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Citation: Chin. Phys. B . 2019, 28(11): 118102 . **doi:** 10.1088/1674-1056/ab4d49
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Chin. Phys. B . 2019, 28(7): 078102 . **doi:** 10.1088/1674-1056/28/7/078102

Effect of growth temperature of $GaAs_xSb_{1-x}$ metamorphic buffer layer on electron mobility of InAs/AlSb heterostructures grown on Si substrate*

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(Received 4 June 2019; revised manuscript received 20 September 2019; published online 30 October 2019)

The InAs/AlSb heterostructures with step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layers grown on Si substrates by molecular beam epitaxy are studied. The step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layers are used to relax the strain and block defects at each interface of the layers. Meanwhile, adding Sb to GaAs is also beneficial to suppressing the formation of dislocations in the subsequent materials. The influences of the growth temperature of the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer on the electron mobility and surface topography are investigated for a series of samples. Based on the atomic force microscopy (AFM), high resolution x-ray diffraction (HRXRD), reciprocal space map (RSM), and Hall measurements, the crystal quality and composition of $GaAs_xSb_{1-x}$ layer are seen to strongly depend on growth temperature while keeping the Ga growth rate and V/III ratio constant. The results show that the highest electron mobility is 10270 $cm^2/V{\cdot}s$ and the roughness is 4.3 nm for the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer grown at a temperature of 410 °C.

Keywords: Si, sticking coefficients, growth temperature, $GaAs_xSb_{1-x}$ metamorphic buffer

PACS: 81.05.Ea, 81.10.–h, 81.70.–q **DOI:** 10.1088/1674-1056/ab4d49

1. Introduction

The integration of III–V materials on Si substrate has been an active research field for many years.[1,2] In the III–V compounds, the growth of InAs/AlSb heterostructures has been explored for over thirty years due to the advantageous electron mobility and sheet electron density in the InAs channel, as well as due to the large conduction band offset between InAs and AlSb.[3] Therefore, it is significant to investigate the growth of InAs/AlSb heterostructures on Si substrates for their potential important applications in the field of high mobility transistors.

Although InAs/AlSb heterostructures have been successfully grown on GaAs and InP substrates by using an AlGaSb buffer,[4,5] the reports on the growth of such heterostructures on Si substrates are limited. The growth of InAs/AlSb heterostructures on Si substrates remains a challenge because numerous defects are generated due to the large difference in lattice constant (13%), thermal expansion coefficient (88%), and inconsistent polarity between the two material systems. Therefore, an appropriate buffer between the AlGaSb buffer layer and the Si substrate is needed to prevent the dislocations from propagating, as well as reduce the degradation of the material and device quality. In previous reports, a thick Si/Ge/GaAs stacked buffer layer,[6] GaP buffer layer,[7] GaAs buffer layer,[8] GaSb or AlSb initiation layer[9] on Si were used to accommodate the lattice mismatch. In addition, it is easier to release strain by using ternary compounds, for example, the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layers are used. Meanwhile, adding Sb into GaAs is also beneficial to suppressing the formation of dislocations in the subsequent materials. Moreover, the growth temperature and V/III ratio are crucial to growing the double V elements of GaAsSb buffer layer. Although GaAsSb buffer layer has been reported in some literature,[10,11] the information is still insufficient about the influence of the growth temperature on the electron mobility of the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer for such heterostructures grown on the Si substrate.

In this paper, the effects of the growth temperature on the electron mobility and surface morphology of the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer for InAs/AlSb heterostructure on Si are investigated for a series of samples. By optimizing the growth temperature of the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer, the surface topography and electrical properties of InAs/AlSb heterostructures are

*Project supported by the National Defense Advanced Research Project, China (Grant No. 315 xxxxx301), the National Defense Innovation Program, China (Grant No. 48xx4), the National Key Technologies Research and Development Program, China (Grant No. 2018YFA0306101), the Scientific Instrument Developing Project of the Chinese Academy of Sciences (Grant No. YJKYYQ20170032), and the National Natural Science Foundation of China (Grant No. 61505196).

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improved and also confirmed by the atomic force microscopy (AFM), high resolution x-ray diffraction (HRXRD), reciprocal space map (RSM), and Hall measurements.

2. Experimental procedures

The InAs/AlSb heterostructure with step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layers is grown on a vicinal Si (100) wafer with a nominal miscut of 4° with respect to the [110] direction by molecular beam epitaxy (MBE). After the regular outgassing process in the preparation chamber, the wafers were transferred into the deposition chamber. Prior to growth, the Si substrates were heated to 700 °C for 10 min and 1100 °C for 20 min under arsenic flux to achieve oxygen desorption.

Figure 1 shows the detailed layer structure for each of all the samples prepared for this study. The growth ofeach sample started with a 3-nm-thick GaAs layer grown at 300 °C using migration-enhanced epitaxy, followed by a step-graded $GaAs_xSb_{1-x}$ buffer layer with different compositions, each with 300 nm in thickness. The As/Ga and Sb/Ga beam ratio of $GaAs_{x1}Sb_{1-x1}$ in the first layer were 20 and 2, respectively. As well as the As/Ga and Sb/Ga beam ratio of $GaAs_{x2}Sb_{1-x2}$ in the second layer were 20 and 4, respectively. No interruption was performed during the growth of the step-graded $GaAs_xSb_{1-x}$ buffer layer. The growth temperatures investigated were 380 °C, 410 °C, 430 °C, 460 °C, 520 °C, and 580 °C. The InAs/AlSb heterostructures with different growth temperatures were named samples A, B, C, D, E, and F, respectively. Then a 50-nm GaSb buffer layer, a 200-nm AlSb buffer layer, a 700-nm $Al_{0.75}Ga_{0.25}Sb$ as buffer layer, a 50-nm AlSb bottom barrier layer, a 15-nm InAs channel layer, a 10-nm AlSb upper barrier layer, and a 5-nm InAs cap layer were deposited on the 300-nm $GaAs_xSb_{1-x}$ buffer layer in turn. The growth temperature of GaSb, AlSb, $Al_{0.75}Ga_{0.25}Sb$, and InAs materials were 540 °C, 560 °C, 560 °C, and 500 °C, respectively.

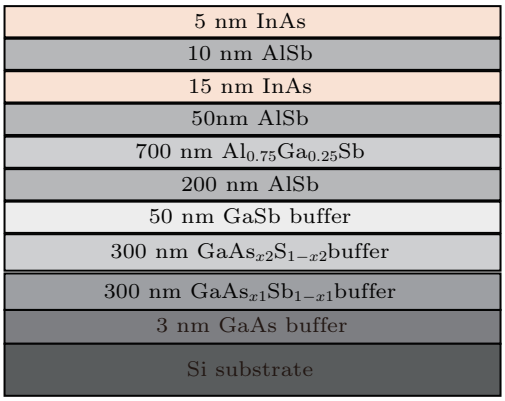


Fig. 1. Schematic diagram for investigated sample.

AFM was used to examine the surface morphologies of all samples. The crystalline quality of the layer was characterized by HRXRD RSM measurement. Hall measurements were conducted at room temperature with the Van der Pauw pattern.

3. Results and discussion

The effect of growth temperature of step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer on surface morphology is investigated by AFM. It can be seen from Fig. 2(b) that sample B has a flat surface with a root mean square (RMS) roughness value of 4.3 nm, while the surface of sample A and samples C–F present a very rough surface with an RMS roughness value of 18.74 nm, 7.16 nm, 8.4 nm, 15.8 nm, and 33.9 nm, respectively. Thus, there is a relationship between the surface morphology and the substrate temperature. At the low substrate temperature of 380 °C (sample A), the adatoms cannot migrate sufficiently and the nucleation growth is likely to occur in the nucleation centers such as defects and kinks on substrate surface. In addition, as is well known, the large difference in thermal expansion coefficient is also a major factor affecting the epitaxy quality of $GaAs_xSb_{1-x}$ on Si. Thus, when the growth temperature is high, such as 580 °C (sample F) and 520 °C (sample E), the crystal grains of the film are coarsened, which increases the thermal stress in the film, thereby affecting the growth quality of the film and resulting in poor surface morphology. Therefore, to utilize step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer for InAs/AlSb heterostructure on Si, growth condition should be carefully controlled to achieve desired crystalline quality of step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer, which is sensitive to growth condition.

The crystalline quality for each of the samples is studied by using HRXRD with Cu $K\alpha 1$ radiation ($\lambda = 1.5406$ Å). Figure 3 shows the HRXRD rocking curves of the symmetrical 004 reflections and asymmetrical 115 reflections for all samples. Apart from the Si substrate peak, three main peaks can be observed in each scan curve, where the narrower peak corresponds to $Al_{0.75}Ga_{0.25}Sb$ buffer layer and the broader double peak corresponds to the $GaAs_xSb_{1-x}$ buffer layer. The $GaAs_xSb_{1-x}$ buffer layer can provide greater flexibility for strain design by adjusting the lattice mismatch extent between $Al_{0.75}Ga_{0.25}Sb$ buffer layer and Si substrate. Typically, the 004 and 115 peak positions for a fully relaxed $GaAs_xSb_{1-x}$ crystal are located at 30.37–33.02 °C and 41.35–45.07 °C, respectively. However, it can be seen that the growth temperature has a great influence on the composition and crystal quality of $GaAs_xSb_{1-x}$, which further affects the growth quality of subsequent materials, such as $Al_{0.75}Ga_{0.25}Sb$ buffer layer. Epitaxial growth is performed at the substrate temperature of 380–580 °C. When the substrate temperature is below 380 °C, spot patterns appear in the reflection high-energy electron diffraction (RHEED) patterns. In a previous report, a similar situation of the GaAs film grown on Si substrate has been reported by Choi *et al.*[12] As can be seen from Fig. 3, the diffraction

intensity of $GaAs_xSb_{1-x}$ is lowest for the sample prepared at 380 °C, which is because the low growth temperature leads Ga atoms to be unable to migrate sufficiently on the surface, resulting in poor growth quality of $GaAs_xSb_{1-x}$ layer. When the substrate temperature is higher than 380 °C, just after the onset of growths, the RHEED patterns indicate that the deposited film occasionally includes a twin and as the growth proceeds the film becomes single crystalline. A similar situation in $GaAs_{1-x}P_x$ alloy was studied by Matsushima and Gonda.[13] The compositions of As of all samples except sample A in each step-graded $GaAs_xSb_{1-x}$ buffer layer are verified by HRXRD of the symmetrical 004 reflections and asymmetrical 115 reflections as shown in Table 1. The variation of composition ratio with substrate temperature may be due to the variation of sticking coefficient. When the growth temperature rises from 410 °C to 520 °C, the sticking coefficient of As increases, while the desorption rate of Sb increases. As a result, the composition of As in $GaAs_xSb_{1-x}$ layer increases, while the peaks positions of 004 and 115 of GaSb change into those of GaAs. As can be seen from Table 1, the lowest As fractions of the $GaAs_{x1}Sb_{1-x1}$ and $GaAs_{x2}Sb_{1-x2}$ buffers in sample B are determined to be 64.62%–68.15% and 18.5%–26.57%, respectively.

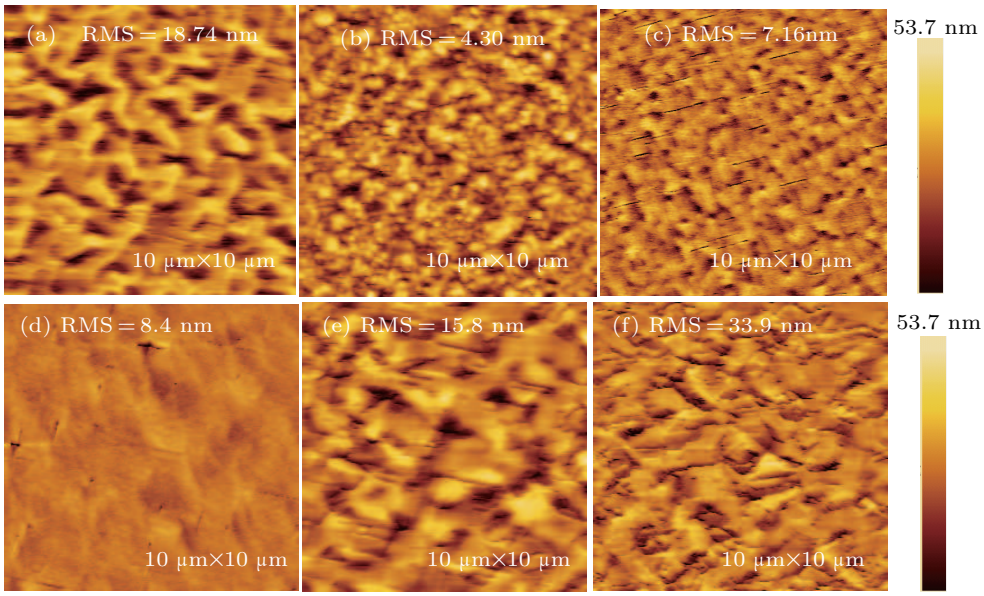


Fig. 2. 10 μm×10 μm AFM images of (a) sample A, (b) sample B, (c) sample C, (d) sample D, (e) sample E, and (f) sample F.

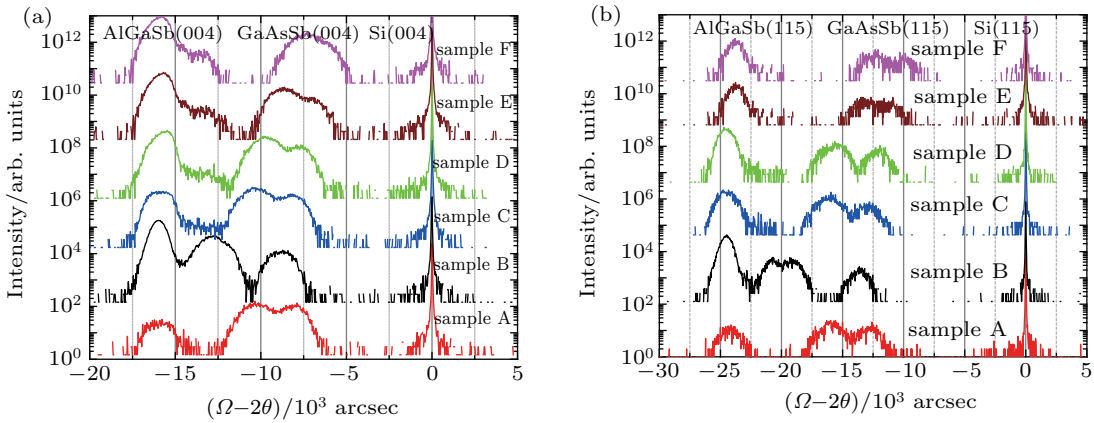


Fig. 3. HRXRD rocking curves of (a) (004) peak and (b) (115) peak for various samples.

Table 1. Compositions of As in $GaAs_xSb_{1-x}$ from HRXRD measurements.

Sample	Growth temperature/°C	Value of $x1$/%	Value of $x2$/%
B	410	64.62–68.15	18.5–26.57
C	430	73.08–73.69	50.01–54.89
D	460	76.84–79.16	54.5–57.22
E	520	84.27–86.04	69.6–74.45
F	580	82.85–92.46	82.8–89.72

Of the samples B, C, D, E, and F, it is also observed that sample B has the Bragg angle peaks of $GaAs_xSb_{1-x}$ and $Al_{0.75}Ga_{0.25}Sb$ closest to each other, indicating that the lattice constant mismatch between $GaAs_xSb_{1-x}$ and $Al_{0.75}Ga_{0.25}Sb$ is small, which would imply that sample B contains the fewest misfit dislocations. As can be seen from Fig. 3, at a

growth temperature of 410 °C, the $GaAs_xSb_{1-x}$ has the highest diffraction intensity and the narrowest full width half maximum (FWHM), which indicates that this temperature is most suitable for growing the $GaAs_xSb_{1-x}$ layer. The $GaAs_xSb_{1-x}$ layer then acts as a template for the succeeding growth of thick $Al_{0.75}Ga_{0.25}Sb$ bulk layer. Therefore, it can be inferred that the quality of $Al_{0.75}Ga_{0.25}Sb$ in sample B is best.

The $Al_{0.75}Ga_{0.25}Sb$ buffer layer can release the strain caused by the lattice mismatch between $GaAs_xSb_{1-x}$ and InAs channel layer. Thus, the quality of the $Al_{0.75}Ga_{0.25}Sb$ material also directly affects the overall quality of the InAs/AlSb heterostructure. The FWHMs and diffraction intensities of $Al_{0.75}Ga_{0.25}Sb$ buffer layer for all samples extracted from XRD measurements are listed in Table 2. It can be seen that the $Al_{0.75}Ga_{0.25}Sb$ layer of the sample A exhibits a minimum FWHM,but the weakest diffraction intensity from sample A indicate its poor crystallinity.

Table 2. Diffraction intensity and FWHM of $Al_{0.75}Ga_{0.25}Sb$ from HRXRD measurements. The unit a.u. is short for arbitrary units.

Sample	Diffraction intensity of 004/a.u	FWHM of 004/arcsec	Diffraction intensity of 115/a.u	FWHM of 115/arcsec
A	22	562.5	16	183.6
B	1251	842.4	340	914.4
C	135	1537.2	51	993.6
D	366	1072.8	120	1094.4
E	349	1018.8	41	633.6
F	345	1002.2	40	636.1

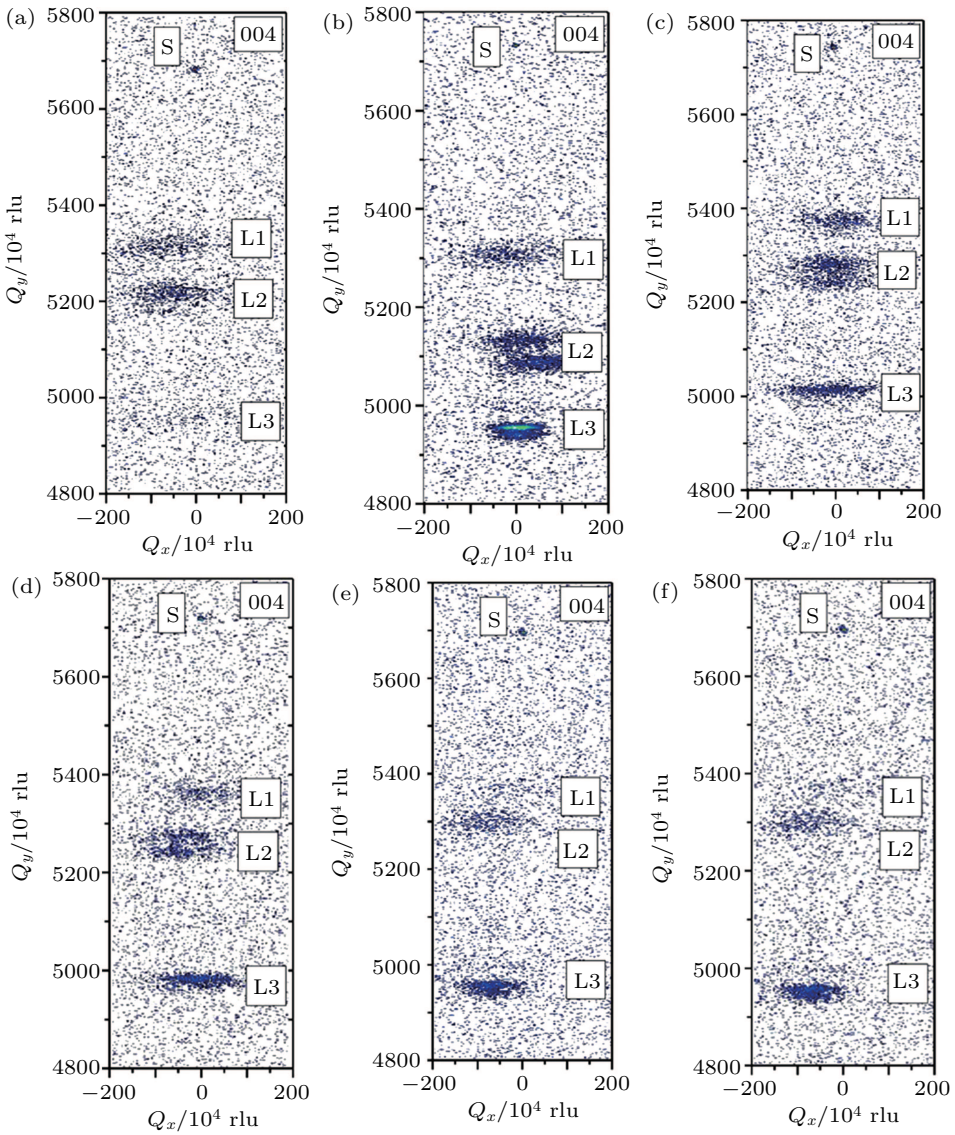


Fig. 4. XRD RSMs of symmetrical (004) for (a) sample A, (b) sample B, (c) sample C, (d) sample D, (e) sample E, and (f) sample F.

However, sample B has the narrowest FWHM and strongest diffraction intensity are observed in the $Al_{0.75}Ga_{0.25}Sb$ layer in all the samples. A suitable growth temperature of $GaAs_xSb_{1-x}$ buffer layer can result in an improvement of the film surface morphology and reduce the density of misfit dislocations inside the $GaAs_xSb_{1-x}$ buffers which migrate inside the $Al_{0.75}Ga_{0.25}Sb$ layer. It could be a possible explanation for the lower FWHM value observed for the sample B.

The crystalline quality of the epitaxial layer is further assessed by XRD RSM measurements. Figures 4(a)–4(f) show the logarithmic XRD RSM of the symmetrical (004) for sample A, sample B, sample C, sample D, sample E, and sample F, respectively. Apart from the Si substrate peak denoted by S, three epitaxial peaks are also identified from Figs. 4(a)–4(f), denoted by L1, L2, and L3, respectively. The epitaxy peaks with relatively strong intensities correspond to the $Al_{0.75}Ga_{0.25}Sb$ buffer layer (denoted as L3), while the weaker L1 and L2 correspond to the $GaAs_xSb_{1-x}$ layers with different compositions. From the analysis in Fig. 3, it can be seen that the epitaxial material of sample A is indeed poorer, while sample B is the best. The $GaAs_xSb_{1-x}$ layer of sample C, sample D, sample E and sample F change their peak positions due to the high growth temperature and the different sticking coefficients of As and Sb. Such a comparison furtherdemonstrates that the quality of sample B is superior to that of other samples.

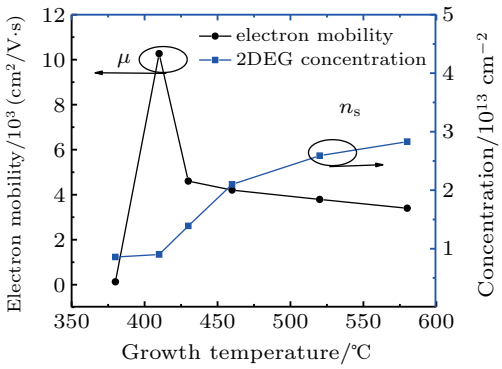


Fig. 5. Electron mobility μ and 2DEG concentration n_s *versus* growth temperature.

The electrical characterizations of the various samples are investigated by examining Hall measurements as shown in Fig. 5. For two-dimensional electron gas (2DEG) concentration, a similar situation was studied by Nguyen[14] in the unintentionally doped InAs/AlSb quantum wells,which was grown on a GaAs substrate. Their study showed that the electrons in the unintentionally doped InAs/AlSb quantum wells come from three different sources: surface donors responsible for a large fraction of the high concentrations usually found in wells with thin top barriers; bulk donors in the AlSb barriers, and interface donors at the InAs–AlSb interfaces of the well. Thus, it can be seen from Fig. 5 that number of electrons is as high as 8.58×10^{12} cm^{-2}–2.83×10^{13} cm^{-2} that accumulate in the quantum well. These electrons source from the surface donors, bulk donor in the undoped AlSb barrier layer, and the AlSb/InAs interface donor.

As the growth temperature increases from 380 °C to 410 °C, the electron mobility at room temperature sharply increases from 129.6 cm^2/V·s (sample A) to 10270 cm^2/V·s (sample B) and then it decreases to 3399 cm^2/V·s (sample F) as the growth temperature is increased from 410 °C to 580 °C. It is found that the growth temperature of the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer plays an important role in determining the electron mobility. By optimizing the growth temperature of the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer, electron mobility is obtained to be as high as 10270 cm^2/V·s (sample B) and the sheet electron density is 9.01×10^{12} cm^{-2} at room temperature. The reason why the sample B can achieve the highest electron mobility can be explained as follows. First, the composition of $GaAs_xSb_{1-x}$ layer is strongly dependent on the growth temperature under a certain Ga growth rate and V/III ratio due to the fact that As and Sb possess different sticking coefficients. At a growth temperature of 410 °C, the small lattice mismatch between $GaAs_xSb_{1-x}$ and $Al_{0.75}Ga_{0.25}Sb$ buffer layer implies that sample B contains fewer misfit dislocations, which is corresponding to the analysis in Fig. 3. The misfit dislocations in the film layer act as scattering centers and reduce the electron mobility. Thus, there is the least density of misfit dislocations in sample B grown at 410 °C, leading to the highest electron mobility. Second, the suitable growth temperature is beneficial to the diffusing and sticking of atoms between $GaAs_xSb_{1-x}$ buffer layer and Si substrate, which means that the growth temperature is important for improving the crystal quality of $GaAs_xSb_{1-x}$ buffer layer. The $GaAs_xSb_{1-x}$ buffer layer will act as a template for succeeding grown epitaxy layer of $Al_{0.75}Ga_{0.25}Sb$ buffer layer and InAs/AlSb active layer, therefore the quality of succeeding layers depends greatly on the $GaAs_xSb_{1-x}$ buffer layer as well.The analysis of AFM, XRD and RSM measurement show that the sample B has a more flat surface and a better crystal quality than the other samples. Therefore, the low electron mobility of samples A, C, D, E, F could be associated with the poorer epitaxial layer quality of $GaAs_xSb_{1-x}$ buffer layer and larger lattice mismatch between $GaAs_xSb_{1-x}$ and $Al_{0.75}Ga_{0.25}Sb$ buffer layer. Lin *et al.*[6] and Desplanque *et al.*[7] demonstrated that their samples have an electron mobility larger than 10000 cm^2/V·s, but our electron mobility is lower. However, it should be noted that their growth methods were different from ours. In their studies they mainly used metal–organic chemical vapor deposition (MOCVD) or Metal organic vapor phase epitaxy (MOVPE) to grow buffer layer and then MBE to grow InAs/AlSb heterostructures. The InAs/AlSb heterostructures with step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layers dis-

cussed in this paper are grown on Si substrates solely by using the MBE. Although the electron mobility of sample B is greatly improved, there is clear indication that better material quality can be expected if the growth condition of each layer is further optimized.

4. Conclusions

In the present research, a series of samples in which step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layers are used for InAs/AlSb heterostructures to be grown on Si substrate is investigated for ascertaining the effects of the growth temperature on the electron mobility and surface topography. The HRXRD and RSM measurements show that the As fractional compositions of step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer in samples are seen to be different for different growth temperatures, which can be attributed to the difference in sticking coefficient between As and Sb at different growth temperatures, which then affects the crystal quality. The flat surface and high electron mobility can be obtained at an optimized growth temperature, which is confirmed by AFM and Hall measurements, respectively. The results show that the highest electron mobility currently achieved is 10270 $cm^2/V{\cdot}s$ and the RMS value is 4.3 nm, in which the step-graded $GaAs_xSb_{1-x}$ metamorphic buffer layer is grown at a temperature of 410 °C. The result of this study is also applicable in the field of various electronic devices, particularly for high electron mobility transistors.

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