Applied Surface Science 360 (2016) 547–552

Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Surface reconstruction: An effective method for the growth of mismatched materials

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ARTICLE INFO

Article history:
Received 7 September 2015
Received in revised form 15 October 2015
Accepted 26 October 2015
Available online 10 November 2015

Keywords:
Heteroepitaxy
Mismatched materials
Surface reconstruction

ABSTRACT

The crystalline quality of epitaxial films depends on the degree of lattice match between substrates and films. Here, we report a growth strategy for large mismatched epi-films to grow GaSb films on Si(1 1 1) substrates. The epitaxial strategy can be influenced by controlling the surface reconstructions of Sb-treated Si(1 1 1). The film with the best quality was grown on Si(1 1 1)-$(5\sqrt{3}\times 5\sqrt{3})$-Sb surface due to the stress release and the formation of a self-assembled 2D fishbone structure. Controlled surface engineering provides an effective pathway towards the growth of the large mismatched materials.

1. Introduction

Advances in the semiconductor industry are vitally dependent on the availability of techniques for the growth of films with high quality [1]. Currently, there are plenty of techniques available in literature for the growth of lattice matched materials, although the techniques for growing severely mismatched ones are scarce. For example, the lack of a proper substrate for a given material of interest prevents the realization of their epi-film with high quality. The degree of lattice match between substrate and epi-film is one of the most important factors in fabrication of high quality crystalline films. Fabrication of high quality epi-film with large lattice mismatch is therefore a daunting challenge in the semiconductor industry. Generally, large mismatched material films are grown on a buffer layer in which the mismatched stress is progressively released [2]. But the application of a buffer layer reduces the device performance.

For epitaxial growth of large mismatched materials without buffer layer, it is possible to form an epitaxial interface described by a coincidence lattice when the film and substrate have the lattice spacings close to an integer ratio n/m [3,4] [Fig. 1(a)]. However, in this configuration many edge dislocations will appear at the interface and the overall crystalline quality is therefore reduced. Erwin et al. have shown that the edge dislocations can be significantly reduced (if not eliminated completely) in the case of Fe epi-film on GaN grown along a tilted crystallographic orientation [5]. Based on this mechanism, we find that there always exists a proper tilt angle to completely eliminate all the edge dislocations as shown in Fig. 1(b). Recently, Boschker et al. found a surface reconstruction-induced coincidence lattice formation for Sb_2Te_3 films grown on Si [6]. The reconstructed surfaces make it possible to create solid–solid interfaces with interface structures and bonding configurations by which twin domains are greatly reduced and crystalline quality are improved [7]. However, very little is known on the effect of substrate surface atomic structure on the growth of large mismatched materials by the tilt mechanism.

GaSb epi-films have potential applications in optoelectronic devices in the near IR regions [8] as well as high speed solid state electronics [9]. However, because of the lattice mismatch issues, the growth technique is limited to limited number of substrates [10,11]. Especially, the growth of GaSb films with high quality on Si substrate needs more effort [12,13]. In this study, we use GaSb films on Si(1 1 1) as an example to illustrate the tilt mechanism for the large lattice mismatch epitaxy relied on substrate's surface reconstruction [14]. We found that not only the mode of lattice matching at interfaces but also the mechanism of stress release are closely tied to the surface reconstruction of Si(1 1 1) substrates. The lattice fringes of GaSb epi-film are aligned with Si substrates at a tilt angle of 14°. GaSb epi-films with the best quality, achieved on the Si(1 1 1)-$(5\sqrt{3}\times 5\sqrt{3})$-Sb surface, will open up a broad prospect for the applications of GaSb-based integration devices. Moreover, this paper offers an effective way for the heteroepitaxial growth of mismatched materials.

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http://dx.doi.org/10.1016/j.apsusc.2015.10.198

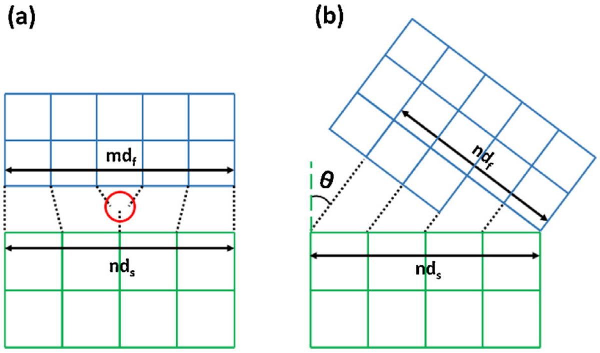

Fig. 1. Schematic view of the interface between a film with lattice constant d_f and a substrate with a lattice constant d_s. (a) For forming the coincidence-site lattice, there exists a relation, $md_f = nd_s$ wherein will form $|n-m|$ edge dislocations as shown in red circle. (b) When the epi-film grows at a tilt angle of θ, every lattice of the epi-film matches well with one lattice of the substrate. So, in principle all edge dislocations can be eliminated completely. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

2. Experiment

Prior to growth, 2 in. p-type Si(1 1 1) wafers with room temperature resistivity of 1 ∼ 10 Ω m were chemically cleaned using standard Shiraki clean procedures [15]. The cleaned wafers were immediately loaded into the molecular beam epitaxy (MBE) load-lock chamber and were degassed at 200 °C at a final pressure of 5×10^{-8} Torr for 2 h. Growth was carried out in a SVTA III–V reactor equipped with valved cracking cell for Sb and effusion cell for Ga. The antimony cracking zone temperature was fixed at 1000 °C for all growths, providing atomic antimony and Sb_2 [16]. The base pressure maintained in the growth chamber was $\sim 10^{-10}$ Torr. The V/III beam equivalent pressure ratio is fixed at 2.0.

For the first one, the Si(1 1 1)-(7 × 7) reconstruction was obtained by annealing the substrates at 800 °C for 10 min. Following the annealing, the substrates were subjected to the following two treatments. For the second one, Si(1 1 1)-($\sqrt{3} \times \sqrt{3}$)-Sb surface, it was obtained by keeping the Sb flux and cooling down to 650 °C at a rate of 20 °C/min. At 650 °C the Sb shutter was closed and the substrate was directly cooled down to the deposition temperature. For the third one, Si(1 1 1)-($5\sqrt{3} \times 5\sqrt{3}$)-Sb surface, it was obtained by annealing the substrate at 650 °C for 20 min before cooling down to the deposition temperature.

In all cases, the growth started immediately after surface reconstructions formed. Before starting the GaSb growth, Sb shutter was open for 10 s to avoid Ga droplet formation [17,18]. The three samples were respectively grown on (7 × 7), ($\sqrt{3} \times \sqrt{3}$)-Sb, ($5\sqrt{3} \times 5\sqrt{3}$)-Sb surfaces at 340 °C. The epi-films grew at a rate of 3.1 nm/min to a final thickness of 200 nm. Surface morphologies and crystal quality were analyzed by scanning electron microscopy (SEM) and high-resolution X-ray diffraction (HRXRD). The specimens for high-resolution transmission electron microscopy (HRTEM) were prepared by focused ion beam (FIB). The amorphous layers induced by ion irradiation were cleaned at a low voltage of 5 kV for 10 s. The lattice matching at interfaces were studied by selected area electron diffraction (SEAD).

3. Results and discussion

Cross-sectional HRTEM is used to study the interfacial properties of GaSb/Si hetero-interfaces in detail. All the images in Fig. 2 show well delineated interfaces between the GaSb epi-films and Si substrates. For understanding the mode of lattice matching, the lattice fringes are marked by different color lines: green for substrates and red for epi-films. Inverse Fast Fourier Transformation (IFFT) images at the interfaces are shown in Fig. 2(d–f). In the epi-film grown on Si(1 1 1)-(7 × 7) surface, the orientation of epi-film lattice is in parallel with that of substrates. Due to $9d_{GaSb} \approx 10d_{Si}$, and it forms a coincidence lattice epitaxial interface with single edge dislocation [19]. Then periodic edge dislocations [11,12] which are marked by purple circles appear at the interface in Fig. 2(d). While for epi-films grown on Si(1 1 1)-($\sqrt{3} \times \sqrt{3}$)-Sb and ($5\sqrt{3} \times 5\sqrt{3}$)-Sb surface, the orientations are no more in parallel. They grow along a tilted crystallographic orientation [20] with no edge dislocations at the interfaces and every lattice fringe of the epi-films matches well with one lattice fringe of the substrate. It can be concluded

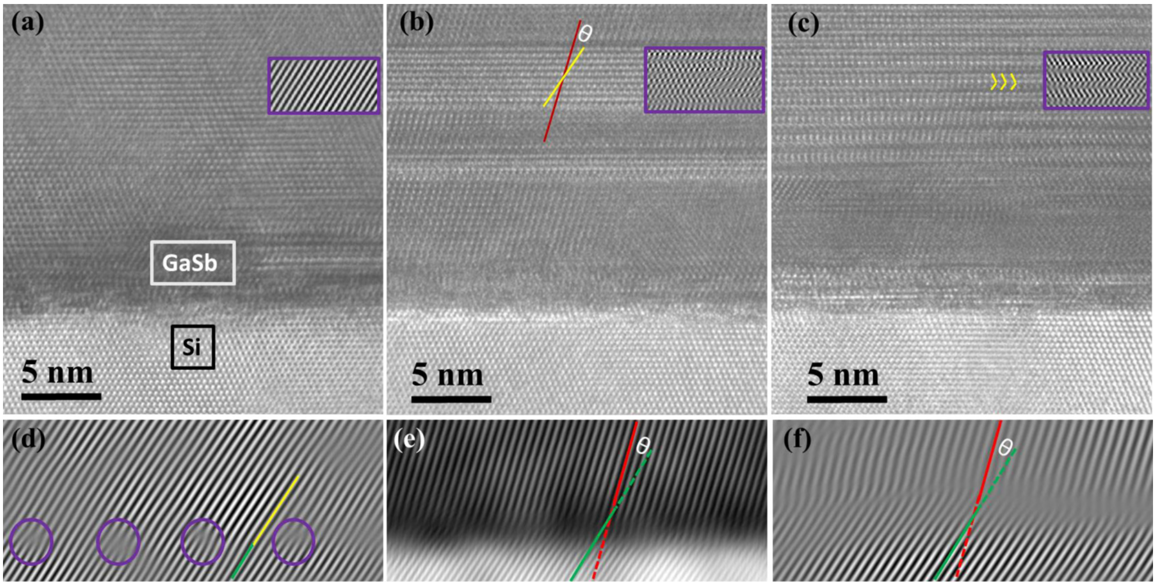

Fig. 2. Cross-sectional TEM images for the interfaces of GaSb films grown on Si(1 1 1) (a) (7 × 7), (b) ($\sqrt{3} \times \sqrt{3}$)-Sb, (c) ($5\sqrt{3} \times 5\sqrt{3}$)-Sb surface. Graphs (d), (e) and (f) show the inverse fast fourier transformation images at the interfaces of (a), (b), (c) respectively. Green lines represent the orientation of Si lattice fringes and the red ones are for GaSb epi-films'. They are in parallel in film grown on (7 × 7) surface in which periodic edge dislocations marked by purple circles appear for the large mismatch, while they intersect with an angle of 14° for films grown on ($\sqrt{3} \times \sqrt{3}$)-Sb and ($5\sqrt{3} \times 5\sqrt{3}$)-Sb surface. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)