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Development of an In-Situ Method of Fabricating Artificial Atom Structures on the Si(100) Surface

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We have investigated adsorption of Ga on the hydrogen terminated Si(100)-2 $\times$ 1-H surface using scanning tunneling microscopy (STM). Thermally deposited Ga atoms preferentially adsorb on the hydrogen-missing dangling bonds. We are able to desorb hydrogen atoms by STM current to fabricate atomic-scale dangling-bond wires and thermally deposit Ga atoms on the dangling-bond wires to fabricate atomic-scale Ga wires on the Si surface.

1. Introduction

Scanning-tunneling-microscope (STM)[1] and its use for atom manipulation[2] has opened up a new field in basic science and technology. In 1960, Feynman proposed an idea of forming switching devices on the atomic and molecular scale[3] well before the invention of STM. More recently, a nanoscale device made of atom wires and a switching atom, Atom Relay Transistor (ART), has been proposed.[4]

The hydrogen terminated Si(100)-2 $\times$ 1-H surface has been systematically studied by STM and the 2 $\times$ 1-H monohydride surface structure is well understood.[5] This surface is one of the promising substrates for atomic-scale structures and nanoscale devices because of the following properties: (a) Hydrogen atoms on the surface can be desorbed by using the tunneling current of the STM and nanoscale dangling bond patterning has been demonstrated.[6] (b) An atomically flat surface is routinely obtained. (c) The bulk conductivity can be reduced enough for characterizing physical properties (conductivity, for instance) of the atomic structures by either using a low dopant level or by reducing the temperature of the sample. (d) Reactivity to some of the metal atoms is low enough and the surface mobility of those metal atoms is expected to be high.[7] Adsorption of Ga on the clean Si(100)-2 $\times$ 1 surface was studied by STM and formation of the Ga dimer rows on the surface was reported after annealing the surface at 750K.[8,9]

We report on the STM observation of the Ga atoms thermally deposited on the hydrogen terminated Si(100)-2 $\times$ 1-H surface. We show that the Ga atoms preferentially adsorb on the dangling bonds left on the surface as missing-hydrogen defects. This selectivity is used to demonstrate a novel method of fabricating atomic-scale Ga wires on the Si(100) surface by adsorbing Ga atoms on to the dangling bond wire.

2. Experimental

Silicon samples were cut from a commercial Si(100) wafer (n type, 0.007-0.013 Ω·cm) into 2 $\times$ 14-mm^2 rectangles and were set on a sample holder made of tantalum. After introducing the samples into the UHV of the preparation chamber, a series of resistive heatings up to 1260°C following the overnight outgassing at 700°C was used to obtain the clean Si(100)-2 $\times$ 1 surface, which was checked by STM observation.

In order to obtain the hydrogen terminated Si(100)-2 $\times$ 1-H surface, the clean surface was exposed to atomic hydrogen flux of typically 3×10^{-2} ML/s (1 ML here is referred to as the number of the Si atoms on the bulk-terminated ideal Si(100) surface; 6.78×10^{14} atoms/cm^2) for 10 min while the sample was kept at approximately 350-400°C.[6] A Ga dispenser made of tungsten filament and a small amount of Ga metal was placed 2 cm away from the sample and heated to 600-650°C in order to deposit Ga on the sample.

We used scanning tips electrochemically etched from $\langle 111 \rangle$ oriented single crystal W wires. Each tip apex was cleaned and shaped into hemisphere using field ion microscope (FIM)[11,12] *in situ* in the preparation chamber. We also have used sharp needle structures on the sample surface, which were made by applying ramped voltages of typically 10.0 V while keeping the tunneling current constant, to counter image the scanning tip with an atomic resolution (Needle Formation and Tip Imaging = NFTI method).[13] The STM images presented here were taken at sample bias voltage V_s of -3.0-+3.0 V and constant tunneling current I_t of 20-100 pA.

3. Results and Discussion

Figure 1 describes a method of connecting atomic structures to the bulk electrodes in order to measure the property of the atom structures and evaluate the performance of the atomic devices. We have used micron order metal mask and have formed metal wires as well as bonding pads on the Si(100)-2x1-H surface by thermally evaporating Ti *in-situ* (Fig. 1(a)). It is known that Ti has a large affinity to Si and other metal atoms, and it is used for a glue material. We have found that Ti atoms do not migrate on the hydrogen terminated Si surface and adsorb randomly and stably on the surface, thus the metal patterns are formed without disturbing the hydrogen-terminated area masked by the metal mask.

Among the metal elements, Ga is the one which shows surface adsorption even after annealing.[9] We, thus, have chosen Ga for atomic-scale metal-wire fabrication on the silicon surface. In Fig. 2(a), we observe several dangling bonds on the hydrogen-terminated Si(100)-2 $\times$ 1-H surface imaged as small protrusions surrounded by moats. This pattern can be understood as a Friedel oscillation of the density of states resulted from the charge localized at the dangling bond, similar to the case of Si dopants near the GaAs(110) surface recently reported by van der Wielen *et al.*[14] It is interesting to note that a dangling bond changed its position from one of the Si of a dimer to the other Si during STM scanning.[15] Also, several

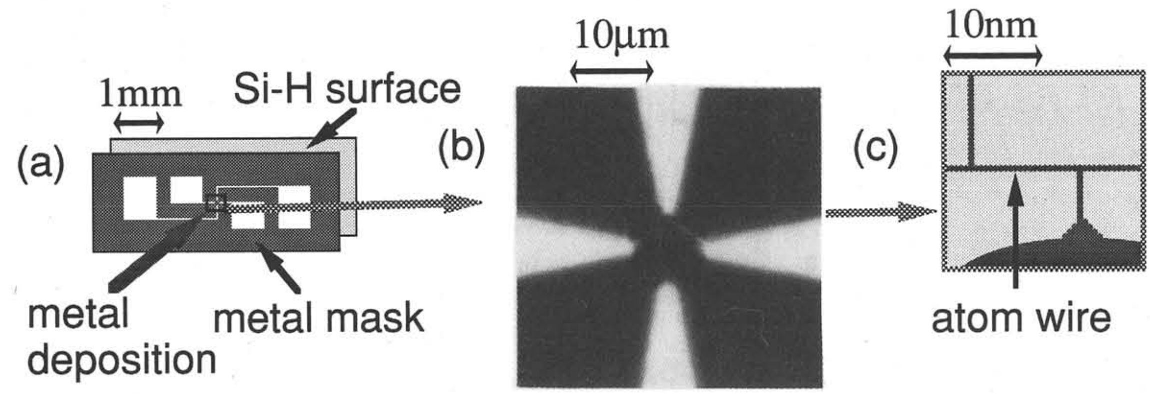

Fig. 1. Schematics describing the method of *in-situ* formation of bulk connection to atom structures. (a) Schematic of the metal deposition process on the Si(100)-2x1-H surface through a metal mask, (b) micrograph of the enlarged center part of the metal mask and (c) schematic of the further enlarged center part with fabricated atom wire.

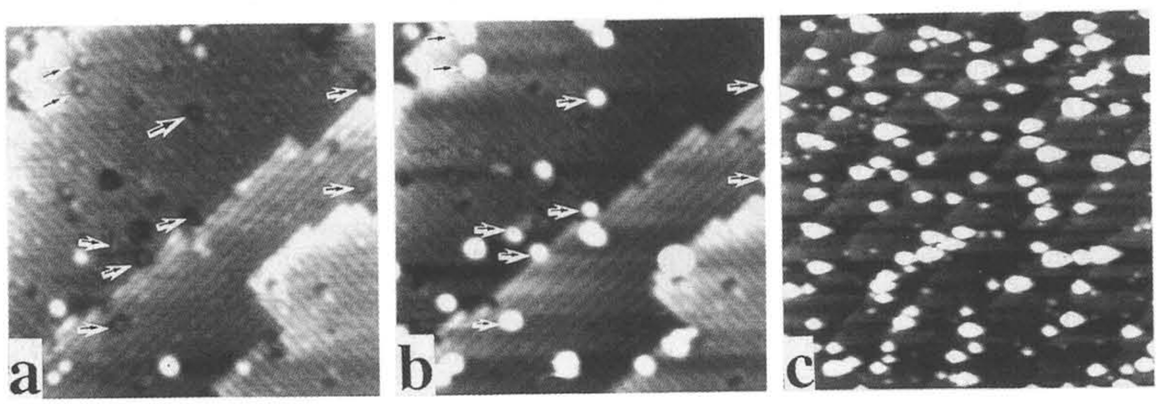

Fig. 2. STM images showing adsorption of Ga on the hydrogen-terminated Si(100)–2 × 1–H surface. (a) Before adsorption. Individual dangling bond is imaged as a small protrusion surrounded by a moat ring. Also, several impurity adsorption are imaged as protrusions (27 nm × 27 nm, V_s = +1.8 V, I_t = 20 pA). (b) Same area as (a) with 0.005ML of Ga. Ga atoms adsorb preferentially on the dangling bonds (shown by arrows in (a) and (b)). Also, the impurity adsorbates are imaged larger in (b) indicating adsorption of Ga on them. (c) Large scale STM images after 2ML of Ga deposition showing cluster formation of Ga (120 nm × 120 nm, V_s = -2.0 V, I_t = 20 pA).

impurity adsorbates are imaged as round protrusions.

Figure 2(b) shows the same area after thermally depositing 0.005ML of Ga. It is clearly observed that Ga atoms preferentially adsorb on the dangling bonds (shown by arrows in (a) and (b)). We notice that there are different heights of the protrusions, indicating clustering of Ga atoms on the dangling bond position. Also, some impurity adsorbates are imaged larger in (b) indicating adsorption of Ga atoms. Further deposition of Ga results in the further growth of Ga clusters, which is shown in Fig. 2(c). The results clearly indicate a high mobility of Ga atoms on the hydrogen-terminated Si surface, in contrast to the Al adsorption.[16)] Our preliminary first-principal calculation has shown the barrier height of Ga atoms for surface migration to be approximately 0.3 eV.[7)] We do not observe preferential adsorption at the step edges nor missing-dimer defects, which indicates hydrogen passivation at the step edges and missing-dimer defects.

Groups at Illinois University have shown that the hydrogen atoms on this surface can be desorbed by electron exposure from the STM tip.[6)] We have fabricated dangling bond wires using the same method and have thermally deposited Ga atoms in order to demonstrate a method of fabricating atomic-scale metal wires on the silicon surface. The results are summarized in Fig. 3. In the left part of Fig. 3, we show ball stick models of the method we propose in this letter. The method consists of three steps: (1) Prepare the hydrogen-terminated Si(100)–2×1–H monohydride surface. (2) Fabricate dangling bond wire using STM current. Typically, sample bias of V_s = +3.8–+4.0 V, tunneling current of I_t = 750–900 pA, and electron dose of typically 30 C/cm are used in order to fabricate dangling bond wires with less than one to two dimer width. (3) Thermally deposit Ga to cover the dangling bond wire. Examples of STM images corresponding to three steps are shown in Figs. 3(a), (b) and (c). The dangling bond wire shown in Fig. 3(b) is

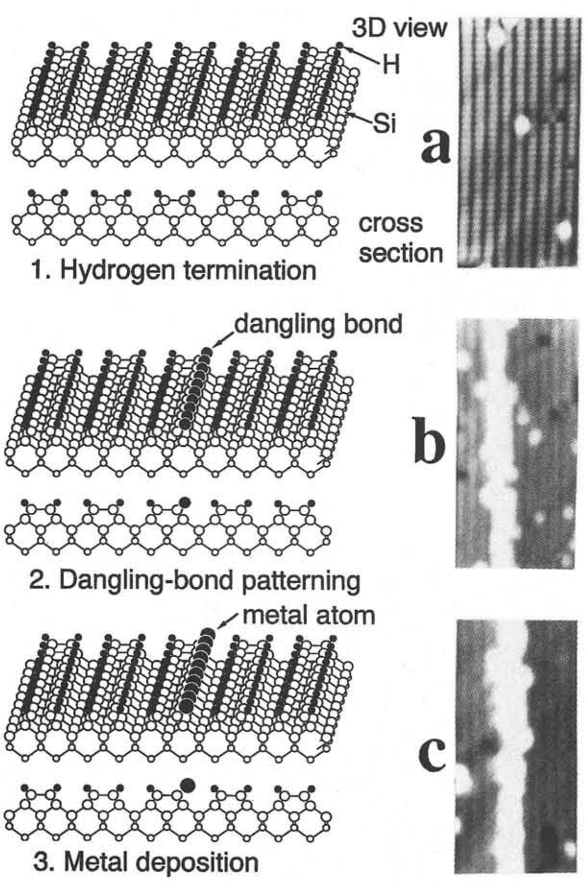

Fig. 3. Ball stick models and corresponding STM images (7 nm $\times$ 15 nm, V_s = -2.0 V, I_t = 20 pA) showing a method of fabricating a atomic metal wire on the silicon surface. (1) and (a) Hydrogen termination of the surface, (2) and (b) dangling bond wire fabrication by STM current, and (3) and (c) thermal deposition of Ga atoms on the dangling bond wire. Note that STM images are from different sample areas.

one or two Si dimer wide (0.8–1.6 nm). It is shown by theoretical calculation that the dangling bond wire itself may have electron conduction.[17] Figure 3(c) shows another example of dangling bond wire after Ga deposition. Since the Ga atoms preferentially adsorb on the dangling bonds, an atomic scale structures of Ga atoms on the silicon surface has been realized. However, the width of the Ga wire is not constant, indicating that a part of the wire has the width of two or more Ga atoms. Also some part of the wire is missing Ga atoms. Individual dangling bond manipulation and/or individual Ga atom manipulation are under investigation in order to reshape the Ga wire. Preliminary spectroscopy (STS) measurement have shown that a part of the Ga wire has metallic character (non zero density of states at Fermi level). This indicates that some Ga atoms have adsorption arrangement where one Ga atom adsorbs on the surface bonding to two dangling bonds. Detailed theoretical and experimental investigation will be published elesewhere.[18]

4. Conclusion

In conclusion, scanning tunneling microscopy has been used to investigate adsorption of thermally deposited Ga on the hydrogen-terminated Si(100)–2×1–H surface. The Ga atoms on the monohydride phase are mobile and stable adsorption of Ga is observed preferentially on the dangling bonds and on the impurity adsorbates. We have demonstrated a method of fabricating atomic-scale Ga wires on the silicon surface using dangling bond patterning by STM current and thermal deposition of Ga onto the dangling bond patterns.

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