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Fabrication of well-aligned Er nanowires on vicinal silicon(001) surfaces

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Abstract

Using vicinal Si(001) surfaces with a 4° miscut angle towards the [110] direction as templates, an approach to fabricating well-aligned nanowires of Er silicide is demonstrated. At Er coverage of 0.1–0.3 nm and annealing temperature of 600–700 °C, ordered nanowires are obtained on the surface several hundreds of nanometres in length. STM images and LEED patterns reveal that the nanowires are all oriented along the $[1\bar{1}0]$ direction. The size, shape and density of the nanowires depends upon annealing temperature and duration as well as coverage. The experimental evidence also suggests a transition of bulk atomic structures between AlB_2 and $ThSi_2$ for Er silicide nanostructures. The alignment of the Er nanowires will make the measurements of their physical properties practicable.

1. Introduction

The formation of nanometre-scale electronic structures has received considerable attention for many years due to their unique physical properties. These nanostructures may have potential applications in novel nanoelectronics and optoelectronics, and spatially ordered nanostructures are desired in many cases [1, 2]. Of the methods built on many efforts for fabricating such nanoscale structures, self-organization is a powerful technique and uses the strain energy of a lattice-mismatched epitaxial layer [3–5]. This technique has the advantages of low cost and high throughput.

It is known that Er silicide will form through a diffusion-determined reaction between Er and Si, when Er is deposited on the Si(001) surface and annealed at elevated temperature. In the previous studies, it was found that the nanowire-like features of Er silicides can be grown in the form of hexagonal crystalline structure, with annealing at 600–700 °C [6–8]. The hexagonal

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Er silicide has a lattice mismatch of +6.5% along the Si dimer row direction and of −1.3% perpendicular to the dimer row direction with respect to Si(001). These nanowires on the substrate terraces are elongated along the directions perpendicular to the dimer rows, i.e. along the direction of minimum lattice mismatch. Due to the tetrahedral bonding configuration in the diamond lattice, (2×1) and (1×2) domains usually coexist on the Si(001) surface, separated by single-layer steps [9]. The Er nanowires appear randomly along two orthogonal [110] directions in the previous experiments.

To open up more promising opportunities in device applications, it is essential to accomplish the controlled fabrication of nanowires. Nanowires with the same orientation are the starting point for our subsequent study. By means of forming electrodes on the substrate in advance, we will be able to implement the measurements of the electrical properties of nanowires with different lengths. Er nanowires perpendicular to Si dimer rows suggests a way of synthesizing long Er nanowires with ordered orientation. It is known that surface misorientation can lead to different surface structure and morphology on a Si(001) surface [9]. The surface will display single (1×2) domains separated by double-layer steps when the miscut angle is 4°–6° in the [110] direction. On the terrace, the dimer row direction is perpendicular to the surface step. On a vicinal surface, the results can also supply more useful information about the silicide growth.

In this work, Si(001) surfaces with a 4° miscut towards the [110] direction are utilized to fabricate well-aligned long Er nanowires. After heating treatments, the substrate exhibits a surface with single (1×2) domain. The scanning tunnelling microscopy (STM) images and the low-energy electron diffraction (LEED) patterns reveal that all the nanowires have the same orientation toward the $[1\bar{1}0]$ direction. The size of the nanowire depends strongly upon the deposited coverage of Er. Annealing temperature and duration also have effects on the formation of nanowires.

2. Experiments

Experiments were carried out in an Omicron ultrahigh-vacuum STM system. It was also equipped with four-grid optics for LEED [7], and its base pressure was lower than 1.0×10^{-10} mbar. Er was evaporated on the substrate surface at room temperature, from a source heated by an electron beam. A typical deposition rate of 0.06 nm min^{-1} was monitored with a quartz-crystal microbalance. The nominal coverage of Er was determined by exposure time and was also calibrated using STM images. After deposition, the sample was annealed at 580–700 °C for 5–15 min, and then cooled down to room temperature for STM imaging. The tips were prepared by electrochemical etching of the polycrystalline W wires.

3. Results and discussion

Substrates were cut from Si(001) commercial wafers with a 4° miscut angle toward the [110] direction. After an overnight outgassing at 600 °C, the substrates were cleaned with direct-current heating above 1200 °C for few seconds in several cycles. It is shown the atomically flat terraces have single domains with (1×2) dimer reconstruction separated by double-layer atomic steps, and the steps extend along the $[1\bar{1}0]$ direction with respect to Si(001). The average width of the terrace is 4.0 nm. This starting surface displays an area density of 'defect' lower than 5%. The 'defects' here are the small patches exhibiting (2×1) dimerization, i.e. (2×1) domains, on the terraces.

Figure 1 is a STM image of a sample with 0.12 nm Er deposited on the substrate followed by subsequent annealing at 650 °C for 10 min. This image clearly shows that many self-ordered

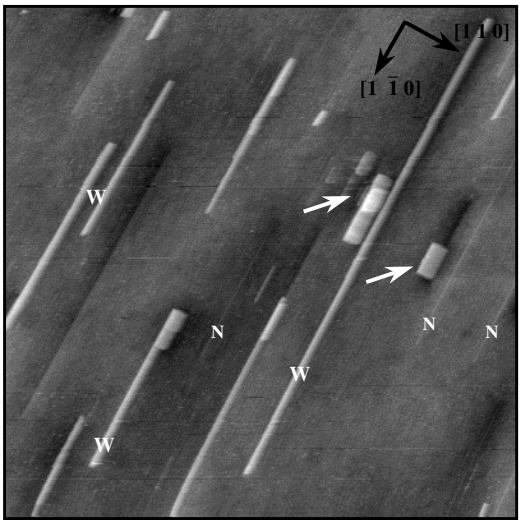

Figure 1. A STM image obtained on the sample with 0.12 nm Er deposited on the substrate. The post-growth annealing is operated at 650 °C for 10 min. The scanning area is 480 nm × 480 nm. The sample bias is 1.8 V and the tunnelling current 0.6 nA.

Er nanowires are grown on the surface. All of the nanowires are oriented toward the [1$\bar{1}$0] direction. According to STM measurements, these nanowires are several hundred nanometres long. The longest one is about 490 nm. There are two kinds of nanowire with different widths: wide (W) and narrow (N) as labelled in the figure. The wide nanowires usually stretch across the steps to neighbouring terraces. They are 6.1–9.0 nm wide and about 1.3 nm high which is the average height from the surface of the nanowires to the substrate surface. It is also observed that usually the height of Si double step does not change as the wide nanowire goes across from one terrace to the other. The widths of narrow ones are less than 2 nm and the apparent heights are about 0.3 nm. The rectangular islands in this figure are generally associated with significant perturbation of the step distribution on the surface, as marked by the arrows.

In order to understand the growth mechanism of nanowire structures, many experiments have been done at different growth conditions. It is found the Er coverage has a great effect on the size of the nanowires. The average lengths of the nanowires will increase as the Er coverage decreases. But the density and shape of nanowires depend strongly upon the temperature and duration of annealing. High temperature and long annealing time will induce nanostructures appearing in the form of rectangular islands or three dimensional (3D) islands with low area density. The detailed effects of the growth condition will be discussed elsewhere, here attention is paid to the surface morphology and crystal structures.

Figure 2 is a 240 nm × 240 nm STM image taken on the sample with 0.6 nm Er and postannealed at 580 °C for 10 min. It shows that many nanowires grow close together into bundles of nanowires, forming a wide nanowire. Sometimes the additional layers of Er silicide can be seen to grow epitaxially on the top of these nanowires, such as nanowire AB in the figure. If the width of a wide nanowire is more than 10 nm with aspect ratio smaller than 5, it becomes a rectangular island. When the sample with high Er coverage is annealed at higher than 650 °C for more than 15 min, nanowires always evolve into rectangular islands, and even into 3D islands. Similar nanostructures have been observed for the Dy/Si(001) system [10].

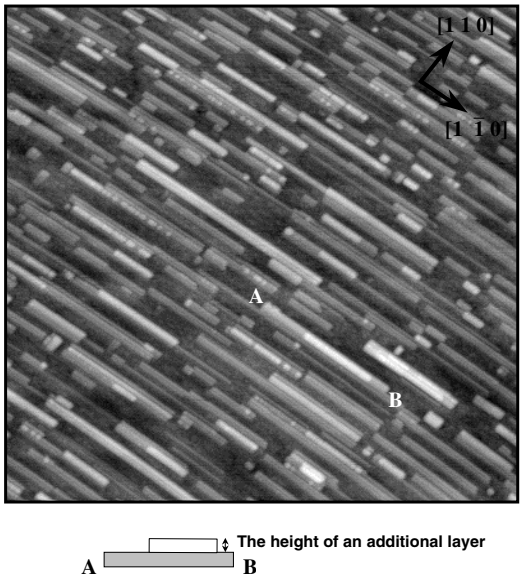

Figure 2. A 240 nm × 240 nm STM image taken on the sample with 0.6 nm Er and postannealed at 580 °C for 10 min. The sample bias voltage is −1.8 V, and the tunnelling current is 0.6 nA.

Usually a 3D island has a smaller aspect ratio ($\leqslant$1.5) and a larger height than a rectangular island. On the top of these two islands, Er silicide grows in a layer-by-layer mode. It is interesting that the heights of single additional layers are different on these two islands. For the rectangular island the heights are multiples of 0.33 nm, but for the 3D island the height unit of an additional layer frequently has a measurement of 1.2–1.4 nm. LEED observations reveal that the surface structures change from a (1 × 2) reconstruction of the clean surface to (4 × 2) and finally to c(2 × 2). In most cases, these reconstructions coexist, but it is obvious that the c(2 × 2) reconstruction appears along with the 3D islands. Er-induced (4 × 2) comes from the regions unoccupied by nanowires and islands [8]. In the STM images acquired on the 3D islands, not on nanowires, c(2 × 2) reconstruction is also observed with atomic resolution.

It is established that two crystalline structures exist for bulk Er silicide: one is the tetragonal structure ($ThSi_2$) and the other is the hexagonal structure (AlB_2). These two types of structure are closely related and the $ThSi_2$-type structure can be derived from the AlB_2-type structure [11]. The nanowires are self-organized on the Si(001) surface in the form of the hexagonal crystalline structure, as illustrated in the previous studies [6, 12], with $ErSi_{2-x}(1\bar{1}00) \parallel Si(001)$ and $ErSi_{2-x}[0001] \parallel Si[\bar{1}\bar{1}0]$. The height of one layer for the hexagonal silicide nanowire along the (001) direction of the substrate is 0.328 nm, but that for the tetragonal silicide is 1.326 nm. The discoveries in this experiment give a clear picture of the crystal structures for nanowires, rectangular islands and 3D islands. It is believed that Er silicides self-assemble into the nanowires in the AlB_2-type structure, some nanowires grow into bunches and form the wide nanowires, then the wide nanowires develop into the rectangular islands. This rectangular island also has an AlB_2-type crystalline structure. But for most 3D islands, a transition of crystalline structure presumably occurs. As mentioned above, the experimental results obtained in this work show that the heights of an additional layer of Er silicide are different grown on the top of a rectangular island and a 3D island. For a rectangular island, it is 0.33 nm or multiples of 0.33 nm, coinciding with the height of one layer of AlB_2-type silicide along the (001) direction. But for a 3D island, the smallest height is the same

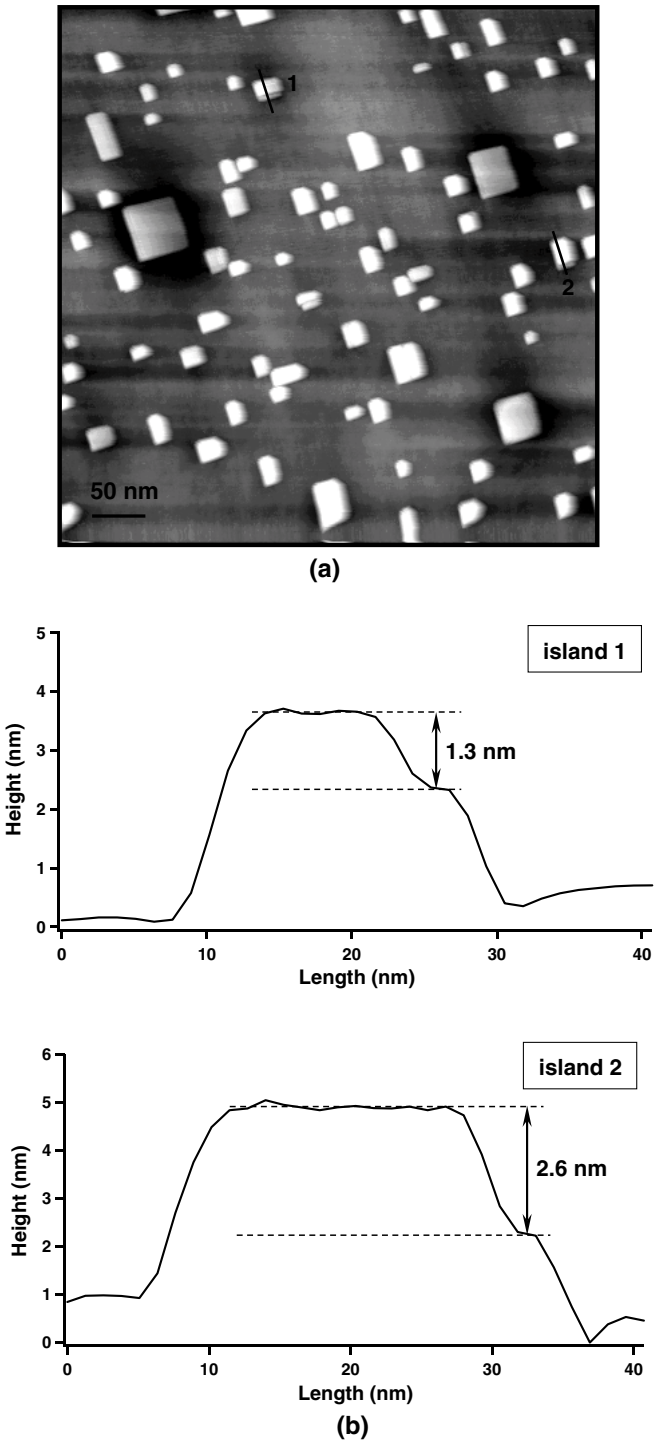

Figure 3. (a) 3D islands formed on the vicinal surface of Si(001) with 0.8 nm Er and annealed at 760 °C for 10 min. The image is acquired at 2.0 V and 0.4 nA. (b) Line profiles of 3D islands labelled as 1, 2 in (a).

as the lattice parameter of the $ThSi_2$-type silicide in *c* axis. X-ray diffraction measurements of the samples with thicker Er silicide films manifest plainly that 3D islands have the $ThSi_2$-type structure [7, 13]. Frangis *et al* also found that the $ThSi_2$-type phase can grow on top of the AlB_2-type phase [11]. It is therefore reasonable that on the top of a nanowire bundle or a rectangular island with the AlB_2-type structure, Er silicides organize in the $ThSi_2$-type structure and grow into a 3D island, as shown in figure 3.

Figure 3(a) displays a 500 nm × 500 nm STM image obtained on the vicinal surface of Si(001) with 0.8 nm Er and annealed at 760 °C for 10 min. The islands on the surface have widths in the range 15–55 nm. The heights of these islands are 3–6 nm, and that is the reason we call them 3D islands. It is clearly exhibited that most islands are very nearly square. For the tetragonal Er silicide, the two lattice mismatches along two orthogonal [110] directions are 3.1% with respect to the Si(001) surface. A square shape is the most possible form that an epitaxial layer will take in the growth on the Si(001) substrate, with the same lattice mismatches along two [110] directions. It is also noted that step structures exist on the top surface of two islands, labelled as 1 and 2 in figure 3(a). The step height can be distinguished easily from the line profiles in figure 3(b). The step height is 1.3 nm for island 1 and 2.6 nm for island 2. This means that double additional layers of tetragonal Er silicide are developed on the top of island 2. These results also testify that the 3D islands are Er silicide in tetragonal phase.

4. Conclusions

Er nanowires were grown on a vicinal Si(001) surface studied with STM and LEED. The well-aligned Er nanowires were self-organized along the $[1\bar{1}0]$ direction, with lengths of several hundred nanometres. It is found that Er coverage, post-annealing temperature and duration have an effect on the formation of nanowires. Based on the experimental results, a transition of bulk atomic structures between AlB_2 and $ThSi_2$ is proposed for Er silicide nanostructures. Well-aligned nanowires are the starting point to fulfill measurement of their electrical properties in subsequent works.

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