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Formation of Bi-Dimer Linear Chains on a Si(100) Surface Studied by STM

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We report results of a scanning-tunneling-microscopy investigation of the bismuth-induced structures on Si(100) surfaces. Bismuth atoms, adsorbed on the surface at 480°C, form long linear belts on the Si terraces. Each belt consists of two chains of bismuth-dimers, and stretches perpendicular to the Si-dimer rows. This is a self-assembled structure formed by an enhanced migration of atoms along the chains. Atomic hydrogen adsorbs on the bismuth-induced structure to cut chains of bismuth-dimers. In the case of heavier depositions of bismuth (~3 ML) at 480°C, long linear structures with an arrangement of bismuth chains similar to the belt on the Si terraces are formed on the bismuth terraces. This indicates that the bismuth atoms deposited on the surface are substituted for Si atoms on the terraces.
Key words: Bismuth, Nanowire, Si(100) surface, STM, Surface structure

1. INTRODUCTION

The fabrication of atomic-scale structures using scanning tunneling microscopy (STM) has attracted much attention from a viewpoint of making atomic-scale devices on the semiconductor surface. Hashizume et al. succeeded in fabricating Ga atom wires on a Si(100) surface [1]. In their method of making one-dimensional structures, they desorbed hydrogen atoms on a mono-hydride Si(100) surface by the STM tip to fabricate atomic-scale dangling-bond wires. When Ga atoms were deposited on the surface, they were preferentially adsorbed on the dangling-bond wires. However, such a technique as the fabrication using STM tips may not be suitable for making a lot of atomic-scale devices on the substrate.

We investigated the atomic structure of Bi films on the Si(100) surface by STM and low-energy electron diffraction (LEED), and found for the first time a formation of long linear chains consisting of Bi-dimers [2,3]. Soukiassian et al. reported a formation of Si wires on SiC(100) surfaces [4]. These one-dimensional structures have been self-assembled and the technique is not relevant to the above-mentioned fabrication.

There seem to exist some differences between the former Bi wires and the latter Si wires. The Bi wires are involved in the substrate terrace in contrast to the Si wires formed on top of the SiC surface. Long linear structures are also formed on the Bi-covered terrace. Bi atoms tend to induce selectively one-dimensional reactions on the Si(100) surface. In the present paper, we report experimental results by STM regarding the reaction of Bi atoms at the Si(100) surface and discuss a unique role of Bi atoms in the process of self-assembled surface re-structuring.

2. EXPERIMENTAL

The experiment was carried out in an ultra-high vacuum chamber under a base pressure of 1×10^{-8} Pa. The chamber was equipped with a commercial STM (JEOL JSTM-4500XT), a rear-view LEED and sample-preparation facilities including heating, Bi deposition and hydrogen adsorption. The STM observations were performed at room temperature. Tips for STM were made from tungsten wires (0.3 mm in diameter), which were etched using 2M NaOH in a Pt loop electrode in DC mode. The tips were baked out before being used for scanning.

The Si(100) samples of $1\times7\times0.38$ mm^3 were cut from a *p*-type wafer and cleaned in situ by direct-current heating at 900°C followed by brief flashing at 1200°C. After the cleaning procedure, well-developed STM images and (2×1) LEED patterns were observed. The sample temperature was measured in the range of 250~1000°C with an optical pyrometer. Pure Bi (99.999 % purity) was deposited from a crucible made of thin Ta foil. The rate of Bi deposition was approximately 1 ML/min, where 1 ML was defined as the Si density on the ideal (100) plane.

Atomic hydrogen was produced by the decomposition of molecular hydrogen with a tungsten filament at 1700°C which was placed at 20 cm away from the sample. The flux of atomic hydrogen was not measured, but the background H_2 pressure was recorded by a B-A gauge.

3. RESULTS AND DISCUSSION

Figure 1(a) shows a filled-state STM image taken from a clean Si(100)(2 × 1) surface. We can distinguish clearly each Si-dimer row. There exist some vacancy-defects on the terrace. We performed the experiments of Bi deposition on the only Si(100) surfaces where a low defect density was checked beforehand. Therefore, the results described below could not be directly caused by the initial Si defects.

Figure 1(b) shows a filled-state STM image taken from a surface with Bi deposited for 120 s at the

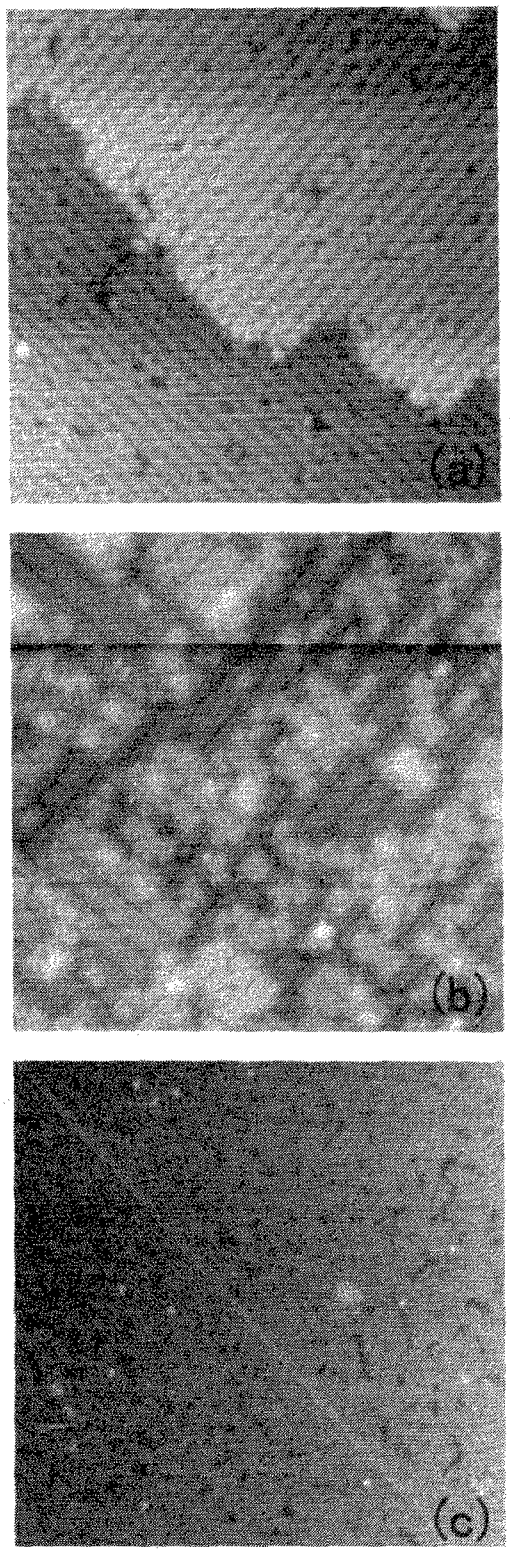

Fig. 1. STM images of Bi/Si(100) surfaces. (a) Clean surface. The image was taken at sample bias V_s = -1.6 V, at tunneling current I = 0.3 nA and from the area $S = 25 \times 25$ nm^2. (b) After Bi deposition for 120 s at 400°C. There is a noise spike in the figure. V_s = -2.0 V, I = 0.3 nA, $S = 35 \times 35$ nm^2. (c) After Bi deposition for 120 s at room temperature followed by annealing at 480°C. V_s = -2.2 V, I = 0.3 nA, $S = 70 \times 70$ nm^2.

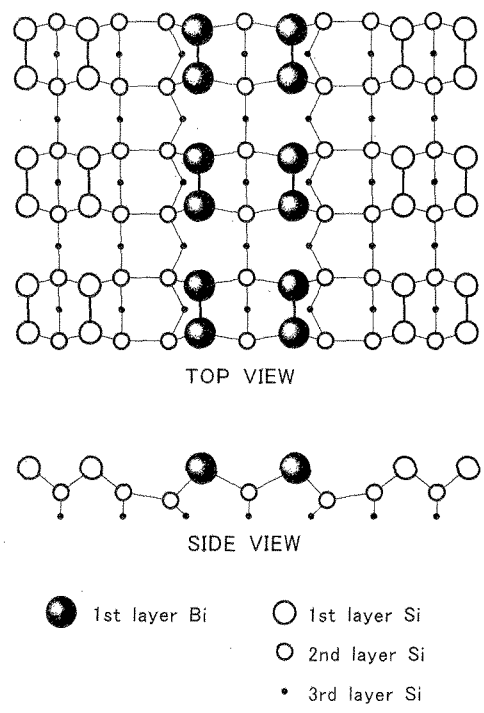

Fig. 2. A ball and stick model of a linear chain of Bi-dimers on the Si(100) surface. The Bi chains stretch perpendicular to the Si-dimer rows.

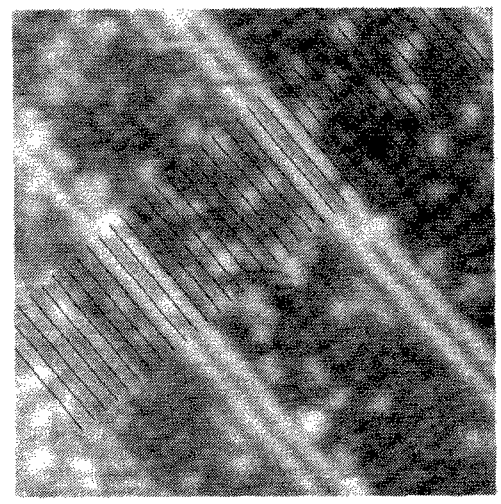

Fig. 3. An STM image taken after hydrogen adsorption (H_2: 18 L) on the Si(100) surface with linear chains of Bi-dimers. The Bi chains have been cut by the adsorption of atomic hydrogen. V_s = -2.0 V, I = 0.3 nA, $S = 12 \times 12$ nm^2.

substrate temperature of 400°C. In the Bi deposition at such high temperatures, adsorption and desorption of Bi atoms compete at the surface [5,6]. We cannot, therefore, know Bi coverages quantitatively in the present stage. The height difference between the brightest and the darkest regions in Fig. 1(b), corresponding to three atomic layers, is measured to be about 0.4 nm. This image corresponds to a surface with $(2\times n)$ $(n\sim 6)$ Bi layers, by referring to our previous observation [2]. The Bi atoms, adsorbed on the Si(100) surface at 400°C, form a film of diamond-like structure with a thickness of more than two layers, under the influence of substrate structure. In the filled-state STM mode, the structure of Bi layers is imaged with a $(1\times n)$ periodicity instead of $(2\times n)$. There are few defects on the terrace of the Bi layers.

We show in Fig. 1(c) an STM image after Bi deposition for 120 s at room temperature followed by annealing at 480°C. There appears the terrace with a straight belt and some vacancy defects. The belt is imaged as consisting of adjoining two bright lines. According to our previous studies [2,3] and to the observation by Miki et al. [7], each bright line consists of Bi-dimer chain, where the direction of Bi dimerization is parallel to the Bi-dimer chain. The structure model of the Bi-dimer linear chains is shown in Fig. 2. In this model, the Bi-dimer chains are involved in the Si(100) topmost layer. The direction along the Bi chains is perpendicular to the direction of the Si-dimer rows.

Figure 3 shows a filled-state STM image taken after hydrogen adsorption on the Si(100) surface with Bi-dimer linear chains at room temperature. We can see well-resolved dimer units on the Si terrace. This corresponds to a region with the mono-hydride phase, by comparing with a work by Boland [8]. We observed that the Bi chains were cut by the adsorption of atomic hydrogen. When hydrogen atoms adsorb on the Bi-deposited Si(111) surfaces, Bi atoms are displaced from their original positions [9]. The decomposition of the linear Bi chains is attributed to the breaking of Bi-Si bonds on the attack of atomic hydrogen.

In order to analyze precisely the structure of Bi chains, we depicted parallel black lines on the position of the Si atoms in the first layer shown in Fig. 3. The distance between two adjacent lines is 0.38 nm, which agrees with the lattice constant of the Si(100) surface. We found the two Bi-dimers are substituted for four Si-dimers on the terrace. Miki et al. proposed the model of Bi chains [7], where the two Bi-dimers are substituted for three Si-dimers. The present STM results contradict to their model.

From an X-ray photoelectron diffraction measurement, the separation of two Bi-dimer chains in the same belt is estimated to be larger than the unit separation 0.38 nm [10]. We propose the model shown in Fig. 2 by taking this result into account.

Figure 4 shows an STM image taken after Bi deposition for 180 s at 480°C. We can see long linear structures and rectangular-shaped islands in the figure. These islands should consist of Bi-dimers, by judging from this image with unresolved dimer rows and by recalling the unresolved Bi-dimer rows in the

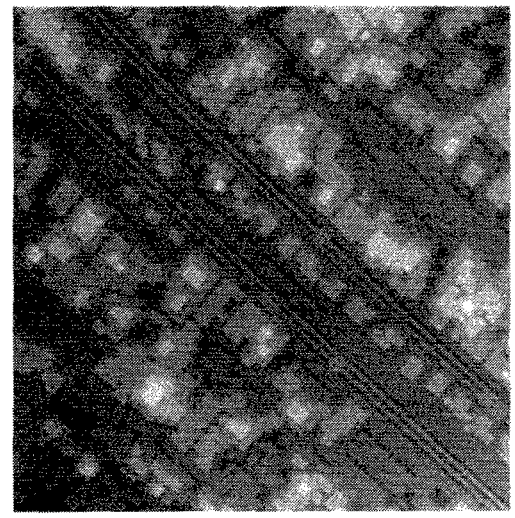

Fig. 4. An STM image taken after Bi deposition for 180 s at 480°C. There appear linear chain structures in the Bi-covered terrace. V_s = -2.2 V, I = 0.3 nA, S = 40 $\times$40 nm^2.

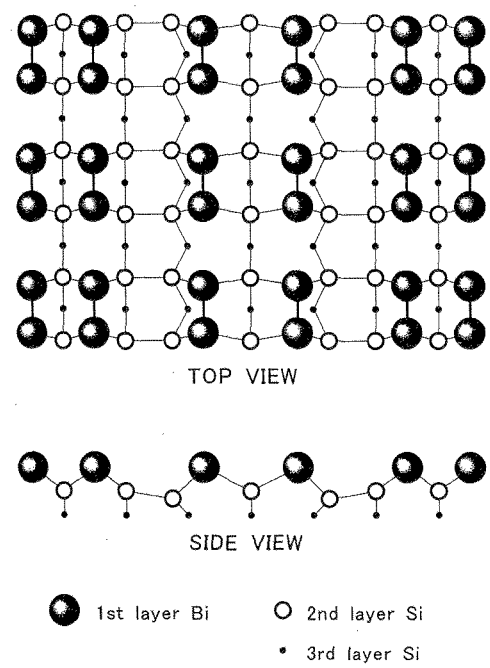

Fig. 5. A ball and stick model of a linear chain of Bi-dimers in the Bi terrace.

filled-state STM images (Fig. 1(b)) in contrast to the resolved Si-dimer rows (Fig. 1(a)). In our previous study [3], we observed a structure with Bi-dimer linear chains on the Si terraces after Bi deposition for 120 s at 480°C. The STM image shown in Fig. 4 corresponds to the surface obtained after Bi deposition on the surface with Bi chains. We speculate Bi atoms deposited on the surface are substituted for Si atoms on the terraces of the substrate. The structural model of the surface is shown in Fig. 5.

We can see a group of four-bright protrusions on the Bi-dimer linear chains in Fig. 4. This has been observed rather frequently on the Bi chains. We suggest that it is a key of understanding enhanced migration of the atoms along the Bi chains. A detailed mechanism will be discussed elsewhere [11].

4. CONCLUSION

The STM investigation revealed the formation of new surface structures induced by Bi adsorbates at the Si(100) surface. Long linear chains of Bi-dimers are formed on the Si(100) surfaces and even on the Bi-covered surface by Bi deposition. These phenomena are caused by self-assembling of adsorbates. We have shown the unique character that Bi atoms possess at the Si(100) surface. It would be essential to understand such characters of individual atoms in order to apply those to creating nano-scale electronic devices.

5. ACKNOWLEDGEMENTS

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