Adatom Displacement Using the Scanning Tunneling Microscope

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Abstract:

Tunneling electrons in a scanning tunneling microscope were used to displace silicon (Si) adatoms on a Si(111) 7×7 surface at 78K. The displacement was observed to occur using both positive and negative bias voltages. Five topography levels of the displaced adatom were observed, each corresponding to a different configuration of Si adatoms in the half unit cell directly beneath the microscope tip.

Introduction:

The scanning tunneling microscope (STM) is a powerful tool for nanoscale characterization and manipulation of individual atoms on both metallic and semiconducting surfaces. The STM can accurately probe the atomic structure of various conductive surfaces [1]. The Si(111) 7×7 surface reconstruction was the first semiconductor surface imaged with atomic resolution by STM [2]. Atomic scale manipulation experiments have shown that specific Si adatoms on the bare Si(111) 7×7 surface can be reversibly laterally displaced under the influence of both tunneling and field emitted electrons [3]. Stipe et al. reported that the center silicon adatom in both the faulted half (FH) and unfaulted half (UFH) of the unit cell can be displaced to a neighboring metastable threefold site (T4 site) with a sample bias above +2.0 V. This phenomenon as been touted as the basis for a single atom switch [5].

Experimental Procedure:

In this paper, we report new findings on the adatom displacement phenomenon by observing the Si(111) 7×7 surface with low temperature STM. Unlike previous experiments, the displacement can be induced with both positive and negative voltage pulses applied with respect to the sample. Figure 1(A) shows an STM image of the Si(111) 7×7 surface at 78K. The dimer-adatom-stacking-fault (DAS) structure is visible, a single unit cell is highlighted, and the scan voltage of -1.0 V highlights the contrast between the FH and UFH unit cell. A schematic of the surface layer is shown in Figure 1(B). In the top adatom layer, there are six Si atoms in "corner" sites and six Si atoms in "center" sites, each of these atoms lies on a T4 site of the "rest atom" layer underneath the surface. Positive and negative voltage pulses above approximately +2.0 V or below -2.0 V cause a transfer of the center site adatom to a neighboring metastable T4 site, as shown in Figure 2. Stipe et al. studied this phenomenon and found that at temperatures below 175K, voltage pulses above +2.0 V induce a single adatom transfer or return in the half unit cell of the (7×7) structure, with the displacement probability in the FH being 100 times greater than the UFH. Furthermore, the transfer and return rate of the adatom depends on sample bias, tunneling current, temperature, and excitation is not localized beneath the STM tip. Our experiments on the Si (111) 7×7 surface were consistent with these observations, but with the exception that the adatom displacement could be induced by applying negative voltage pulses.

Experiments were performed in an ultrahigh vacuum STM with base pressure of approximately 5×10^{-9} Pa, operating at 78K. The samples used were n-type Si(111), phosphorus doped, with a resistance of 0.01 Ω cm. The surface was cleaned by flashing to a temperature of 1200K, followed by an annealing step to produce the 7×7 reconstruction. Electrochemically etched tungsten tips were used for imaging. Topographical images were typically scanned with a sample bias of ± 1.0 to 1.5 volts and 0.2 nA tunneling current.

The frequency of the adatom displacement was measured by positioning the STM tip above a selected center atom in the FH. The bias voltage was increased to a predetermined value, and the z position (tip height above surface) of the STM tip was measured as a function of time. This produces a frequency trace corresponding to the measured local density of electronic states (LDOS) directly underneath the tip. Figure 2 presents a series of z-height traces as a function of time when the bias voltage was increased to +2.0, 2.6, and 3.0 volts respectively. During the time of increased tip-sample bias, the z position of the tip fluctuates between several height states, each corresponding to a transfer of adatoms among metastable sites within the half unit-cell. Observation of the tip height during the voltage pulse reveals five distinct height steps, denoted by lines a, b, c, d, and e in Figure 3.

Previous experiments have analyzed the mechanics between only the two topographic states corresponding to a "single hop" or the z position of a center adatom in the "normal" position, and in the "vacancy" position [3]. However, we have

observed the underlying mechanics to be further complicated given the five possible z-height positions measured. As shown in Figure 4, these steps correspond to (a) the center adatom in its "normal" position, (b) an "adatom vacancy" underneath formed underneath the tip, (c) contrast enhancement due to a "single hop" of a neighboring center atom in the same half unit cell into an adjacent T4 site, (d) contrast enhancement due to a "double hop" of the other two center adatoms into the adjacent T4 sites, and (e) a "depressed adatom" where a decrease in topographic contrast is observed when an adatom vacancy is created in the adjacent UFH unit cell. It is worth noting that the local electronic structure and surface potential of the depressed adatom differ from those on a clean surface [4,6].

Results and Conclusions:

In summary, adatom displacement experiments using on the clean Si(111) 7×7 surface have been performed using the STM. These experiments proved that center adatom displacement in the faulted half unit cell is possible at both positive and negative sample bias voltages. Additionally, five distinct topographic states have been observed for bias voltages above + 2.0 V while the STM tip is placed directly above a center adatom in the faulted half unit cell. Future work will focus on a detailed understanding of the physical mechanism for the adatom displacement phenomenon and the resulting changes in the electronic structure of the Si(111) 7×7 surface.

Acknowledgements:

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References:

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[5] B. C. Stipe, M. A. Rezaei, and W. Ho, Science 279, 1907 (1998).

[6] An in-depth discussion on the electronic structure of the depressed adatom will be provided in a separate paper.

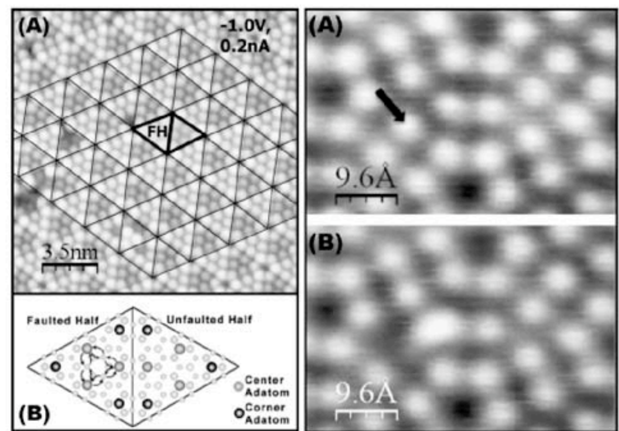

Figure 1, left: (a) STM image of Si (111) 7x7 surface at 78 K. (b) Schematic of DAS model of Si(111) 7x7 surface showing detail of center adatom displacement between neighboring T4 sites, adapted from Sagisaka et al.

Figure 2, right: (a) STM image of Si(111) at 78K showing 7x7 unit cell. The tip is positioned above the denoted adatom and the bias voltage increased until a change in z position is observed. (b) Rescan over same area shows the center adatom has been displaced to a neighboring metastable T4 site.

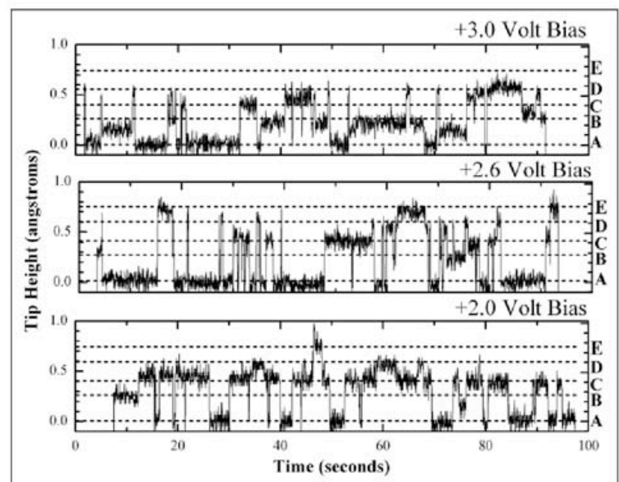

Figure 3, right, middle: Z-height trace of the STM tip height over a center adatom in the faulted half of a unit cell showing evidence of five topographical states. The levels correspond to: adatom vacancy (A), depressed adatom (B), normal position (C), single hop (D), and double hop (E).

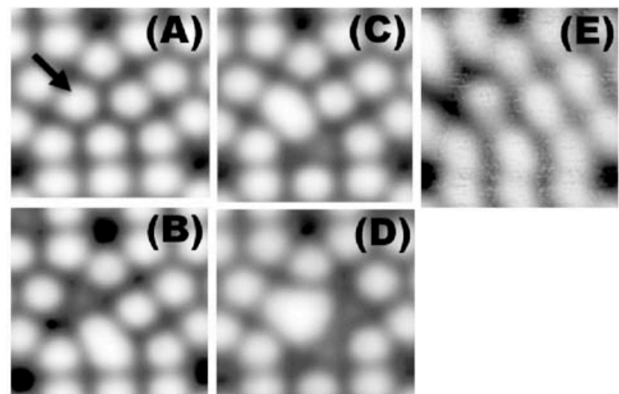

Figure 4, right, bottom: STM images of the five possible topographic states of the center atom in the faulted half unit cell denoted by black arrow. These correspond to: (a) normal position, (b) adatom vacancy, (c) single hop, (d) double hop, and (e) depressed adatom.