surface. On the bare Ge(001) surface the flip-flop motion of the dimers is induced by phasons, which perform a one-dimensional random walk along the substrate dimer rows. The phasons on the Au induced nanowires ridges are pinned and therefore only a limited number of dimers exhibit flip-flop behavior for the Au/Ge(001) system.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The silicon and germanium semiconductor group IV (001) surfaces are, because of their relevance for the semiconductor industry, among the most frequently studied surfaces [1, 2]. The unreconstructed, bulk truncated Si and Ge(001) surfaces have two broken bonds (dangling bonds) per surface atom. Such a high number of dangling bonds per surface atom is energetically unfavorable, since the free energy per unit area of a surface strongly depends on the number of broken bonds per surface atom. In order to minimize the surface free energy, the (001) surfaces reconstruct by the formation of surface dimers. This dimerization leads to a reduction of the number of dangling bonds from two per surface atom in the unreconstructed case to only one dangling bond per surface atom in the reconstructed, i.e. dimerized, case. The short-range interaction that is responsible for the dimerization gives rise to a (2×1) surface reconstruction of the (001) surfaces. Higher-order surface reconstructions, such as $p(2 \times 2)$ and $c(4 \times 2)$ can occur as a consequence of weaker, long-range interactions [3].

In 1985 the first scanning tunneling microscopy (STM) images of the Si(001) surface [4, 5] revealed that most of the surface dimers have a symmetric appearance, i.e. they seem not to buckle. Since the late seventies it has, however, been well established that the lowest energy configuration is not a symmetric dimer, but a buckled dimer [6]. The dimers that appear symmetric in the STM images are actually rapidly flip-flopping between their two possible buckled configurations, see figure 1. The first direct evidence for this flip-flop motion was provided by Sato *et al* [7]. They demonstrated that the tunneling current recorded on-top of one of the atoms of a dimer of the Ge(001) surface exhibited telegraph like noise. A few years later similar experiments were reported for Si(001) by Hata *et al* [8], Yoshida *et al* [9] and Pennec *et al* [10]. The latter measurements demonstrated that the flip-flop motion of the dimers can be interpreted in terms of a so-called phason. Several groups reported that such phasons can be created by bias voltage control [8–13].

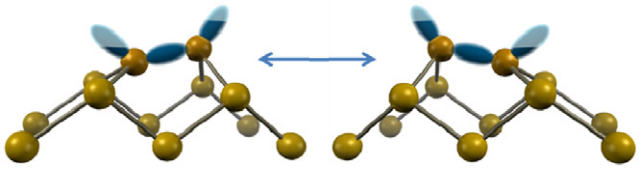

Figure 1. Schematic representation of the flip-flop motion between the two buckled configurations of a surface dimer of Ge(001) or Si(001). The tilt angle of the dimer bond of a buckled dimer is about 10°–20°.

A phason is a phase defect or anti-phase boundary in the zigzag buckling order of the dimers within in dimer row. At an anti-phase boundary two adjacent dimers are buckled in the same direction, rather than in an opposite direction (see figure 2). If at an anti-phase boundary one of the dimers flips to its other buckled configuration, the phason effectively moves by one lattice spacing, see figures 2(a)–(c), which at sufficiently high temperatures leads to a thermally activated random walk of the phason, i.e. a phason diffuses along the substrate dimer row. A dimer which is positioned under an STM tip will thus flip to its other buckled configuration each time that a phason traverses the tunnel junction. Such an event will lead to a jump in the tunneling resistance and thus to a jump in the tunneling current, resulting in a telegraph like signal.

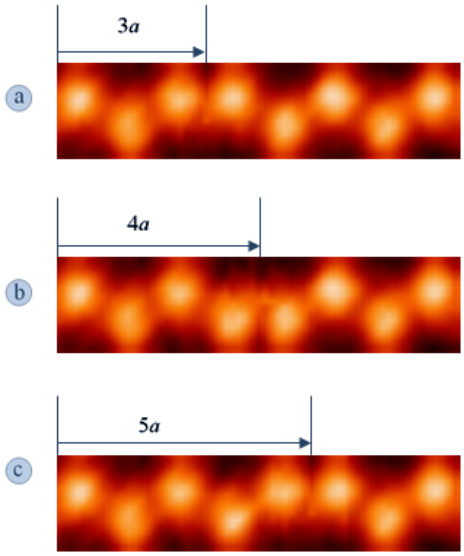

Figure 2. Animation of a diffusing phason in a substrate dimer row. The phason diffuses from 3*a* (a) to 4*a* and 5*a* in (b) and (c) respectively. One diffusion 'step' of a phason corresponds to a single flipping event of one of the constituting dimers of the phason.

Here we study this flip-flopping behavior of Ge dimers by means of open feedback loop scanning tunneling microscopy. We will elaborate on the role of phasons in the flip-flop process for both the clean Ge(001) surface as well as the Au modified Ge(001) surface.

2. Experimental details

Experiments were performed with a room temperature Omicron STM1 operating in ultrahigh vacuum (UHV). Ge(001) substrates were cut from nominally 3 inch by 0.3 mm, about 25 Ω cm resistance, single-side-polished n-type wafers. Samples were mounted on Mo holders and contact of the samples to any other metal during preparation and experiment has been carefully avoided. The Ge(001) samples were cleaned by prolonged 800 eV Ar^+ ion sputtering and annealing via resistive heating at 1100 (±25) K. The temperature was measured with a pyrometer. After several cleaning cycles the Ge(001) samples were atomically clean and exhibited a well ordered $(2 \times 1)/c(4 \times 2)$ domain pattern (observed in STM images) [14]. For the Au/Ge(001) system an equivalent of 0.20–0.30 monolayer of gold was deposited onto the cleaned Ge(001) surface at room temperature. Au was evaporated by resistively heating a W wire wrapped with high purity Au (99.995%). After Au-deposition the sample was annealed at 650 (±25) K and then cooled down to room temperature by radiation quenching before placing it into the STM for observation.

3. Results and discussion

3.1. Phasons in Ge(001)

Figure 3 shows a room temperature STM image of the Ge(001) surface. The surface shows ordered $c(4 \times 2)/(2 \times 1)$ regions as well as some regions where the buckling registry is disturbed by the presence of adsorbates and missing dimer defects. Some interesting observations are outlined by arrows, lines and ellipses:

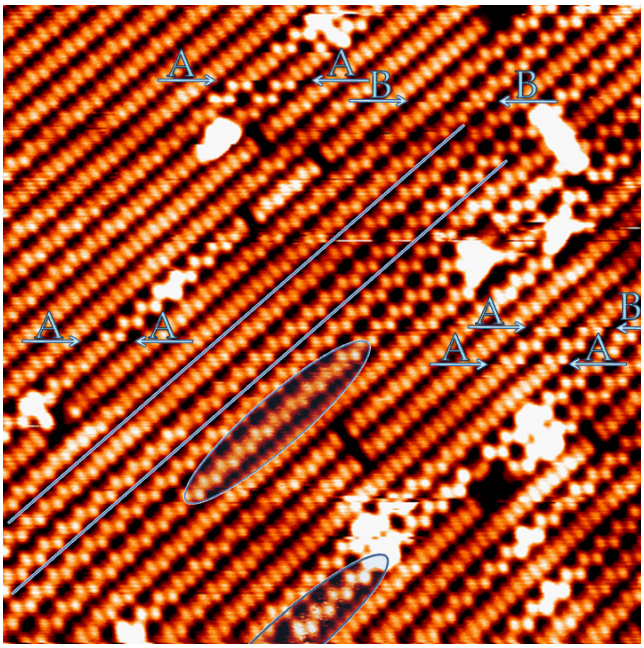

Figure 3. Filled state STM image (20×20 nm^2, bias voltage −1.5 V, tunneling current 0.4 nA) of Ge(001) recorded at room temperature. Abrupt changes in the surface topography are indicated by arrows. The rows highlighted by the ellipses exhibit some flickering, while the neighboring rows do not exhibit this flickering. In the dimer rows between the lines the reconstruction changes from $c(4 \times 2)$ in the upper part of the image to $p(2 \times 2)$ in the lower part of the image.

- The arrows A and B point at abrupt changes in periodicity of the substrate dimer rows. These abrupt changes occur very locally and therefore we ascribe these features to the passage of a phason, rather than an STM tip induced effect. In some of the changes (marked A) the $c(4 \times 2)$ reconstruction (zigzag rows) is changed to a (2×1) reconstruction (symmetric appearance), whereas in the other case (marked B) the zigzag appearance is maintained.
- Within the two dimer rows, which are enclosed by long lines in figure 3, an interesting change in buckling registry is observable: the dimer rows buckle out-of-phase in the upper part of the image, giving rise to a local $c(4 \times 2)$ reconstruction, while they buckle in-phase in the lower part of the image, resulting in a $p(2 \times 2)$ reconstruction. In the middle part of the image one of the dimer rows shows a (2×1) reconstruction. In this dimer row a phason is trapped between the $c(4 \times 2)$ and $p(2 \times 2)$ domains. The rapid diffusion of this phason is too fast to be imaged in real space with our STM. The latter leads to a symmetric appearance of the dimers.
- The dimer rows located in the ellipses reveal a flickering appearance, whereas the neighboring dimer rows are properly imaged. The flickering can therefore not be ascribed to an unstable STM tip, but must be attributed to dynamics of the dimers. We suggest that this flickering appearance is induced by rapidly diffusing phasons.

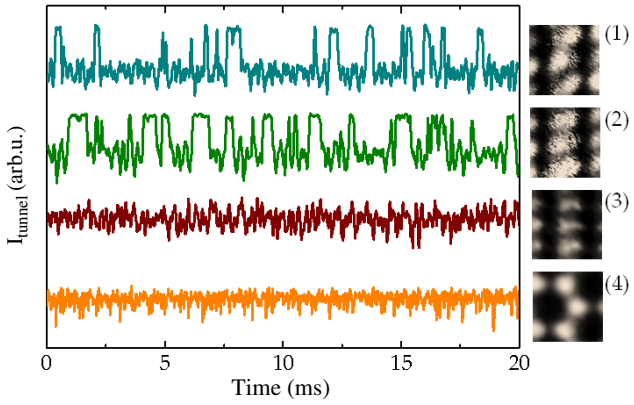

Figure 4. Tunneling current traces measured on a flickering asymmetric dimer (curve 1), on a flickering symmetric dimer (curve 2), on a nonflickering symmetric dimer (curve 3) and on a nonflickering asymmetric dimer (curve 4). Typical images of the probed dimers are shown in the panels on the right. The measurements are performed at room temperature. The sampling rate is 50 kHz. Current set points are 0.40 nA for curves 1–3 and 0.55 nA for curve 4.

Cooling of the substrate will lower the diffusion speed of the phasons, which makes it possible to image them in real space [15] and thus provide direct evidence for their existence. At room temperature, where the diffusion is too fast to be imaged properly, we will make use of open feedback loop current–time measurements [15–17].

Figure 4 shows typical current–time traces measured on a flickering asymmetric dimer (curve 1), a flickering symmetric dimer (curve 2), a nonflickering symmetric dimer (curve 3) and a nonflickering asymmetric dimer (curve 4). In figure 5 the distribution of residence times for a flickering symmetric (A) and a flickering asymmetric dimer (B) are shown. For a flickering symmetric dimer the distribution of residence times in both states is about same, whereas a clear asymmetry in the residence times of both buckled states is present in the asymmetric case. The ratio of these average residence times results in an energy difference of 22 ± 2 meV between the two buckled configurations [17].

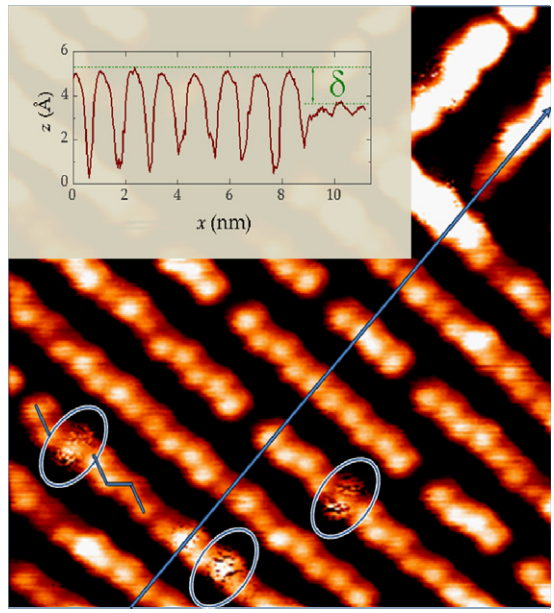

Figure 6. STM image (10.0×10.0 nm^2, sample bias -1.0 V, tunneling current 0.6 nA, $T = 293$ K) of an area with Au induced nanowires on Ge(001). The nanowires show up as bright stripes in the images, the troughs between the nanowires are dark. The inset shows a line profile along the blue arrow in the image. The depth of the troughs is about 0.4–0.5 nm and involves several atomic layers. The monatomic step height on Ge(001), δ(=0.14 nm), is also indicated. The features marked by the ellipses show a flickering behavior.

3.2. Phasons in the giant missing row reconstruction on Au/Ge(001)

Phasons are not necessarily mobile. In the Au/Ge(001) system immobile phasons are observed. Recently the Au/Ge(001) system has attracted quite a bit of attention, because of its complicated and intriguing surface reconstruction [18–26]. Upon the deposition of Au on Ge(001) and subsequent annealing, a surface reconstruction with deep nanogrooves can be observed, see figure 6. The Au induced nanowires appear as bright rows in the image. Careful inspection reveals that the ridges of the rows exhibit a zigzag character. Occasionally one observes defects in the rows. One also finds occasionally

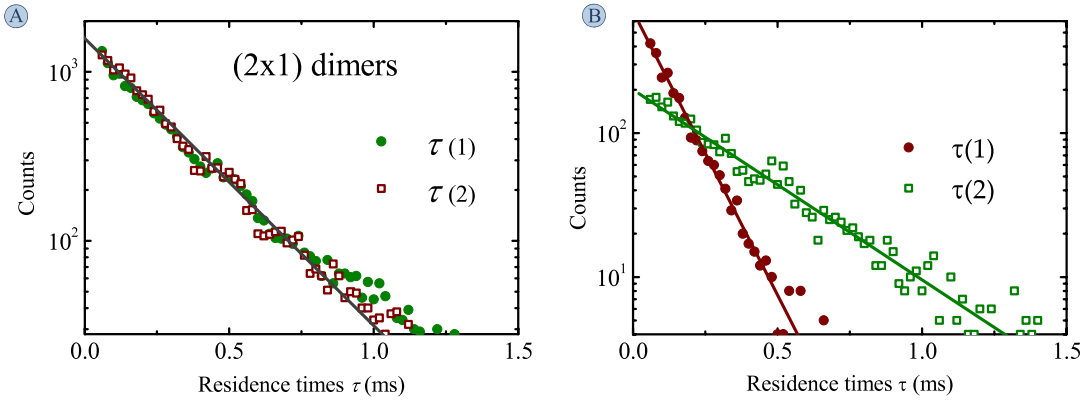

Figure 5. Histograms of the residence times of the two buckled states of a flickering dimer that appears symmetric (A) and of a flickering dimer that appears asymmetric (B). The lines are theoretical fits for a fully random process (Poisson distribution). $\tau(1)$ and $\tau(2)$ are residence times of the two buckled states.

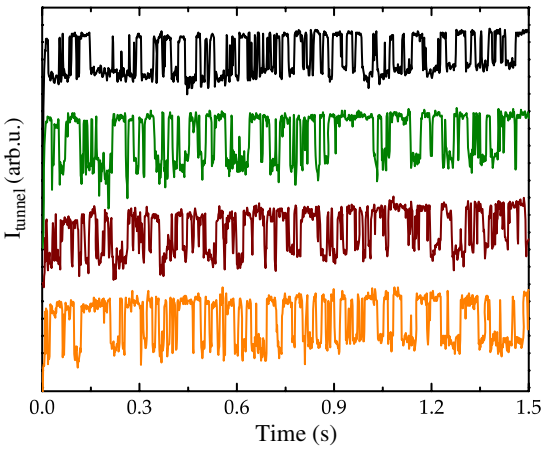

Figure 7. Tunneling current traces measured over four different immobile phasons in the Au/Ge(001) system. The measurements are performed at room temperature. The sampling rate is 666.7 kHz, the set point current is 0.8 nA and the sample bias −0.6 V.

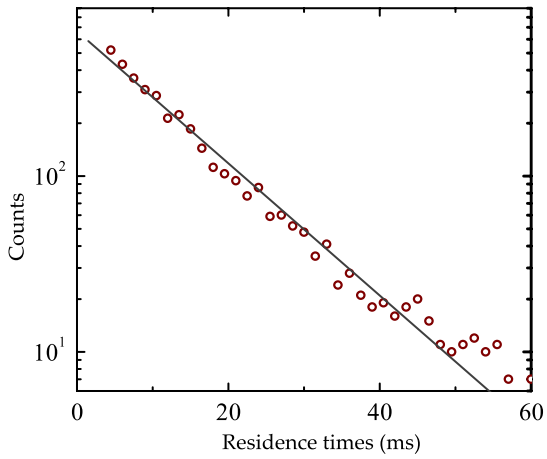

Figure 8. Histogram of the residence times recorded on immobile phasons of the Au/Ge(001) system. The measurements are performed at room temperature. The sampling rate is 666.7 kHz. The gray line is the theoretical fit for a fully random process.

noisy, flickering dimers in the rows (marked by ellipses). A line profile recorded in a direction perpendicular to the nanowire direction is shown in the inset of figure 6. The troughs are surprisingly deep (about 0.4–0.5 nm) and thus involve several atomic layers. In [21] we presented a detailed model for the Au induced reconstructed Ge(001) surface, which we will briefly discuss here. The deposition of Au leads to nanofaceted Au decorated (111) grooves. These grooves have a width of 1.6 nm and are perfectly aligned along the substrate dimer row directions of the (001) surface. High resolution STM images of the Au decorated (111)-nanofacets revealed a $(\sqrt{3} \times \sqrt{3})$R30° periodicity which is reminiscent of a Au decorated Ge(111) surface [27]. Since here we are not interested in the exact details of this complicated surface reconstruction we restrict ourselves to the structure of the top ridges of these nanowires. The zigzag appearance and the measured width of the nanowires suggest that the ridges are comprised of dimers, with their dimer bond aligned in a direction perpendicular to the nanowire direction, rather than atoms. The electronic structure of these 'ridge' dimers is determined by scanning tunneling spectroscopy [21]. Their electronic structure is very similar to the electronic structure of buckled dimers of the bare Ge(001) surface and therefore we believe that the ridges are comprised of regular buckled Ge dimers rather than Au or mixed Ge/Au dimers [21, 28].

The flickering dimers (see figure 6) are always observed at an anti-phase boundary in the zigzag pattern. STM images are recorded in a bias voltage range from −2 to +2 V and flickering phasons are observed at all bias voltages. The behavior of these phasons can be studied by time-resolved $I(t)$ measurements. $I(t)$ traces recorded on different phasons are depicted in figure 7. Each measurement reveals two distinct current levels, similar to the phasons of the bare Ge(001) surface. It is also clear from figure 7 that the flip-flop frequencies of different phasons of the Au/Ge(001) system are very comparable in magnitude (0.1 ± 0.05 kHz). The latter is in marked contrast to the pristine Ge(001) surface where flip-flop frequencies are measured in a broad range of frequencies. The measured flip-flop frequencies are independent of the magnitude of the tunneling current, i.e. the flip-flop movement is not current induced. Figure 8 shows a histogram of the residence times of the flip-flop motion. The solid line in figure 8 refers to the residence time distribution for a fully stochastic flip-flop process. Hence our data clearly reveals that we are dealing with a stochastic process. In addition, the symmetric appearance of these noisy dimers reveals that both buckled state are roughly equally populated.

Among the many similarities between the flickering dimers of the pristine Ge(001) surface and the flickering dimers of the Au/Ge(001) system, there is also a striking difference: the phasons of the Au/Ge(001) system are immobile. Since an anti-phase boundary in the $(\sqrt{3} \times \sqrt{3})$R30° Au overlayer structure is always accompanied by a phason in the top ridge, we tentatively propose that the phasons are pinned by the structural details of the faceted grooves. Proper imaging of the faceted sides of the nanogrooves is a far from trivial task, since the troughs are extremely deep and narrow. One thus needs a very sharp and asymmetric STM tip to image these facets properly. In figure 9(a) we depict a schematic representation of such an STM tip. A strongly asymmetric image with atomic resolution is shown in figure 9(b). Due to the asymmetry of the tip apex one is only able to image one side of the nanogrooves properly. The position of a phason in the ridge of one of the nanowires is marked by an ellipse. Exactly at this position there is also an phase boundary in the $(\sqrt{3} \times \sqrt{3})$R30° Au overlayer structure. A few other phase boundaries in the $(\sqrt{3} \times \sqrt{3})$R30° Au overlayer structure are outlined by arrows. These phase boundaries are not accompanied by a flickering phason in the Ge dimer row due to the presence of a missing dimer defect in the ridge of the nanowire.

4. Conclusions

In summary, the flip-flop motion of Ge dimers of the Ge(001) surface and the Au/Ge(001) system have been studied using scanning tunneling microscopy and time-resolved scanning tunneling spectroscopy. The flip-flop motion is for both systems directly related to the presence of anti-phase

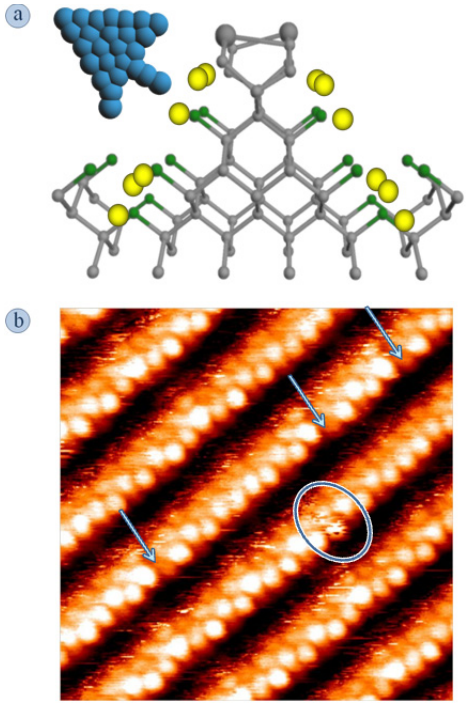

Figure 9. (a) Cartoon of the Au/Ge(001) model and an asymmetric STM tip. (b) Filled states STM image (7.4 × 7.4 nm^2, bias voltage −0.6 V, tunneling current 0.8 nA) recorded with an asymmetric STM tip. Note that only one of two sides of the grooves is resolved. The ellipse marks a phason. Note that exactly at this position there is a phase boundary in the $(\sqrt{3} \times \sqrt{3})$R30° Au overlayer structure of the facet. The arrows point at several other phase boundaries in the $(\sqrt{3} \times \sqrt{3})$R30° Au overlayer structure.

boundaries in the buckling registry of the dimer rows. In case of the pristine Ge(001) surface the phasons are mobile, whereas in the case of the Au/Ge(001) surface the phasons are pinned.

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