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Surface reconstructions on Sb-irradiated GaAs(0 0 1) formed by molecular beam epitaxy

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Abstract

Reconstructed surfaces on Sb-irradiated GaAs(0 0 1) formed by molecular beam epitaxy have been studied by *in-situ* scanning tunneling microscopy (STM). The reflection high-energy electron diffraction patterns showed (2×3) [or weak (4×3)] structure. The step density was about five times higher than that of GaAs(0 0 1)-$c(4\times4)$ surface. It was found that there were swinging dimer rows along to the $[1\bar{1}0]$ direction, which seemed not to consist of a specified reconstruction. We proposed two (2×3)-structure models for these swinging dimers. By first-principles calculation, we found that the proposed models were stable and with energy difference was 0.17 eV, indicating the coexistence of the two structures. Moreover, we proposed three (4×3) reconstruction models based on these (2×3) models. The electron counting rule was applied for these models, indicating that there was an excessive amount of electrons. By two bias-alternative STM images, it was found that the many spots appear only in empty-state. These might be segregated Ga or Sb cluster and strongly relate to the excessive amount of electrons.

Keywords: Molecular beam epitaxy; Scanning tunneling microscopy; Sb; GaAs; Surface reconstruction; Reflection high-energy electron diffraction; Electron counting rule; First-principles calculation

1. Introduction

The fine deposition control of various semiconductor materials by molecular beam epitaxy (MBE) has enabled to fabricate the quantum-size effect devices. III–V semiconductor materials such as GaAs and InP have used as diverse devices, in particularly, optoelectronic device applications. Recently, the novel fabrication method that irradiates antimony (Sb) on GaAs(0 0 1) surface and forms Sb-terminated layer by As–Sb exchange reaction have been devised [1]. Sb irradiation brings that surface reconstruction changes from $c(4\times4)$ to $(n\times3)$ (n–1, 2, 4). The new application of Sb/GaAs(0 0 1) have been proposed that InAs quantum dots grown on Sb-irradiated GaAs(0 0 1) by MBE obtained high density and high uniformity [2,3]. However, a detailed structure of this surface has not been investigated. Although surface reconstruction of Sb-terminated GaAs(0 0 1) have been reported existing (2×4) [4,5] and (2×8) [5] so far, $(n\times3)$ surface reconstruction has not been reported yet. The $\times3$ ordered reconstructions have also been studied for in Sb-passivated GaAs(0 0 1) at room temperature [6–8]. Although STM observation of Sb-passivated surface-(1×3) [8] and GaSb on GaAs(0 0 1)-$c(4\times4)$ [9] have been reported, any reconstruction model is not discussed for these $\times3$ ordered reconstructions, including (2×3) or (4×3). In this paper, using *in-situ* STM and first-principles calculation, we investigated on the surface reconstructions on Sb-irradiated GaAs(0 0 1) formed by MBE and proposed its structure models.

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2. Experimentals

It was used a non-doped GaAs(0 0 1) just-oriented substrate. After the oxide layer removal, a GaAs buffer layer of 200 nm was grown at 570 °C under As_4 pressure of 5×10^{-5} Pa and Ga pressure of 3.3×10^{-6} Pa. Next, under As_4 flux, the substrate was set up to irradiation temperature of 435 °C. The $c(4\times4)$ reconstruction of the As-rich surface was confirmed by the reflection high-energy electron diffraction (RHEED). When the Sb shutter was opened, simultaneously closing the As shutter, an Sb_4 flux of 1.0×10^{-6} Pa was irradiated on the As terminated GaAs so that As–Sb exchange reaction was carried out [1]. The irradiation amount depends on RHEED pattern changing from $c(4\times4)$ to (2×3) or (4×3). The substrate was annealed over 10 min at the same temperature after the irradiation. The (4×3) or (2×3) reconstructions were unchanged during substrate quenching to 200 °C. The sample was observed at the same temperature on the same substrate heater by the *in-situ* STM located inside MBE growth chamber [10]. STM experiments used a tungsten tip and were performed under the background pressure of 8×10^{-8} Pa. All STM images were acquired by a constant current of 0.1 nA, a scan speed of 250 nm/s and a tip bias of +3 V. Then, first-principles density-functional total-energy calculations were performed based on the density-functional theory using the Vienna *ab initio* simulation package [11]. We used the local-density approximation for the exchange correlation and the projector augmented wave [12,13] pseudopotentials. The Ga 3d electrons were treated as part of the valence band. The cutoff energy for the plane-wave basis was 400 eV. We employed supercells containing six atomic layers of GaAs and two layers of GaSb where the bottom side of the slab was terminated with fractionally charged hydrogen in order to maintain bulk properties.

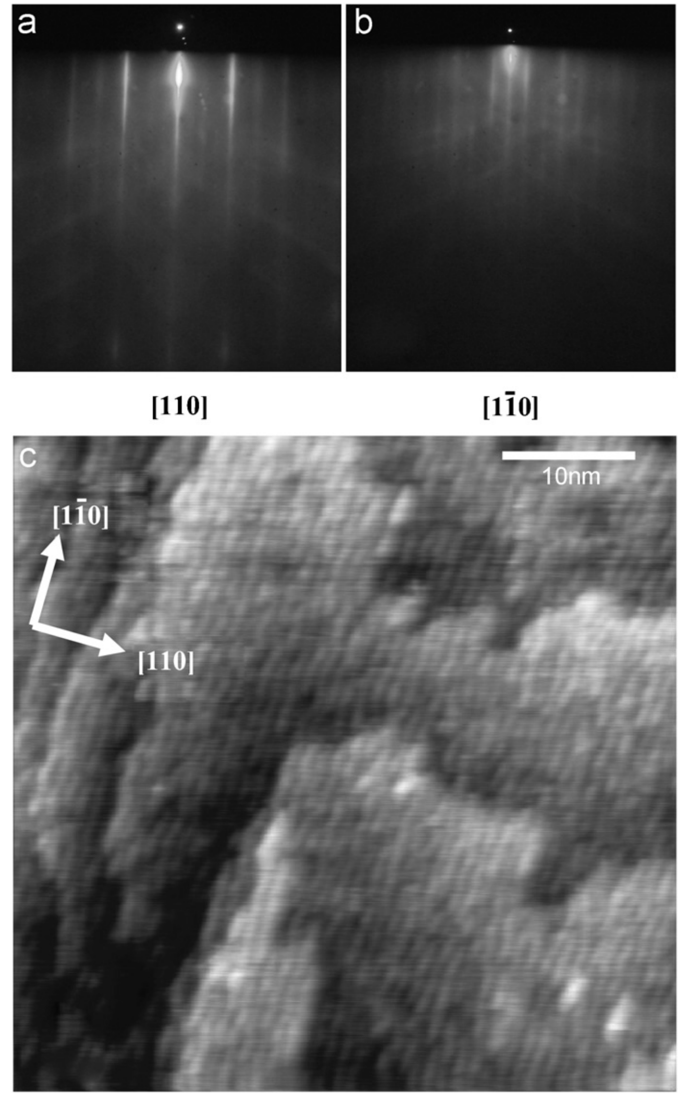

Fig. 1. The RHEED patterns of Sb-irradiated GaAs(0 0 1). (a) Slightly obscure two-fold in [1 1 0] azimuth and (b) three-fold in $[1\,\bar{1}\,0]$ azimuth. (c) The STM image at 200 °C, tunneling current of 0.1 nA, tip bias of +3 V, scan size of 50×50 nm, scan speed of 250 nm/s and background pressure of 8×10^{-8} Pa. The height range of the surface is approximately 1.0 nm. The periodicity perpendicular to the $[1\,\bar{1}\,0]$ direction is 1.2 nm.

3. Results and discussions

Fig. 1 shows RHEED patterns in the [1 1 0] and $[1\,\bar{1}\,0]$ azimuth and a filled-state STM image on Sb-irradiated surface. The RHEED patterns indicated three-fold order distinctly in the $[1\,\bar{1}\,0]$ azimuth (Fig. 1(a)) and weak $2\times$ and very weak $4\times$ in the [1 1 0] azimuth (Fig. 1(b)) so that the surface is dimerized (2×3) [or (4×3)]. STM image (Fig. 1(c)) shows that anisotropic islands are formed with multi-layer behavior and kinks that result from steps. The step density of this surface, defined here as the total length of step edges per unit area, is 183 μm^{-1}, whereas that of GaAs(0 0 1)-$c(4\times4)$ is 40 μm^{-1} [14]. This Sb-irradiated surface was thus found to be rough, which agreed with the ribbon-like structures reported by Zinck et al. [7]. They suggested that the additional growth of GaSb of 2.5 ML on GaSb of 1 ML (3.5 ML total)/GaAs(0 0 1) surface enhances the anisotropy of the surface attributed to the direction-dependent strain associated with the dimer-based surface reconstructions of the wetting layers. Our result reinforces their suggestion because of the anisotropy along to the $[1\,\bar{1}\,0]$ direction. The Sb irradiation causes an increase of surface step density. The same phenomena is reported in the co-deposition of Sb and Si on Si(0 0 1) [15] and AlAs on GaAs(0 0 1) [16]. The high QD-density can be achieved by using these high-step-density surfaces since dangling bonds on the step edges play a role of nucleation sites [3,16]. However, the incorporation mechanism of InAs deposition into Sb/GaAs(0 0 1) and the segregation mechanism of Sb remain unclear. Therefore, it is important to know its initial surface which means the (2×3) [or (4×3)] reconstructed Sb-terminated GaAs(0 0 1).

Fig. 2 shows a high-resolution empty-state image of Sb-irradiated GaAs(0 0 1). We confirmed $\times3$ structure of approximately 1.2 nm periodicity perpendicular to the