

Surface dynamics studied by perturbing the surface with the tip of a scanning tunneling microscope—Si(100) at 80 K

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We have utilized the tip of a scanning tunneling microscope to perturb a specific local structure (the C defect) of Si(100) at 80 K, and observed the dynamical symmetric \leftrightarrow buckled transition of the surrounding dimers. The observed large-scale transition implies that the configuration of the dimers is determined by a detailed balance among many elastic long-range forces generated by the surrounding C defects. © 1998 American Institute of Physics. [S0003-6951(98)03727-9]

The ability of the scanning tunneling microscope (STM) is not only restricted to imaging the static atomic structure of the surface. By manipulating the tip of the STM and applying a controlled electric field to a specified target, transfer of single atoms and fabrication of nanoatomic structures have been demonstrated.¹⁻³ Since the concept of atomic manipulation was introduced, this technique has been applied to many surfaces, for example, to fabricate atomic structures of desired design,¹ to confine electrons to artificial nanostructures,² and to extract Si adatoms.³ The technique of atomic manipulation can also be used as a method to perturb a specified local atomic structure and to excite a portion of the surface into a nonequilibrium state. Another, and important, application of the STM is its ability to visualize real-time dynamical processes on surfaces.⁴ *In situ* observations of crystal growth, adsorption, and atomic diffusion have revealed a wealth of information inaccessible by other methods.

Combining the technique of atomic manipulation and dynamic visualization STM would give a unique opportunity to study the surface dynamics through observation of the local excited state and its relaxation to an equilibrium stage. In this letter we report on an application of these techniques to Si(100) at 80 K to study the dynamics of dimers. On Si(100) at low temperatures (80 K), a special target (C defect) was perturbed by positioning the STM tip above it and applying a controlled electric field. The response of the surrounding dimers was dramatic and an avalanche type dynamical symmetric \leftrightarrow buckled phase transition of the dimers was observed. It can be understood by the fact that the surface is forced into an excited (metastable) state by the perturbation. If an appropriate temperature is chosen, it is possible to observe, by subsequent scanning, both the excited state and the dynamical relaxation of the surface in response to the localized perturbation until a new ground state is established. Direct observation of the dynamical transition reveals a wealth of important implications concerning surface dynamics.

Si(100) samples were phosphorus doped with a conduc-

tivity of 0.005 Ω cm. After the sample was prebaked at ~ 700 °C for one night, it was flashed to 1200 °C for several seconds and cooled down to 80 K.

An example of the perturbation and the accompanying dynamical transition of the dimers is displayed in a set of consecutive STM images in Fig. 1. Figure 1(a) shows the surface before perturbation. The white region at the lower left represents a step edge and an upper terrace. The C defect in the center indicated by an arrow is the target. Every time, before perturbation, the surface was scanned with both negative and positive surface bias to confirm that the target has the characteristics of the C defect mentioned afterward. The tip of the STM was positioned above the target C defect, and a ramped bias (typically -2 – 2 V, 7 ms) was applied several times (~ 16 rounds). By this procedure we could destruct the

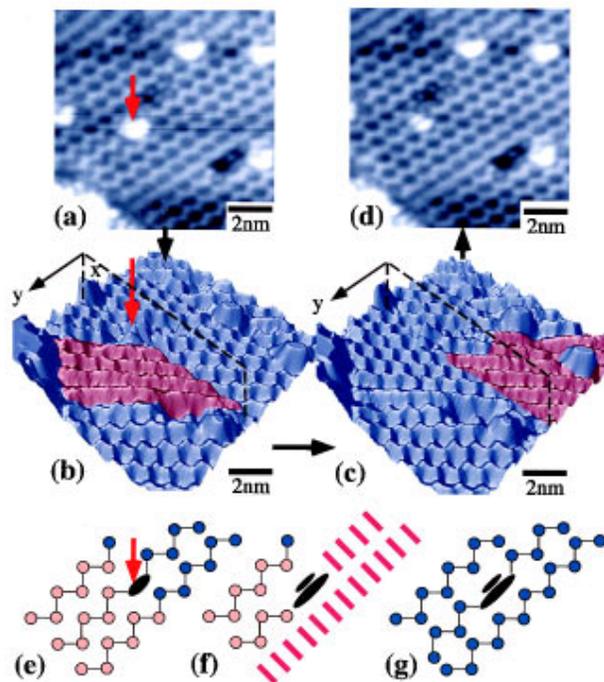


FIG. 1. Four STM images showing the dynamical response of the surface to a perturbation. The red regions show the symmetric dimer domains induced by the perturbation. Tunneling conditions: 0.6 V and 1 nA. The schematics show the stick and ball atomic structure of the initial, excited, and final states.

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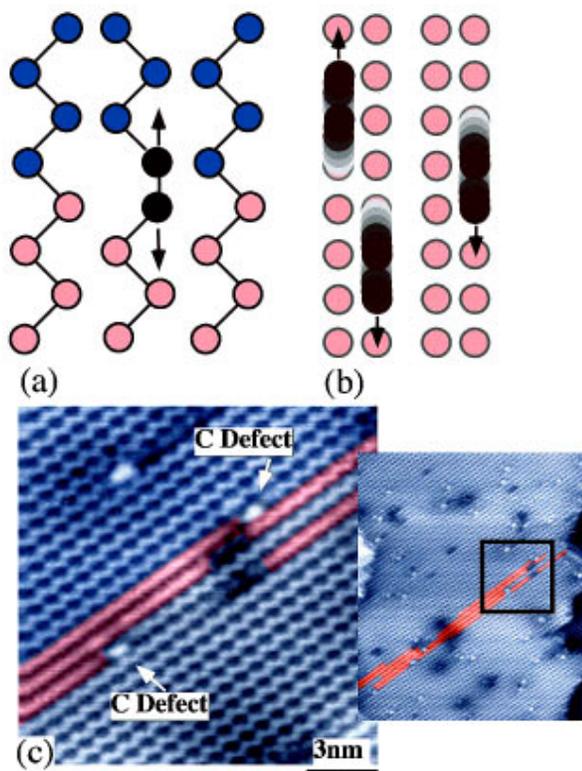


FIG. 2. (a) Stick and ball model showing the down (up) atoms of the buckled dimers. Red and blue represent the $c(4 \times 2)$ and $p(2 \times 2)$ phases, respectively. The schematic structure of the C defect and P defects is represented by the black atoms. (b) Schematic showing many P defects migrating along the dimer rows resulting in an apparent symmetric configuration of dimers observed by STM. (c) The STM image on the left shows a wider region of the STM image on the left (region surrounded by a box). Tunneling conditions: 0.6 V and 1 nA.

C defect routinely with a probability estimated roughly at 50%. Never did the same perturbation induce a noticeable transition when the tip was located above the dimers. It is important to realize that STM images are not snapshots of the surface. Ordinary scanning was halted when the tip came above the target, and the C defect was perturbed. After that, scanning was resumed. The x axes of the scanning are represented by the dotted lines in Figs. 2(b) and 2(c), while the black arrows show the y direction. An increase in the y coordinate not only means a change in location but also an increase in time. Considering these facts, it is possible to understand that the excited state is composed of the lower part of Fig. 2(b) below the dotted line and the upper part of Fig. 2(c) above the dotted line. At the moment of perturbation, the upper part of the perturbed dimer row and three buckled dimer rows on the right turned into a symmetric configuration, seen in red. Dynamical relaxation from the excited state was observed 3 min after perturbation as shown in Fig. 1(c). In the course of the dynamical relaxation, the newly born symmetric dimer rows returned into a buckled configuration as shown in Fig. 1(c). Figure 1(d) shows the new ground state established.

Before giving a detailed analysis, we want to describe the characteristics of the symmetric and buckled dimers observed at 80 K by the STM. The basic building block of the Si(100) reconstruction is a buckled dimer. Buckled dimers align in an antiferromagnetic order making up a dimer row.

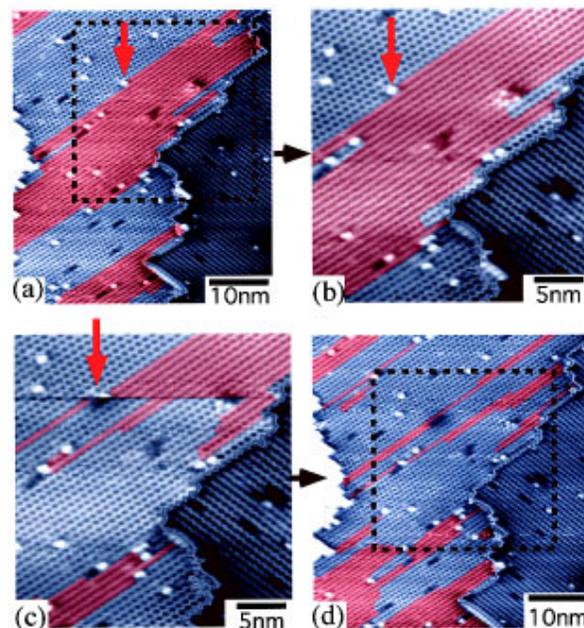


FIG. 3. Another example of perturbation. (a) A large scale STM image showing an overview of a large symmetric region (red). (b) A closeup showing the boundary of the symmetric and buckled dimer domains. (c) The C defect located at the boundary indicated by the red arrows was perturbed. (d) Final configuration after perturbation. Tunneling conditions: 0.6 V and 1 nA.

An antiphase alignment of these buckled dimer rows gives a surface phase of $c(4 \times 2)$ [blue region in Fig. 2(a)], while an inphase alignment gives a $p(2 \times 2)$ [red region in Fig. 2(a)]. At 80 K, the STM images show surfaces covered with $c(4 \times 2)$ domains with a certain ratio of symmetric dimer domains.^{5,6}

By looking through a number of STM images at low temperatures we reached the conclusion that the configuration of domains is mainly regulated by the defects on the surface, particularly, by the C defects. When probing the filled states, the C defects appear to be two adjacent Si atoms missing along the dimer row direction as shown schematically in Fig. 2(a), and these C defects are observed as bright protrusions in the empty states (this is our definition of the C defect). The C defect is a phase shifter by nature. If one side of the C defect is the $c(4 \times 2)$ phase, the other side must be the $p(2 \times 2)$, as shown in Fig. 2. However, a wide $p(2 \times 2)$ domain is never observed at 80 K, and regions supposed to reconstruct to the $p(2 \times 2)$ phases are usually observed as symmetric dimer domains. A typical example is shown in Fig. 2(c), where two antiphase $c(4 \times 2)$ domains (blue) are regulated by two C defects. The region sandwiched by the two $c(4 \times 2)$ domains, which is supposed to reconstruct to the $p(2 \times 2)$ phase, appears as a symmetric dimer domain (red).

It is proposed that numerous phasons nominated as P defects are migrating along the symmetric dimer rows far faster than the scanning of the STM.⁷ In such a case, basically the dimers are buckled, although they appear symmetric in STM as shown schematically in Fig. 2(b). The crystallographic structure of the P defects is exactly the same as the C defect, although the P defects are movable and do not appear as bright protrusions when probing the empty states. When this P defect moves along a dimer row, the surface

reconstruction switches from the $c(4\times 2)$ to the $p(2\times 2)$ phase or vice versa. In this sense the P defect is a phason. The existence of the P defect was first directly confirmed by STM observations at 6 K.⁸ At 80 K, the symmetric dimer regions can be regarded as a “sea” of these phasons imprisoned by the C defects.

At this stage, we return to the result of Fig. 1 and interpret the data in terms of the concept of the P defect in symmetric dimers. Structural models of the initial, the excited, and the final state around the target C defect are presented in Figs. 2(e), 2(f), and 2(g). By comparing the configuration of dimers of the perturbed dimer row in Figs. 2(e) and 2(f), we can see that, by perturbation, the C defect has been converted into an unidentified defect which is not a phase shifter. This means that a P defect has been created by the perturbation, which carries the phase shifter ingredient of the C defect. We suppose that the newly born P defect has migrated upward, and is the origin of the symmetric dimers observed there in the excited state. In the course of the dynamical relaxation, not only did the symmetric dimers convert into buckled dimers, but the $p(2\times 2)$ phase observed at the left side of the C defect also switched into a $c(4\times 2)$ configuration. Indeed, we assume that the existence of this $p(2\times 2)$ phase is the direct cause of the dynamical relaxation, because, at this temperature, the $c(4\times 2)$ phase is favored. The transition can be explained in two ways: (i) the P defect has migrated downward into the step edge, and associated with this migration, the $p(2\times 2)$ phase converted into a $c(4\times 2)$ phase; (ii) a new P defect was produced at the step edge and migrated upward, uniting with the P defect produced by perturbation. In both cases, the perturbed dimer row is left with no P defects, corresponding to the dissipation of the symmetric dimers in the final ground state.

When the weak interaction among the dimer rows is considered, it is surprising to find that the effect of perturbation extends to other dimer rows. In the excited state, symmetric dimers emerge not only in the perturbed dimer row but also in adjacent rows. This suggests that phasons have come into being even in the adjacent rows. At 80 K, it is reported that phasons in adjacent rows have a strong tendency to form pairs,⁹ which is explained, in first-order approximation, as a reduction of the total $p(2\times 2)$ area by this pairing. Experimental results of Fig. 1 imply that the artificially created phason has induced another phason in the adjacent row to form a pair with it. A new single counterpart single phason is created by this process because phasons form in pairs. We assume that this newly born single phason again induces another phason in the adjacent row. A chain reaction of these processes would induce a large-scale dynamical transition as was observed.

It should be noted that the remainder of the C defect was always a defect which is not a phase shifter. This suggests that the C defect is an unfavorable factor in a set of buckled dimers as was reported before.¹⁰ In other words, the C defect highly stresses the surrounding buckled dimers by pinning

down the buckled dimer domain and forces the surface into a metastable state. We believe that when the C defect is strongly perturbed, the pinning effect is released, resulting in the observed large-scale dynamical transition.

Since Figs. 1(a) and 1(d) are quite similar, one might conclude that the initial and new ground states are quite similar, but this is not correct. By comparing STM images of wider regions before and after perturbation (not shown), it became clear that a new symmetric dimer domain has emerged in the upper region which was once a wide buckled dimer domain. This means that the influence of the perturbation has extended a long distance. This example is not an exception. Frequently we observed a dynamical transition induced by perturbing a single C defect, in which thousands of dimers changed their configuration. An example is shown in Fig. 3. At the beginning, there exists a large symmetric dimer domain [colored red in Figs. 3(a) and 3(b)]. The C defect located at the boundary of the buckled symmetric dimer domain indicated by the arrow was perturbed as shown in Fig. 3(c). At the moment of destruction, the wide symmetric dimer domain converted into a buckled dimer domain. Numerous changes occurred and the final configuration became very different from the initial state as shown in Fig. 3(d), the large symmetric dimer domain has been replaced by a buckled dimer domain and a new symmetric domain has emerged in the lower part of the terrace.

We can regard the surface morphologies before and after perturbation as representing the equilibrium surface configuration with and without the C defect. Therefore comparing the two configurations will give a unique opportunity to study the influence of the C defects on the buckled dimers. The drastic difference between the two configurations indicates that the elastic stress produced by the C defect extends a long distance and that dimer configuration is determined by a detailed balance among many long-range forces produced by the surrounding defects.

In conclusion, we have combined the technique of atomic manipulation and the dynamic visualization STM and applied them to Si(100) at 80 K to study the dynamics of dimers. By perturbing the C defect, an avalanche type symmetric \rightleftharpoons buckled phase transition of dimers was observed.

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