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Si atom wire growth for quantum information processing

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Abstract

We report on the experimental realization of straight atomic wires of Si on a vicinal Si(111) substrate. Atomic-kink-free steps with an identical structure are formed on the clean substrate by prolonged annealing around 800 °C. The direction of the annealing DC current that is effective to extend the straight step region is the so-called *kink-up* direction. Furthermore, the step-edge structure obtained is serendipitously suitable for the exclusive growth of the single adatom wires by molecular beam epitaxy. An isotopic version of such a structure is expected to be the most basic building block for a silicon-based quantum computer.

Keywords: Silicon; Nanostructures; Scanning tunnelling microscopy; Molecular beam epitaxy

1. Introduction

In recent years, quantum information processing has been extensively studied alongside the development of nanoscience and nanotechnology. Taking advantage of the fact that natural silicon (^{nat}Si) is composed of three stable isotopes having nuclear spins of 0 (^{28}Si and ^{30}Si) and 1/2 (^{29}Si), the present group has proposed a Si nuclear-spin quantum computer [1,2]. If we regard the up and down states of the ^{29}Si nuclear spin as quantum 1-bit states, then ^{29}Si isotope precisely positioned in a ^{28}Si matrix becomes an attractive candidate for the ultimately small bit-carrier. An overview and the operating principles of this quantum computer [1,2] are presented in Fig. 1. There are several promising paths to achieving the three fundamental quantum-computing procedures, i.e., *initialization*, *manipulation* and *readout* of the qubits, as described in Fig. 1. However, successful fabrication of perfectly straight atomic wires of ^{29}Si in a matrix of ^{28}Si has not been reported to date. Thus, we have proposed a self-assembly procedure [1], in which a regular array of straight steps on a ^{28}Si(111) substrate is used as a template for linear chains of ^{29}Si atoms, as shown in Fig. 2.

Because arrangement of the self-assembled ^{29}Si atoms depends on the step-edge structures of the ^{28}Si substrate, they have to be atomically well-defined. Viernow et al. and Lin et al. have achieved a parallel array of straight steps with very low density (0.12 μm^{-1}) of 7×7 unit-cell wide kinks on a vicinal ^{nat}Si(111) surface, by a thermal procedure in ultra-high vacuum for a wafer with $\sim 1°$ miscut towards the $[\bar{1}\bar{1}2]$ direction [3,4].[1] Although the straight-edge substrates prepared in this manner have proven useful as templates for many nanostructures [5], our goal to form atomically straight single wires of ^{29}Si on ^{28}Si poses stricter requirements: Defective kinks narrower than the 7×7 unit-cell width must be completely eliminated from the step edges and the lattice displacements across the steps must be the same for all the steps. Therefore, we report here on the fabrication of subnanometer wide ^{nat}Si wires—single lines of adatoms—as well as a new thermal procedure to prepare atomic-kink-free straight step edges of an identical atomic structure, which is ideal as a template for the atomic wires.

2. Experimental

In the present study, ^{nat}Si was used in place of isotope-enriched Si for both the substrate and the molecular beam epitaxy (MBE) source. A commercially available (111) wafer of ^{nat}Si (doped with boron) was polished to obtain a substrate with 1° miscut towards the direction within 3° from $[\bar{1}\bar{1}2]$. Thermal treatment of this substrate and homoepitaxial growth

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[1] In contrast to the $[\bar{1}\bar{1}2]$-oriented steps, $[11\bar{2}]$-oriented steps tend to form step bunches so that regular arrays of single bilayer steps cannot be formed.

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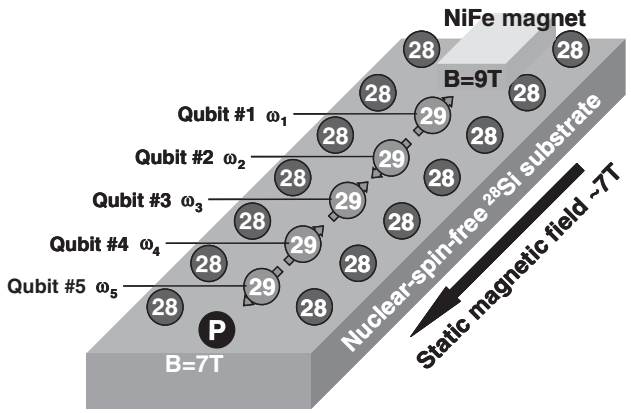

Fig. 1. Overview of the all-Si nuclear-spin quantum computer structure. An atomic chain of ^{29}Si qubits is arranged in a matrix of ^{28}Si. The entire structure is placed in a static magnetic field of ~7 T. A NiFe strip with saturation field of ~2 T is positioned at one end of the ^{29}Si qubit chain. This strip serves (1) as a source of polarized electrons for nuclear spin polarization (*initialization*) through electron-nuclear spin flip scattering and (2) as a local field gradient source giving each qubit a different nuclear-magnetic-resonance (NMR) frequency to allow selective *manipulation* of the qubits. The magnetic field B (9 T) at the edge of the strip must decay to the external one (7 T) in a very short distance along the qubit chain in order to assign a specific NMR frequency ω_i to the ith qubit. *Readout* can be performed either directly by magnetic resonance force microscopy (MRFM) [12] or indirectly via electron spin resonance of a phosphorus donor [13,14] placed at the other end of the qubit chain.

on it were performed in an ultrahigh vacuum (UHV, $<7\times10^{-9}$ Pa) chamber equipped mainly with a scanning tunnelling microscope (STM; Omicron STM-1) and an MBE system. The substrate was heated resistively by passing DC current parallel to steps. After being quenched to room temperature (RT) from 1260 °C flash cleaning, the surface consisted of a number of kinks at the step edges because of a small azimuthal deviation of the miscut direction. In order to reduce the number of kinks and extend the regions of the straight step edges, we applied a thermal procedure modified from that reported previously [3,4]. The key factors in our thermal procedure were prolonged annealing around 800 °C followed by slow cool-down to room temperature and the direction of the heating DC current along the step edges. After this procedure, atomically straight step edges were obtained. Then, ^{nat}Si was deposited from an effusion cell at 1150 °C by MBE on this substrate held at 400 °C to form atomic wires of Si along the well-defined

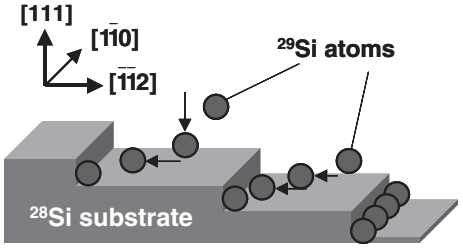

Fig. 2. Fabrication scheme for single straight ^{29}Si wires on a ^{28}Si substrate. A ^{28}Si substrate with a regular array of straight step edges is prepared by a thermal treatment of a vicinal Si(111) substrate. ^{29}Si atoms deposited by MBE in UHV on this substrate at an elevated temperature migrate to the nearest step edges to form atomically straight single ^{29}Si wires in step-flow growth.

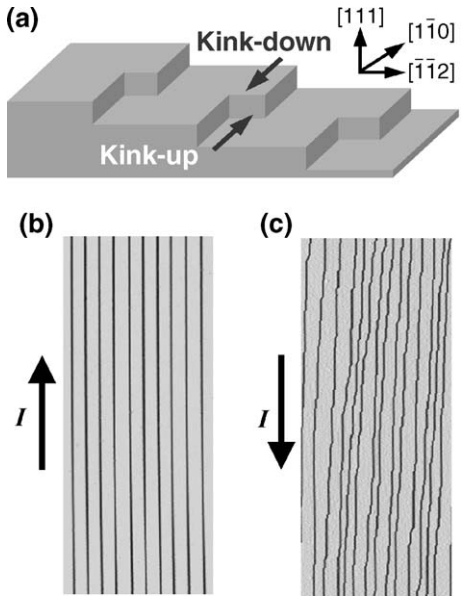

Fig. 3. Step straightness dependent on the heating DC current direction parallel to the steps. Illustration of the two possible directions of the DC current, *kink-up* and *kink-down*. (b) and (c) are STM images after the prolonged annealing at 800 °C by DC current in the (b) *kink-up* and (c) *kink-down* directions, respectively, indicated by the arrows labeled *I*. The derivative of the topography is shown to enhance the steps. Each dark line is a single step descending from left to the right. The area and the sample bias voltage are respectively 400 nm × 160 nm and +1.5 V for both images.

straight step edges. STM images of the surfaces were obtained at RT. The surface temperature was measured with an infrared pyrometer calibrated to read 860 °C (T_c) at the 1 × 1-to-7 × 7 surface phase transition, which was observed by reflection high-energy electron diffraction (RHEED). The homoepitaxial growth rate was measured both from intensity oscillations of specular spot in RHEED and by STM.

3. Results and discussion

After cleaning at 1260 °C, the substrate was annealed around 800 °C for 10 h and subsequently cooled slowly (over

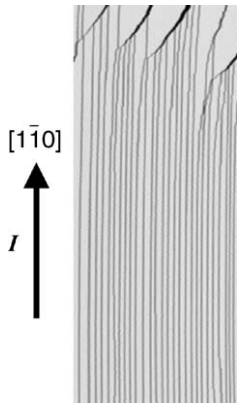

Fig. 4. STM image of the bunched kinks outside the straight steps region after prolonged annealing at 800 °C with the *kink-up* DC current, indicated by the arrow labeled *I*. The area and the sample bias voltage are 320 nm × 750 nm and +1.5 V, respectively.

40 min) to RT. In this thermal sequence, an appropriate choice of the DC current direction between the two opposite directions parallel to the step edges is crucial for step-edge straightening, as shown in Fig. 3. With the *kink-up* current, we obtained atomically straight step edges of single bilayer (BL, 0.314 nm high) without any kinks or excess adatoms, as shown in the STM image of Fig. 3(b). The kink density is evaluated to be less than 0.25 μm^{-1}. Moreover, the first requirement mentioned above—free of atomic-level kinks—is satisfied. In contrast, when the current direction was *kink-down*, more than one kinks per 100 nm remained on each step, as shown in Fig. 3(c). Thus, we conclude that annealing around 800 °C with the *kink-up* DC current for a sufficiently long time is critical to the formation of the straight step edges.

Meanwhile, due to the azimuth miscut of the substrate, kink bunches are formed between such straight step regions by *kink-up* annealing, as shown in Fig. 4. Typical distance in the [1$\bar{1}$0] direction between the kink bunches are roughly 1 μm. This kink bunching phenomena seems a two-dimensional analog of the step bunching phenomena induced by annealing with step-perpendicular DC current [6-9]. Because, at the annealing temperature we used, the current directions inducing the kink bunching and the step bunching are *kink-up* and *step-up*, respectively, the effects of the current direction are similar between the kink bunching and the step bunching. Thus, we propose that the mechanism for the kink bunching or the step-edge straightening is analogous to that for the step bunching. The details of this current-direction effect on the step straightening will be reported elsewhere.

Atomic structure of the straight single-BL step edges was shown in the STM image of Fig. 5(a). The upper step edge is terminated by the dimer wall on the unfaulted half of the 7×7 structure, while the lower corner is not terminated by that on the faulted half. Thus, there is displacement of the 7×7 structure across the step edge: 0a in the step-parallel direction and $(2+2/3)b$ in the step-perpendicular direction. Here, $a=0.384$ nm and $b=0.333$ nm are the side length and the lateral height, respectively, of the 1×1 half-unit-cell triangle. This configuration is referred to as $U(2,0)$, where the notation $U(n,m)$ represents the shifts of $(n+2/3)b$ perpendicular and ma parallel to the U-type step, i.e. <1$\bar{1}$2> step [10]. From this STM image, we propose the structural model illustrated in Fig. 5(b). The same structure was observed at essentially all single-BL step edges in the kink-free regions on similarly prepared substrates. Thus, the second requirement—an identical lattice displacement across the step edges—is satisfied.

After the successful preparation of the substrate, we deposited ^{nat}Si to form atomic wires at the step edges. Fig. 5(c) shows an STM image after growth of 0.097-BL Si on this substrate held at 400 °C. By comparing this image with Fig. 5(a) taken before deposition, it is found that a single linear chain of adatoms is grown along the $U(2,0)$ step edge. As shown in the atomic model proposed in Fig. 5(d), this wire consists of linearly arranged Si adatoms with regular spacing 2a on 2b wide Si BL. Successive rows were not formed in parallel to the first row at the $U(2,0)$ step edge, but excess Si

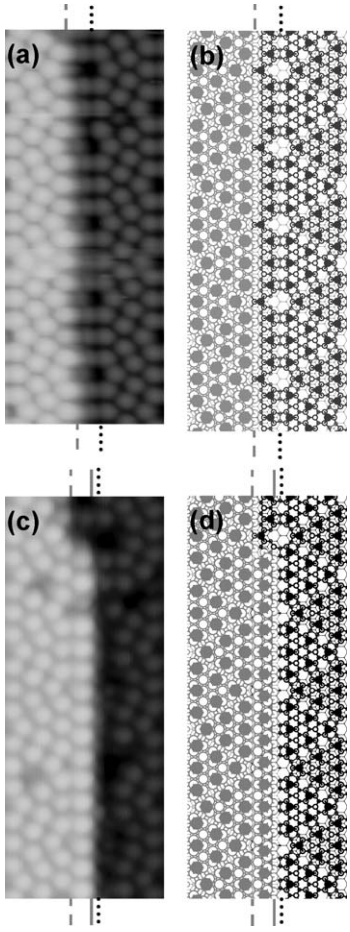

Fig. 5. Atomic structures of the step edges on the vicinal Si(111) substrate. (a) STM image and (b) atomic structure model of the step edge in a kink-free region before the homoepitaxial growth. (c) STM image and (d) atomic structure model of the step edge after deposition of Si atoms. Both STM images were taken with a sample voltage of +1.5 V. The dashed and solid lines indicate the positions of the step edge before and after the wire formation, respectively; the dotted line indicates the dimer line closest to the step edge on the lower terrace. In the models, black and gray indicate atoms in the lower terrace and the upper terrace, respectively. Top-layer atoms on each terrace are indicated with filled circles, while underlying atoms are indicated by open circles of decreasing diameters for deeper ones. The area of each panel is 5.5 nm × 14.0 nm.

atoms formed defective 7×7 structures instead. A similar behaviour has been suggested in homoepitaxial growth at a U-type step [10]. The absence of multiple wires is explained by the width comparison between the transition region at the end of the original lower terrace and the grown wire: The transition region $[(2+2/3)b]$ is wide enough to form a single wire (2b) but too narrow to form a double wire (4b). If the transition region had a width larger than 3b, the faulted halves of the 3×3 structure would be formed instead [11]. It is suggested that the transition region of $U(2,0)$ before growth has no stacking fault to form such a single wire, while the growth of multiple rows is prevented by the presence of the stacking fault in the 7×7 structure beyond the transition region. Therefore, the $U(2,0)$ step-edge structure formed uniformly on the substrate is responsible for the formation of the single wires of Si adatoms.

4. Conclusion

In this study, we have produced single lines of Si adatoms at the edges of atomically straight steps specially prepared on a vicinal Si(111) surface. Annealing around 800 °C with the DC current in the *kink-up* direction is critical to the formation of the straight step edges. The identical step-edge structure obtained is suitable to the formation of the single atomic wire. Such atomic wires are expected to be a basic building block for the silicon quantum computer [1,2].[2] The next step towards realization of that quantum computer is to form an isotopic version of the present results: single wires of ^{29}Si atoms on the vicinal (111) surface of ^{28}Si. This work is currently underway in the present group.

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[2] Although at present we cannot completely exclude the possibility that Si atoms in the substrate are substituted with the deposited Si atoms, such surface diffusion dynamics could be revealed even for homoepitaxial growth if the distinct isotopes (^{28}Si, ^{29}Si, or ^{30}Si) are used for the substrate and the adsorbate.