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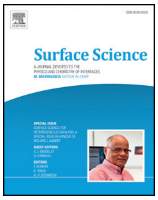

Endotaxial growth of $CoSi_2$ nanowires on Si(001) surface: The influence of surface reconstruction

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Evidence for the influence of Si(001)-(2 × 1) surface reconstruction on the elongation direction of $CoSi_2$ flat islands is discussed in this paper. Step height analysis of these flat islands shows that flat island heights, H_A, follow discrete values of N_A such that $H_A = mN_A + c$, where $N_A = 1, 2, 3, \ldots, m$ is equivalent to the number of monoatomic step height (1.4 Å) of the Si(001) surface, and c is the initial island height when $N_A = 0$. The N_A values were found to be correlated to the flat island elongation direction with respect to the (2 × 1) dimer rows. For a given terrace, the preferred elongation direction of these flat islands is parallel to the Si dimer rows. As a result, orthogonally elongated islands are clearly resolved on adjacent terraces, which are separated by monoatomic steps. The endotaxial growth of these flat islands is thus also influenced by the anisotropic adatom diffusion due to (2 × 1) surface reconstruction.

1. Introduction

To achieve preferential growth and selective control over the morphology of silicon -based heteroepitaxial low-dimensional nanostructures, such as nanowires, requires fundamental insights into the growth dynamics and kinetics [1–3]. Homoepitaxial growth of Si nanowires, for example, on Si(001)-(2 × 1) surface have shown to be influenced by surface reconstruction, where anisotropic Si-adatom diffusion leads to growth of Si islands forming nanowires [4,5]. On the other hand, the formation of heteroepitaxial nanowires, such as rare-earth silicide system [6–9], have been attributed to anisotropic lattice mismatches between islands and substrates. These islands elongate preferentially along the direction with lower lattice-mismatch in order to minimize strain energy. In other cases, the shape transition of compact islands to nanowires driven by strain relaxation have also been reported for material systems such as Ag nanowires [10] and silicide nanowires such as $CoSi_2$ on Si(001) [11–16]. The introduction of nanowires growing epitaxially into the substrate surface (endotaxy) reviewed recently for several systems such as Ni, Co, Pt, and Fe on Si(001), Si(110), and Si(111) surfaces, however, revealed a more complex mechanism for nanowire formation and growth [17–19].

Of particular interest is the formation of $CoSi_2$ low-dimensional structures. Recent works have shown that nanowires on Si(001) are formed not only because of strain-induced shape transition [13,16] but is also a consequence of a thermally activated growth due to endotaxy [18,20–24]. It has been reported that $CoSi_2$ forms two types of islands, ridge and flat, on the Si(001) surface [23]. Briefly, ridge islands form preferentially low energy $CoSi_2\{111\}//Si\{111\}$ interface (Type B) with Si, which appears to show a “twinned” type interface due to a stacking fault. They grow endotaxially because the low energy Type B interface is more energetically favorable than other higher energetic planes along the $<110>$ directions ($CoSi_2\{111\}//Si\{115\}$, $CoSi_2\{115\}//Si\{111\}$, and $CoSi_2\{112\}//Si\{112\}$). Its preferred growth over other interfacial planes results in wire formation. For flat-type islands, they form Type A, i.e., $CoSi_2\{111\}//Si\{111\}$, interface endotaxially with Si. Type A interface, unlike Type B, is “untwinned” where the lattice structure of $CoSi_2$ follows that of Si. These islands are bound by the energetically favorable Type A interface on all sides, resulting in the preferential formation of compact islands. However, growth at low temperature results in wire-like flat islands before compact islands are seen at high temperatures. Although the occurrence of wire-like features have been attributed to the presence of corner barriers [23,25,26], the influence of Si(001)-(2 × 1) surface reconstruction due to the anisotropic diffusion of adatoms along and across dimer rows has not been adequately addressed. Here, we report the anisotropic growth of wire-like flat islands at low growth temperatures between 500 °C and 650 °C. By analyzing the island height with respect to the

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Si(001)-(2 × 1) reconstructed surface, we elucidate the apparent orthogonal elongation directions along <110> of flat nanowires as observed at low growth temperatures—a consequence which we attribute to the influence of surface reconstruction of Si(001).

2. Methods

The STM experiments were carried out *in situ* in an OMICRON Ultra-High Vacuum (UHV) system with base pressure of 2×10^{-10} Torr, equipped with an OMICRON Variable Temperature-Scanning Tunneling Microscope (VT-STM). Si samples were cut from Boron-doped P-type singular Si(001) wafers with resistivity less than 0.1 Ω/cm supplied by Virginia Semiconductors. These samples were chemically etched *ex situ* based on the recipe described by Ong *et al.* [27,28]. They were then dipped in dilute aqueous hydrofluoric (HF) acid solution to terminate the surface with hydrogen prior to outgassing in the UHV chamber for 8 h at ~300 °C. The samples were then progressively annealed in steps of 50 °C to 700 °C and then flashed at 30 s per cycle to 1100–1150 °C. Upon cooling to room temperature, the clean samples' surface morphologies were verified *in situ* using a VT-STM. The samples were then deposited at elevated temperatures (530 °C, 560 °C, 590 °C, and 620 °C) with cobalt (Goodfellow, > 99.99 + % purity) using electron-beam evaporation with a rate of 0.1 ML/min for 1 min. Temperatures and deposition rate were determined using an infrared pyrometer and a quartz crystal monitor (QCM), respectively. The surface morphologies were subsequently characterized *in situ* using the VT-STM. The STM tungsten tips were fabricated using the Omicron Tip-Etching kit and then outgassed in UHV prior to STM scans. All STM images were taken *in situ* at room temperature using constant-current mode, with a tunneling current at −1.0 nA, sample bias of −2.0 V with acquisition done in a unidirectional mode. Drift in between images were kept to a minimum by allowing longer times for the STM tip to scan the surface. The STM scan direction was kept unidirectional from bottom to top. The STM images were background-corrected (planar) and flattened ("Flatten discarding regions") using the WSxM software (Nanotec Electronica) [29]. Analyses and measurements from these images were done using the same software.

3. Results and discussions

3.1. Flat island height evolution and height analyses

Details of the structure of ridge-type and flat-type islands and their epitaxial relationships with the Si(001) substrate have been reported previously [23]. Fig. 1a shows a 500 nm × 500 nm global surface morphology of a Si(001) surface after 0.1 ML of cobalt is deposited at 530 °C. Si dimer rows elongates along the $[1\bar{1}0]$ direction on Si(001)-(2 × 1) surface as shown in the figure. The surface morphology consists only of two types of islands: flat type (labeled "F") and ridge type (labeled "R"), elongating along two orthogonal [110] and $[1\bar{1}0]$ directions. Apart from these islands, the surface is also decorated with "holes" (labeled as "h") surrounding several islands with remnant Si terraces exhibiting (1 × 2) reconstruction (labeled as "t").

Fig. 1b shows the average length to width aspect ratio of the flat islands measured as a function of its growth temperature. The plot represents the shape evolution of the flat islands with increasing growth temperature. Between 530 °C and 650 °C, the average length to width aspect ratio is shown to increase rapidly from 2:1 to 7.5:1. Thereafter, it decreases rapidly back to 2:1 above 710 °C. The increase in the aspect ratio shows the elongation of flat islands at lower growth temperatures. However, interfacial energies of the flat island are reported to be similar on all sides of the island since they are bound at the $CoSi_2\{111\}//Si\{111\}$ interface. The formation of flat islands energetically favors a compact isotropic shape (e.g., square) rather than a nanowire. The elongation of the flat island therefore suggests other factors which kinetically limit the growth and formation of compact flat islands. We proceeded to examine the flat islands in more detail and subsequently reveal the correlation between the flat island's heights and their elongation direction with respect to the Si dimer rows.

Two flat islands from Fig. 1a (labeled as "2a" and "2b"), which appear to elongate parallel and perpendicular to the Si(001)-(2 × 1) dimer rows, were then scanned at higher resolution and shown in Fig. 2a and b. The flat island in Fig 2a elongates along the Si dimer rows with respect to the main Si(001)-(2 × 1) terrace labeled "1," while it is found to elongate perpendicular to the adjacent remnant Si(001)-(1 × 2) terrace labeled "2." The line profile AB shows that the island height is about 2.4 ± 0.2 Å with respect to terrace "2," while the line profile CD shows that the height is 3.8 ± 0.2 Å with respect to terrace "1." Comparing the two line profiles, the height difference between the Si terraces "1" and "2" is thus about 1.4 Å.

Fig. 2b shows the second flat island elongating along [110] perpendicular to the Si(001)-(2 × 1) Si dimer rows. The line profiles EF and GH give the island a height of 3.7 ± 0.2 Å with respect to remnant Si(001)-(1 × 2) terrace labeled "2" and 5.1 ± 0.2 Å with respect to the main Si(001)-(2 × 1) terrace labeled "1." Comparing the two line profiles EF and GH, the height difference between terrace "1" and "2" is also about 1.4 Å. Both flat island measurements suggest that their heights are closely correlated to the monoatomic step height of the Si(001) surface (1.4 Å). The remnant Si terraces in

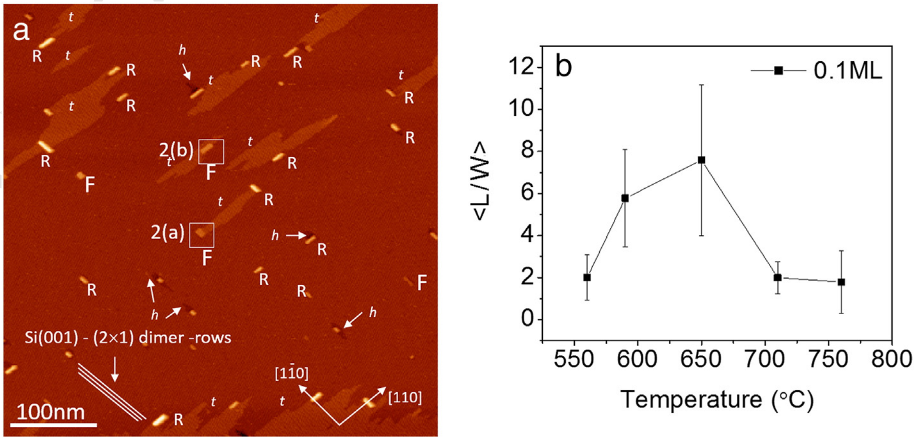

Fig. 1. (a) STM global morphologies of Si(001)-(2 × 1) deposited with 0.1 ML Co at 530 °C (500 nm × 500 nm). Some flat islands and ridge islands are labeled "F" and "R," respectively. Features labeled "h" are holes which formed as Si is consumed during cobalt deposition. Consumption of Si results in the remnant Si(001)-(1 × 2) terraces left after cobalt deposition (labeled as "t"). (b) Average length to width aspect ratio of flat islands measured as function of growth temperature.

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