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Cyclic transformation of one-dimensional structures during homoepitaxy of Si(5 5 12)-2 × 1

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Abstract

In the homoepitaxy of Si(5 5 12) at a finite temperature, 500 °C, it has been found that one-dimensional elements composing of Si(5 5 12)-2 × 1, such as honeycomb (H) chain, tetramer (T) row, and dimer-facing-adatom (D/A) row, transform for themselves with adding Si atoms. It turns out that a Si dimer is a basic building block, and selectively adsorbs on D/A sites of Si(5 5 12)-2 × 1. Dimer-adsorption on a D/A row induces a tensile stress to the neighboring T row to be split to a new D/A row, which can also host Si dimers. The additional Si-dimers arriving at a saturated D/A row transform it to a new H chain. Such a conversion generates a compressive stress causing the neighboring and pre-existed H chain to be broken to a new T row, which can also be split to a D/A row by the external tensile-stress. Under such cyclic transformation among D/A row, H chain, and T row, (1 1 3) facet initially starts to grow from a (1 1 3) seed in Si(5 5 12)-2 × 1 and saturates at the width of four periodicities. Then, a (1 1 2) facet of three periodicities is formed from the opposite side to complete one sawtooth-like facet in one unit-cell of Si(5 5 12). Finally, the valley of sawtooth-like facet is filled and a uniform Si(5 5 12)-2 × 1 terrace is recovered. After one-cycle of such homoepitaxy, the unit-cell of recovered Si(5 5 12)-2 × 1 shifts horizontally by 3.04 Å toward $[\bar{6}\,\bar{6}\,5]$ direction relative to the original one and the effective height increases by 1.36 Å, which costs only 28 atoms per unit cell of Si(5 5 12)-2 × 1. These results imply that the exact growth-direction for an identical reconstruction is toward $[\bar{1}\,\bar{1}\,2]$ and a new layer is formed in the fashion of adding a cell-unit composed of two dimers from $[\bar{1}\,\bar{1}\,2]$ to each of seven (1 1 1)-bilayer step-edges existing in the (5 5 12) surface.

Keywords: Scanning tunneling microscopy; Epitaxy; Surface structure, morphology, roughness and topography; Silicon; High index single crystal surfaces

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1. Introduction

As the dimension of semiconductor device becomes smaller and enters a new world of nanometer scale, it is essential to control down to the atomic scale, to dope abruptly in that scale and to prepare the atomically-flat surfaces with little contamination. In order to satisfy such conditions the immaculate substrate of least defects should be prepared, which might start from successful homoepitaxy. Since the surface reconstruction should influence the epitaxy at the initial atom-adsorption stage, the equilibrium structure of surface must be well-defined prior to homoepitaxy. In other words, as the delicate energy-balance between eliminating dangling-bonds and minimizing surface-stress determines a specific reconstruction, both the available number of dangling-bonds and their relative directions can be determining factors for a specific morphology during homoepitaxy. For example, in the Si(1 1 1) homoepitaxy, the growth mode changes from multilayer to layer-by-layer with increasing Si coverage [1], while, in the Si(0 0 1) homoepitaxy, the growth mode changes from two-dimensional island to step-flow with increasing the substrate temperature [2]. Therefore, the homoepitaxy of a specific substrate-direction under some conditions can give a chance to achieve an ideal template for nano-scale fabrication.

In the present study, Si(5 5 12), which exists between (0 0 1) and (1 1 1), has been chosen for homoepitaxy. Since the reconstructed Si(5 5 12)-2×1 has been known to have one-dimensional symmetry along $[1\bar{1}0]$ and be reconstructed as a relatively planar surface compared to other surfaces existing between (0 0 1) and (1 1 1), it can be a potential template for nanowire fabrication [3]. Up to now, the homoepitaxy of Si(5 5 12) has not been reported. Furthermore, it seems that it is not easy to figure out the exact reconstruction due to its relatively large unit-cell of 0.77 nm $\times$ 5.35 nm. Hence, the studies on Si(5 5 12)-2×1 based upon various experimental techniques have followed, but the satisfying model explaining all of them has not been known [3–5]. In addition to this, as shown in the STM images of Si(5 5 12)-2×1, it has been turned out that a Si dimer is a unique species which adsorbs on a specific site. Then, through homoepitaxial growth at a finite temperature, this dimer species, a potential impurity in future nanowire fabrication, might be removed. In other words, as the adsorbing species in the homoepitaxy is the same kind of atoms as the substrate, its preferential adsorption and related evolution might alter the substrate reconstruction at a finite temperature. Through the present homoepitaxy of Si(5 5 12), the mechanism of structural evolution with increased Si atoms during one cycle of homoepitaxy has been clearly exposed and the structural model of Si(5 5 12)-2×1 recently reported has been confirmed [6].

2. Experimental

The Si(5 5 12) substrate of the size, $13 \times 3 \times 0.25$ mm^3, was prepared through cutting from an n-type (P-doped) wafer and decreasing with organic solvents in the air. It was mounted on a molybdenum sample-holder and introduced to the ultrahigh vacuum (UHV) chamber of a base pressure, 2×10^{-10} Torr. The introduced sample-holder assembly was outgassed at 700 °C for 12 h, and the substrate temperature was monitored by optical pyrometers. After outgassing the introduced substrate, it was flashed at about 1200 °C by resistive heating in order to remove a native-oxide layer, under a pressure less than 3×10^{-10} Torr. Each flashing-period was kept for three seconds and the accumulated flashing period was about five minutes. At the end of flashing, the surface was reconstructed by slow cooling from 900 °C to a room temperature at the rate of one degree per second. Silicon atoms were evaporated onto the substrate held at 500 °C at the rate of 0.2 Å per minute from a resistively heated silicon wafer. For each Si coverage, a reconstructed Si(5 5 12)-2×1 has been confirmed prior to Si deposition. The STM images were acquired at a constant current mode ($I_{\text{tunneling}} = 0.5$ nA), and both topography and error-signal images were obtained at the same time. Error-signal images were obtained through recording the value controlling the z-axis motion in the feed-back process in order to single out the intensity variation [7].