Scanning Tunneling Microscopy of Atomic-scale Dangling-bond Structures Fabricated on the Si(100)-2 × 1-H Surface

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Abstract

Various atomic-scale dangling-bond (DB) wires are fabricated and studied by scanning tunneling microscopy (STM) on a hydrogen-terminated Si(100)-2×1-H surface at low temperature. A single DB and a paired DB on a Si dimer, fabricated by extracting hydrogen atoms from the hydrogen terminated Si surface, are distinguished by STM. For the DB wire made of single DBs, we observe charge redistribution in the DB wire. The DB wires made of paired DBs show a buckling structure seen in a clean Si(100) -2×1 surface. The origins of these structural changes in the DB wires are discussed in this paper.

Introduction

The scanning tunneling microscope (STM) [1] has become useful for modifying surfaces on an atomic scale. It allows us to manipulate atoms one by one [2-4], and has opened up important new fields in both science and technology. This technique has also led us toward the development of atomic-scale electronic/photonic devices [5, 6]. In order to investigate these devices we need to design appropriate device structures and materials as well as improve atomic-scale fabrication techniques.

Si(100)-2×1 surfaces are widely used in semiconductor devices. These surfaces are characterized by Si dimers with one dangling bond (DB) remaining on each Si atom [7, 8]. Boland studied atomic-hydrogen adsorption on the Si(100)-2×1 surface and reported tunneling spectroscopy of the monohydride Si(100)-2×1-H surface [9, 10], which is one of the most promising substrates for fabricating atomic-scale structures through the extraction of hydrogen atoms by STM tunneling current [11, 12] and/or field effect [3, 4]. Hitosugi et al. measured the tunneling spectroscopy of atomic-scale DB wires [13]. Recently, Hashizume et al. reported on the formation of atomic-scale Ga structures on the hydrogen-terminated Si(100)-2×1-H surfaces using DB wires [14].

In this paper we present a STM study of atomic-scale DB structures on the hydrogen-terminated Si(100)-2×1 surface. A row of fabricated DBs forms a pseudo-one-dimensional atomic structure, which confines electrons. We found that spatial distribution of charge shows striking changes in the DB wires. The experimental results were analyzed based on recent first-principles calculations by Watanabe et al. [15, 16]. We think that this structure serves as an instructive example of an atomic-scale structure on a semiconducting surface, as it is the first step in fabricating useful atomic wires.

Experimental

An ultrahigh vacuum(UHV)low-temperature STM was used for sample preparation and STM operation. A Si(100) sample (As-doped, n-type, 7 to 13 mΩcm) was cut from a commercial wafer into a 2×14 mm² rectangle and was set on a sample holder made of tantalum. After being transferred into a UHV sample preparation chamber, an atomically clean Si(100)-2×1 surface was prepared by repeated resistive heating to 1260℃ at a pressure not exceeding 2×10^{-10} Torr. Hydrogen termination was achieved by exposing the clean surface to atomic-hydrogen flux, which was typically 3×10^{-2} ML/s for 5 min (1 ML here is defined as the number of Si atoms on a bulk-terminated ideal Si(100) surface: 6.78×10^{14} atoms/cm²), while the sample was kept at a temperature of approximately 390℃. The atomic hydrogen was obtained by decomposing hydrogen molecules with a heated tungsten filament 5

cm from the sample surface. The sample cleaning temperature was measured with an optical pyrometer and the hydrogen termination temperature was estimated by extrapolating a measured temperature-annealing-power curve using the Stefan-Boltzmann law of radiation.

A<111>oriented single-crystal tungsten wire was sharpened by electrochemical etching and used as the STM tip. The apex of the tip was cleaned and shaped by a field ion microscope (FIM) [17,18]. The base pressure of the STM chamber was 7×10^{-11} Torr during STM observation.

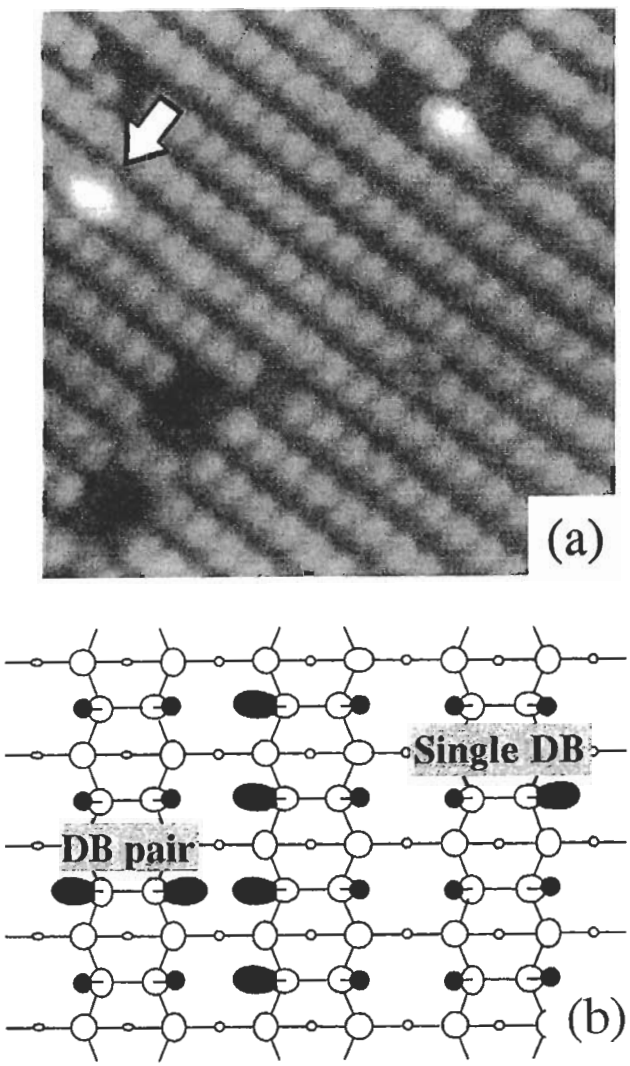

Fig.1 (a) Filled-state gray-scale STM image of the Si(100)-2×1-H surface (96K, 9 nm×9nm, sample bias voltage Vs = -2.0 V, tunneling current It =20 pA). (b) Schematics of a single DB, a DB pair and an ideal DB wire parallel to the dimer-row direction made of single DBs. The open circles, the small solid circles and the large solid circles represent silicon atoms, hydrogen atoms and DBs, respectively.

Results and Discussion

An atomically flat terrace made of Si dimer is observed in a filled-state STM image of the hydrogen-terminated Si(100)-2×1-H mono-hydride surface (Fig. 1(a)). The STM image was obtained at 96K. Cocoon shaped individual Si dimers are resolved in Fig. 1(a). Dimer rows are made of Si dimers and observed as bright lines running diagonally. The topographic maxima which appear as (white) protrusions in the gray-scale filled-state STM images are associated with DBs at the surface. The hydrogen terminated surface is observed lower than DBs, since the surface

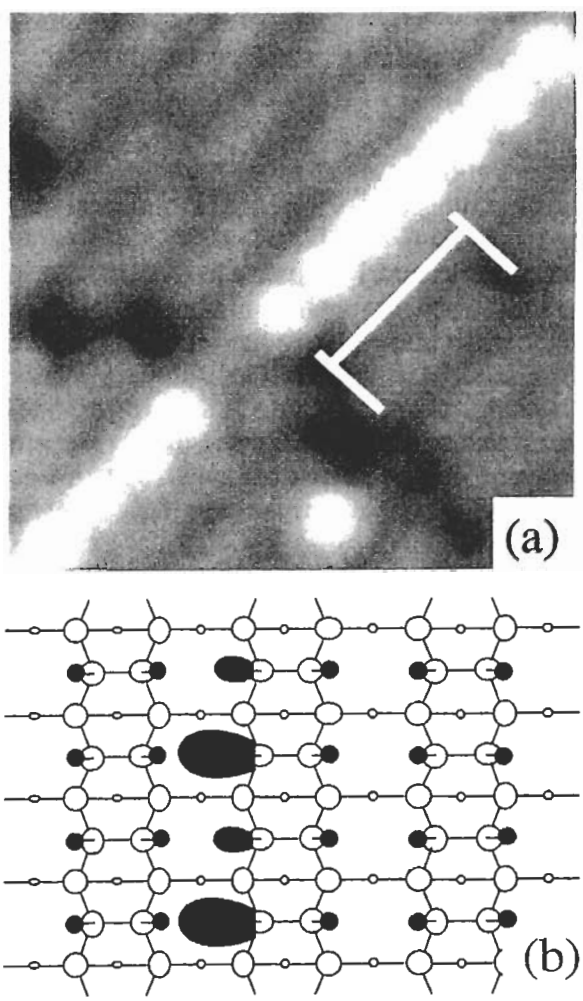

Fig.2 (a) A DB structure fabricated parallel to the dimer row on the Si(100)-2×1-H surface. This wire is made of only single DBs. (110K, 6 nm×6 nm, Vs = -2.0 V, It = 20 pA). (b) Schematics of a DB wire parallel to the dimer-row direction made of single DBs. Notice that DBs are large alternatively.

states of the DBs of Si dimers are passivated by hydrogen adsorption.

A defect with one hydrogen atom missing from a Si dimer is imaged off-center on a dimer row and an example is indicated by the small arrow in Fig. 1(a). We call this a single DB (a ball stick model is shown in Fig. 1(b)). Since a defect with two hydrogen atoms missing from a Si dimer, called a DB pair, is imaged at the center of the dimer row (not shown in (a), but shown in the ball stick model in Fig. 1(b)), we can easily distinguish the two. The dark spots on the surface correspond to missing Si dimers.

A line of DBs on the Si(100)-2×1-H surface was fabricated by applying a large bias and current [11-14]. Fig. 2(a) shows the filled state image of DB structures fabricated at 110K. The tip was addressed on top of the desired hydrogen atom, and moved parallel to the dimer row. We routinely obtained DB wires one- to two-dimers wide (0.8 to 1.6 nm) by moving the tip for 5 to 10 s while applying a sample voltage of Vs = +2.8 V and a tunneling current of It = 0.9 nA. The feedback was off during the tip movement, and the constant tip-sample distance was maintained using the gradient measured just before manipulation. We found that the required tunneling current and sample bias voltage to desorb hydrogen atoms at low temperature was much lower than the required current and voltage at room temperature. At room temperature, the typical sample voltage was Vs = +3.4 V and the tunneling current was It = 1.3 nA. For the bias polarity dependence of the hydrogen desorption, higher voltage and current were required to desorb at the negative sample bias voltage than at the positive sample bias voltage.

The DB wire shown in Fig. 2(a) is parallel to the dimer-row direction and is made of only single DBs. We found that DBs are seen alternately, as schematically shown in Fig. 2(b). This means that DBs are observed as different heights. After the hydrogen desorption, each DB should be equivalent, which means that every DB should be observed at equal heights by STM measurement. Nevertheless, the STM result clearly shows the height modulation of DBs in DB wire.

Figure 3 is an empty state image of the same DB wire. Lines have been introduced to clarify the difference in the lateral positions of the peak between the empty and filled states. In contrast with the filled state image, the dark (lower in height) DBs seen in the filled state image are brighter in the empty state image, and the bright DBs seen in the filled state image are darker in the empty state image. Considering this STM result, we conclude that a change in electronic structure, accompanying charge redistribution, has occurred in this DB wire.

To explain the origin of this charge redistribution, we analyzed experimental results based on recent first-principles calculations by Watanabe et al. [15, 16] Watanabe et al. predicted the existence of a surface-state band resulting from DBs when a DB wire made of single DBs is formed parallel to the dimer-row. They predicted that Peierls distortion stabilizes the system by 14 meV. From this distortion, energies of the DBs and charge distribution may vary, so that certain DBs may be seen at some tip-sample voltages but not at others.

What happens if all hydrogen atoms along a single Si dimer row are extracted? An STM image of the DB wire made of DB pairs is shown in Fig. 4. The part of the DB structure between the two arrows is the DB wire made of DB pairs and both ends are structures made of single DBs, which were discussed previously. We can clearly see the zigzagged buckling structure typically seen on clean Si(100)2×1 surfaces. The buckled dimers are only stabilized near the defects on the clean Si(100)-2×1 surface. In the case of the DB wire in Fig. 4, the buckling is stabilized either by the one-dimensional characteristics of the wire structure (Peierls distortion) or by the side effects.

Detailed theoretical and experimental investigations on these effects are presently under way.

Summary

In summary, we fabricated atomic-scale DB wires by extracting individual hydrogen atoms from the hydrogen-terminated Si(100)-2×1-H surface at around 100K. Charge redistribution was seen for the DB wires made of single DBs. We compared the results with the first-principles calculations and concluded that the origin of this redistribution is Peierls distortion. For the DB wire made of DB pairs, a buckling structure was observed. We believe that the DB structures on the hydrogen-terminated Si surface provide us with a unique and a stimulating system for the study of

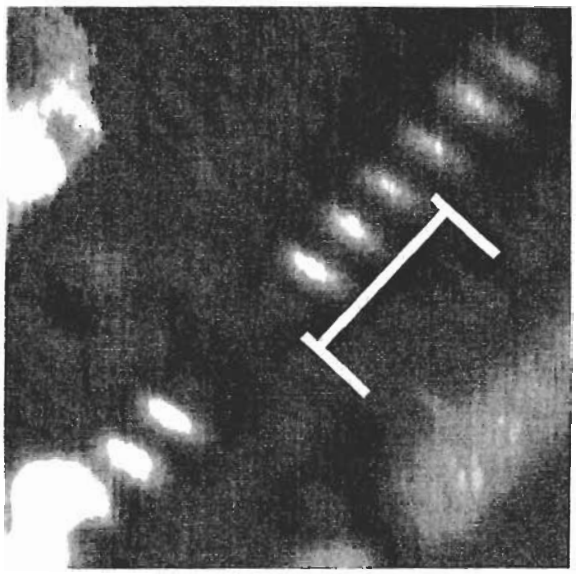

Fig.3 (a) Empty-state STM image of DB wire shown in Fig. 2(a). (6 nm×6nm, Vs =+2.0 V, It = 20 pA). White line is to compare the peak shift with filled-state image.

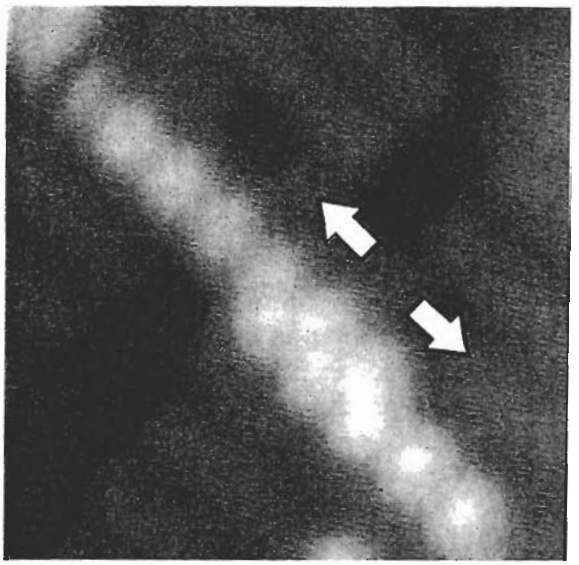

Fig.4 (a) Filled-state STM image of a DB wire (5 nm×5 nm, Vs = -2.0 V, It = 20 pA). The part of the DB wire indicated by arrow is made of DB pairs only. The buckled structure is clearly seen.

pseudo-one-dimensional atomic-scale structures.

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