Molecular Beam Epitaxy of GaSb on GaAs Substrates with Compositionally Graded LT-$GaAs_xSb_{1-x}$ Buffer Layers *

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(Received 11 August 2016)

We investigate the molecular beam epitaxy growth of GaSb films on GaAs substrates using compositionally graded $GaAs_xSb_{1-x}$ buffer layers. Optimization of $GaAs_xSb_{1-x}$ growth parameter is aimed at obtaining high GaSb crystal quality and smooth GaSb surface. The optimized growth temperature and thickness of $GaAs_xSb_{1-x}$ layers are found to be 420°C and 0.5 μm, respectively. The smallest full width at half maximum value and the root mean square surface roughness of 0.67 nm over $2 \times 2\,\mu m^2$ area are achieved as a 250 nm GaSb film is grown under optimized conditions.

PACS: 81.05.Ea, 81.10.Pq, 74.78.Fk, 81.15.−z DOI: 10.1088/0256-307X/34/1/018101

For the lattice matching point of view, an ideal substrate for the growth of Sb-based compounds is the GaSb substrate. However, epitaxy growth of Sb-based compounds on GaAs substrate has garnered considerable interest from researchers and developers since it has several advantages, including high quality with semi-insulating, large area, and low cost compared with substrates of GaSb.[1−4] Additionally, GaSb substrate-based devices are hard to integrate with read-out circuits in a monolithic technology.[5] GaAs substrates afford the possibility of integration for optoelectronics devices.[6,7] In spite of advantage of performances, there is a fundamental problem in the growth of GaSb on the GaAs substrate. The lattice mismatch between GaAs and GaSb is 7.8%. Stress and dislocation in the epitaxial film can be induced by the large difference in lattice constants between the film and the substrate.[8,9]

To overcome this problem, various buffer layers such as compositionally graded layers, superlattices, and low temperature (LT) layers have been widely used.[10−26] Although many kinds of buffer layers were used in various growth, only a few systematic studies on the compositionally graded LT-$GaAs_xSb_{1-x}$ buffers were reported. In this Letter, we investigate the effects of four different buffer layers and then systematically investigate the effects of the growth temperature and thickness of compositionally graded LT-$GaAs_xSb_{1-x}$ buffer layer on the crystal quality and the surface morphology of GaSb epilayers.

We grew our samples on semi-insulating GaAs substrates by the Riber412 molecular beam epitaxy system equipped with valved arsenic (As) and antimony (Sb) cracker cells. Dual-filament effusion cells were used for gallium (Ga). The substrate temperature was measured by a thermocouple calibrated from the GaAs oxide desorption temperature of 580°C. The background pressure of the growth chamber was maintained in the low 10^{-10} torr. The beam equivalent pressures (BEP) of the molecular fluxes were measured using an ionization gauge during each sample growth. Growth rates were 0.5 monolayer/s (ML/s) for all the layers. The V/Ⅲ beam equivalent pressure (BEP) ratio was 11 for GaAs and 8 for GaSb. X-ray diffraction (XRD) measurement was used to evaluate the crystal quality of samples. The surface morphology was characterized by an atomic force microscopy (AFM).

We grew four samples, as listed in Table 1, with four different buffer layers to examine the effect of buffer on crystal quality. Firstly, a 500 nm GaAs buffer layer was grown at 580°C to obtain a smooth GaAs surface for all the samples. Then, a 250 nm GaSb layer was grown directly after 500 nm GaAs for sample A, serving as a reference sample. For sample B, 250 nm $GaAs_{0.715}Sb_{0.285}$ and 250 nm $GaAs_{0.53}Sb_{0.47}$ were grown sequentially after 500 nm GaAs. For samples C and D, 500 nm compositionally graded $GaAs_xSb_{1-x}$ and $Al_{0.5}Ga_{0.5}As_ySb_{1-y}$ layer were grown after 500 nm GaAs, respectively. Lastly, 250 nm GaSb layer was grown for samples B, C, and D. For all the samples, the GaSb layer was grown at the temperature of 530°C, which was proved to be the optimum temperature for GaSb growth. The Sb content of $GaAs_xSb_{1-x}$ and $Al_{0.5}Ga_{0.5}As_ySb_{1-y}$ is changed gradually from 18% to 100%. The valves of Sb and As cracker cells can be controlled to change their flux. During the growth of $GaAs_xSb_{1-x}$ and

*Supported by the National Basic Research Program of China under Grant Nos 2015CB351902, 2015CB932402 and 2012CB619203, the National Natural Science Foundation of China under Grant Nos 61177070, 11374295 and U1431231, and the National Key Research Program of China under Grant No 2011ZX01015-001.

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$Al_{0.5}Ga_{0.5}As_ySb_{1-y}$, we linearly changed the valve from fully opened to closed for As cracker cell and oppositely for Sb cracker cell, to gradually change the composition of As and Sb.

Table 1. The structures of four samples.

Sample A	Sample B	Sample C	Sample D
250 nm GaSb	250 nm GaSb	250 nm GaSb	250 nm GaSb
None	$GaAs_{0.53}Sb_{0.47}$ (250 nm) $GaAs_{0.715}Sb_{0.285}$(250 nm)	500 nm $GaAs_xSb_{1-x}$	500 nm $Al_{0.5}Ga_{0.5}As_ySb_{1-y}$
500 nm GaAs	500 nm GaAs	500 nm GaAs	500 nm GaAs
GaAs substrate	GaAs substrate	GaAs substrate	GaAs substrate

Figure 1 shows the full width at half maximum (FWHM) of the XRD curves of the GaSb layer as a function of four different samples. The FWHM is smallest when the buffer designed is the compositionally graded $GaAs_xSb_{1-x}$ layer. From sample A to sample C, the FWHM result shows that the $GaAs_xSb_{1-x}$ buffer plays a positive rule in improving the quality of the crystal GaSb layer. However, the result of FWHM of sample D shows that the quality of crystal is degraded by inserting Al content. The sample C containing the compositionally graded $GaAs_xSb_{1-x}$ exhibits a mirror surface after GaSb growth. However, sample A without the compositionally graded $GaAs_xSb_{1-x}$ buffer layer has a clouded surface indicating that the GaSb growth was not suitable. These results clearly demonstrate that the compositionally graded $GaAs_xSb_{1-x}$ buffer layer is very useful to improve the GaSb crystal grown on GaAs substrates.

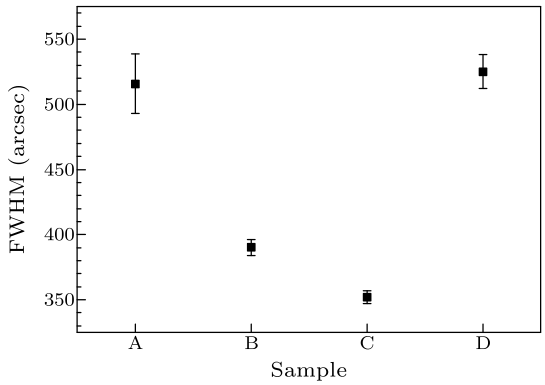

Fig. 1. Dependence of FWHM of XRD curves on four samples with different buffer layers.

To find the optimum growth condition, we investigate the dependence of crystal quality on the growth temperature and thickness of compositionally graded $GaAs_xSb_{1-x}$ buffer layers. We grew another group of samples using the same structure like sample C, including four samples with different growth temperatures of $GaAs_xSb_{1-x}$ layer and four samples with different thicknesses. The temperature of the $GaAs_xSb_{1-x}$ layer was in the range of 360–480℃ and the thickness is in the range of 0.25–1 μm. Figure 2 shows the FWHM of XRD curves of the GaSb epilayer as a function of the growth temperature of the compositionally graded $GaAs_xSb_{1-x}$ layer. The $GaAs_xSb_{1-x}$ thickness was fixed at 0.5 μm. As shown in Fig. 2, the smallest FWHM is obtained at the temperature of 420℃. In the higher-temperature range of 420–480℃, there is a sharp increase in the FWHM, and the corresponding samples' surfaces were clouded. Consequently, 420℃ seems to be the optimum growth temperature of compositionally graded $GaAs_xSb_{1-x}$ buffer layers. Such a low temperature of compositionally graded $GaAs_xSb_{1-x}$ grown is a novel result.

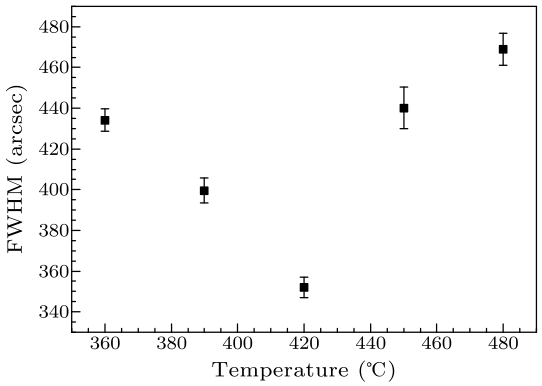

Fig. 2. Dependence of FWHM of XRD curves on growth temperature of the compositionally graded $GaAs_xSb_{1-x}$ buffer layer.

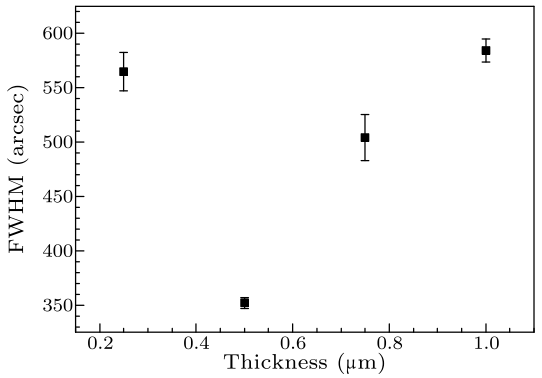

Fig. 3. Dependence of FWHM of XRD curves on the thickness of the compositionally graded $GaAs_xSb_{1-x}$ buffer layer.

To find the optimum thickness of the $GaAs_xSb_{1-x}$ layer, we vary the thicknesses from 0.25 μm to 1 μm.

Figure 3 shows the $GaAs_xSb_{1-x}$ thickness dependence of the FWHM of the XRD curves. The growth temperature of $GaAs_xSb_{1-x}$ was fixed at 420℃. As shown in Fig. 3, the smallest FWHM is obtained by a 0.5 μm $GaAs_xSb_{1-x}$ buffer layer. It is indicated that the $GaAs_xSb_{1-x}$ layer of thinner than 0.5 μm cannot inhibit the threading dislocation adequately. On the other hand, the $GaAs_xSb_{1-x}$ layer of thicker than 0.5 μm, which is grown under the optimized growth temperature, can also degrade the crystal quality of the GaSb epilayer. We define the composition–thickness ratio as the change of Sb composition of $GaAs_xSb_{1-x}$ in every micrometer. In our experiment, the great GaSb quality can be obtained by the composition–thickness ratio of 1.64.

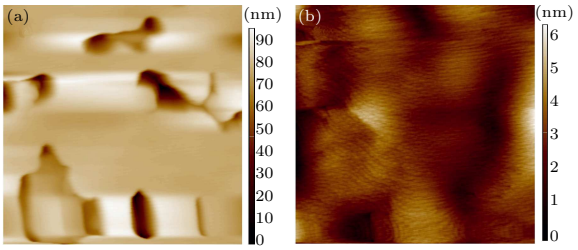

Fig. 4. AFM images ($2 \times 2\,\mu m^2$) of 250 nm GaSb films grown on GaAs substrates without (a) and with (b) a compositionally graded $GaAs_xSb_{1-x}$ buffer layer.

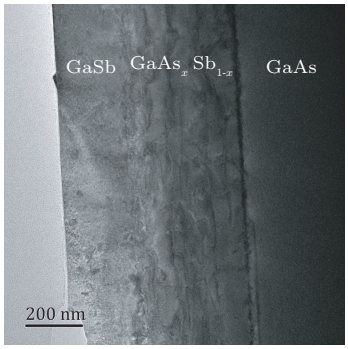

Fig. 5. The TEM image of the GaSb layer on the GaAs substrate with the $GaAs_xSb_{1-x}$ buffer.

We measure the mounds density of the sample with and without GaAsSb buffer layers using a 3D microscope over a $100 \times 100\,\mu m^2$ area. The density of mounds is about $1\times10^{-9}\,cm^{-2}$ for the sample without GaAsSb buffer layers and $1 \times 10^{-7}\,cm^{-2}$ for the sample with GaAsSb buffer layers. This result shows that the GaAsSb buffer layers have a positive role in decreasing density of mounds. Screw dislocations are considered to be the origin of these mounds and make the surface rough.[27] Indirectly, this result proves that GaAsSb buffer layers are able to decrease density of screw dislocation. AFM measurement was performed in a taping mode to study the surface morphology. Figure 4(a) shows the surface morphology of a 250-nm-thick GaSb layer grown directly on GaAs. The surface consists of a large number of mounds. The rms surface roughness is about 10.2 nm over a $2 \times 2\,\mu m^2$ area. As a 0.5 μm compositionally graded $GaAs_xSb_{1-x}$ buffer layer is inserted between the GaSb epilayer and the GaAs substrate, the sample shows an atomically stepped surface, as shown in Fig. 4(b). The atom steps are about 0.4 nm high without step bunching. The rms surface roughness decreases to only 0.67 nm over a $2 \times 2\,\mu m^2$ area. It indicates that the compositionally graded $GaAs_xSb_{1-x}$ buffer layer improves the crystal quality of the GaSb layer greatly. Transmission election microscopy (TEM) measurements were performed to study the origin source of improving GaSb layer quality by inserting the compositionally graded $GaAs_xSb_{1-x}$ buffer layer. From the TEM image (Fig. 5) we can see that massive dislocations exist in the $GaAs_xSb_{1-x}$ buffer layer instead of the GaSb layer. We believe that the insulation of dislocation in the $GaAs_xSb_{1-x}$ buffer layer plays a vital role in improving the crystal quality of the GaSb layer.[28]

In summary, the effect of four different buffer layers on the crystal qualities of GaSb layer has been investigated. The result shows that the compositionally graded $GaAs_xSb_{1-x}$ buffer is the best one in the four samples. Then, the effect of the compositionally graded $GaAs_xSb_{1-x}$ buffer layer to the crystal qualities of GaSb layers is investigated. The smallest value of FWHM is obtained by inserting a 0.5 μm 420℃ compositionally graded $GaAs_xSb_{1-x}$ buffer layer. The surface morphology is strongly improved, and the rms surface morphology is only 0.67 nm over a $2 \times 2\,\mu m^2$ area. It is concluded that the compositionally graded LT-$GaAs_xSb_{1-x}$ buffer layer is really effective in improving the crystal quality of GaSb layers.

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