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Effects of growth temperature and metamorphic buffer on electron mobility of InAs film grown on Si substrate by molecular beam epitaxy*

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The growth of the InAs film directly on the Si substrate deflected from the plane (100) at 4° towards (110) has been performed using a two-step procedure. The effect of the growth and annealing temperature on the electron mobility and surface topography has been investigated for a set of samples. The results show that the highest electron mobility is 4640 $cm^2/V{\cdot}s$ in the sample, in which the 10-nm InAs nucleation layer is grown at a low temperature of 320 °C followed by ramping up to 560 °C, and the nucleation layer was annealed for 15 min and the second layer of InAs is grown at 520 °C. The influence of different buffer layers on the electron mobility of the samples has also been investigated, which shows that the highest electron mobility of 9222 $cm^2/V{\cdot}s$ at 300 K is obtained in the sample grown on a thick and linearly graded InGaAlAs metamorphic buffer layer deposited at 420 °C.

Keywords: InAs, Si, high electron mobility, growth temperature, InGaAlAs metamorphic buffer

PACS: 81.05.Ea, 81.10.–h, 81.70.–q **DOI:** 10.1088/1674-1056/28/2/028101

1. Introduction

Integration of group III–V materials on a silicon platform has been one of the most promising techniques for large-scale integrated circuits.[1–4] In the group III–V compounds, InAs has higher electron mobility, which is several times larger than that of Si. It is one of the best candidate channel materials for the next generation Si-based devices. The growth of InAs epitaxial films on Si substrates is of particular interest in terms of its potentially important applications in the field of various electronic devices, especially in high-mobility transistors.[5]

In general, it is difficult to achieve high-quality InAs epilayers on Si substrates due to the large difference in lattice constant (11.6%), thermal expansion coefficient (74.5%), and polarity. To date, although most studies[6–9] have been devoted to the growth of InAs on Si substrates, the lattice-mismatch-related problems causing low electron mobility have not yet been solved. In the case of InAs growth directly on Si, the electron mobility in the InAs film layer was found to be between 2000 $cm^2/V{\cdot}s$ and 5100 $cm^2/V{\cdot}s$.[10,11] These studies mainly investigated the influence of the layer thickness on the electrical and morphological properties of the InAs film by metalorganic vapor-phase epitaxy (MOVPE). However, the influence of growth and annealing temperature on the electron mobility in the InAs film layer directly grown on Si substrate is rarely reported. In addition, a suitable metamorphic buffer is needed to release the lattice strains with silicon, which plays an important role in overcoming the propagation of threading dislocations and degradation of the material. Linear[12] or step-graded buffer layers[13] and strained superlattices[14] are commonly used to form high-quality metamorphic layers for large mismatch epitaxial growth. Alloys such as graded InAlAs and InGaAlAs are used for standard production of metamorphic high electron mobility transistor on GaAs substrates. Although so many buffer layer methods are used for InAs on Si, there are few reports on the influence of the InAlGaAs metamorphic layer on the electron mobility of the InAs film layer grown on the Si substrate.

In this paper, the growth of InAs film directly on the Si substrate deflected from the plane (100) at 4° towards (110) has been performed using a two-step procedure. A set of samples have been used to investigate the effect of the growth and annealing temperature on the electron mobility and surface topography. The effect of the different metamorphic buffer layer on the electron mobility of the samples has also been investigated, which shows that the electron mobility has been significantly improved via inserting an InAlGaAs metamorphic buffer layer.

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2. Experimental procedures

The high-quality InAs epitaxial film was grown on the Si substrate deflected from the plane (100) at 4° towards (110) by molecular beam epitaxy (MBE). After the normal outgassing process in the preparation chamber, the wafers were transferred to 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 oxide desorption. The oxide elimination control was carried out with the reflection high-energy electron diffraction (RHEED) method. Figure 1 shows the RHEED patterns before and after the oxide elimination.

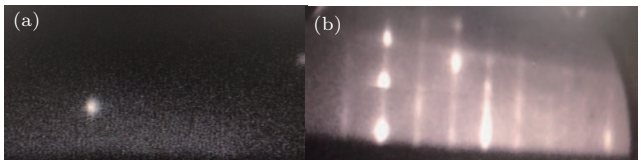


Fig. 1. RHEED pattern of deoxidation process (a) before deoxidation, and (b) after deoxidation.

2.1. InAs film directly grown on Si

The growth of InAs film directly on the Si substrate was implemented using a two-step procedure. To investigate the effect of the growth temperature on the first nucleation layer, a set of samples were grown with high and low temperatures. A 10-nm thick InAs nucleation layer was first deposited at 595 °C, 585 °C, 575 °C, 565 °C, 400 °C, 360 °C, and 320 °C. Then a series of samples were grown by a two-step growth method, consisting of a low temperature ($T_1 \leq 340$ °C) layer followed by the second layer deposition of a 1000-nm thick bulk layer at a higher temperature T_2 between 450 °C and 540 °C, as shown in Fig. 2, to study the influence of the growth temperature on the electron mobility. Also, in order to study the effect of *in situ* annealing on the electron mobility, the growth of the nucleation layer of three samples was performed at a low temperature of 320 °C followed by ramping up to 400 °C, 560 °C, and 580 °C, where the nucleation layer was annealed for 15 min and a second layer was grown at 520 °C.

1000 nm InAs	0.5 ML/s	450 ℃~540 ℃
10 nm InAs	0.1 ML/s	100 ℃~340 ℃
Si substrate		

Fig. 2. Sample structures of InAs film directly grown on Si substrates.

2.2. The growth of InAs film with a metamorphic buffer

In this work, two different structures are used as shown in Fig. 3. After the oxide desorption process, a 930-nm GaAs layer was subsequently deposited by the five-step growth process to smooth out the surface. The 10-nm GaAs buffer layer is formed at a low temperature followed by ramping up to a high temperature and annealed for 6 min, and the growth of the following layers continued by the same approach. The introduction of five buffer layers results in an improvement of the film surface morphology and reduces the density of threading dislocations inside the GaAs buffers, depressing the propagation of defects towards the InAs layer. For one structure (sample A), the InAs film layer is directly deposited on the GaAs buffer layer, as shown in Fig. 3(a). For another structure (sample B), the InGaAlAs layer is grown on the final GaAs buffer, while controlling the linear decrease of gallium concentration and the linear increase of indium and aluminum composition. The V/III flux ratio of InGaAlAs layer is maintained at about 15. The lattice constant is gradually expanded by inserting a 2.5-μm-thick InGaAlAs metamorphic buffer layer, as shown in Fig. 3(b). Next, an InAs film layer is deposited on the top of InGaAlAs layer, while the V/III flux ratio is maintained at about 10. The growth rate and temperature are shown in Fig. 3.

1000 nm InAs	0.3 ML/s	500 ℃
20 nm GaAs buffer	0.64 μm/h	600 ℃
200 nm GaAs buffer	0.64 μm/h	600 ℃
500 nm GaAs buffer	0.64 μm/h	600 ℃
200 nm GaAs buffer	0.3 ML/s	480 ℃
10 nm GaAs buffer	0.1 ML/s	380 ℃
Si substrate		

(a)

1000 nm InAs	0.4 ML/s	500 ℃
2500 nm InGaAlAs	0.6 ML/s	410 ℃~420 ℃
20 nm GaAs buffer	0.64 μm/h	600 ℃
200 nm GaAs buffer	0.64 μm/h	600 ℃
500 nm GaAs buffer	0.64 μm/h	600 ℃
200 nm GaAs buffer	0.3 ML/s	480 ℃
10 nm GaAs buffer	0.1 ML/s	380 ℃
Si substrate		

(b)

Fig. 3. Sample structures of InAs film grown on Si substrates: (a) sample A, and (b) sample B.

The surface morphology of the layers was measured by atomic force microscopy (AFM) with standard tapping mode to make 10 μm×10 μm image. The crystalline quality of the layer was characterized by high resolution x-ray diffraction (HRXRD). Hall electron mobility was measured at room temperature with the Van der Pauw pattern.

3. Results and discussion

3.1. InAs film directly grown on Si

The InAs nucleation layer serves as a template for the subsequently grown thick bulk layer and to accommodate lattice strain caused by the lattice mismatch and thermal mismatch. Therefore, a 10-nm thick InAs nucleation layer firstly deposited at high and low temperatures is used to figure out the effect of the growth temperature on the surface roughness.

Figure 4 shows the AFM images obtained from the seven samples. It is well known that the large difference in thermal expansion coefficient (74.5%) is also a major difficulty affecting the epitaxy of InAs on Si. Thus, when the growth temperatures are high, such as 585 °C and 595 °C, 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. The surface root mean square (RMS) roughness of a sample with the growth temperature at 595 °C is 4.6 nm and it consists of densely packed Stranski–Krastanow or Volmer–Weber coalesced islands. The suitable growth temperature is beneficial to the diffusion and bonding of atoms between InAs films and Si substrates, and contributes to the increase of the adhesion force, which means that the growth temperature is important to improve the surface roughness of InAs epilayers. When decreasing the growth temperature to 320 °C, the surface becomes smooth and the morphology is improved greatly. In this case, the RMS value decreases to 1.4 nm. Therefore, the growth temperature of the first nucleation layer should be at a low temperature.

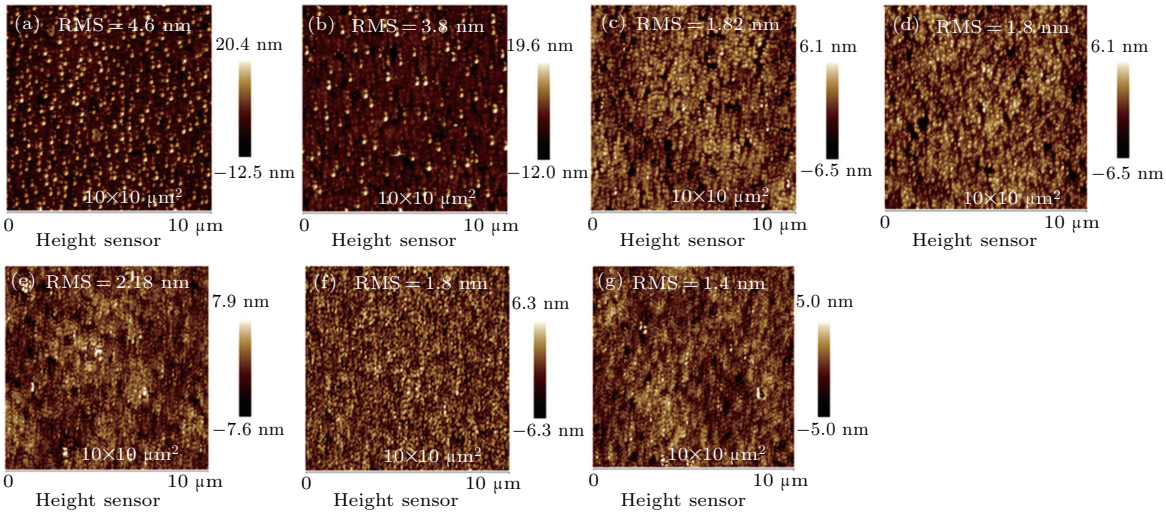


Fig. 4. 10 μm×10 μm AFM images of InAs directly grown on Si at (a) 595 °C, (b) 585 °C, (c) 575 °C, (d) 565 °C, (e) 400 °C, (f) 340 °C, and (g) 320 °C.

Then, adopting a series of samples obtained by a two-step growth method consisting of a low temperature ($T_1 \leq 340$ °C) prelayer followed by deposition of a 1000-nm thick bulk layer at higher growth temperatures T_2 between 450 °C and 540 °C, the influence of the growth temperature on the electron mobility has been investigated. The test results from Hall measurements of InAs materials grown at different growth temperatures are shown in Fig. 5.

As can be seen from Fig. 5, when the growth temperature T_2 is 450 °C, the mobility of samples increases from 1239 $cm^2/V{\cdot}s$ to 2600 $cm^2/V{\cdot}s$ as the first growth temperature T_1 increases from 100 °C to 320 °C, and it decreases from 2600 $cm^2/V{\cdot}s$ to 2368 $cm^2/V{\cdot}s$ as the first growth temperature T_1 increases from 320 °C to 340 °C. This is because MBE is a non-thermal equilibrium process controlled by surface chemistry and surface reaction, which involves the adsorption, decomposition, migration, binding, and desorption of incident atoms on the substrate surface. Therefore, when the first growth temperature T_1 is too low ($T_1 < 320$ °C), the energy provided from the heating chamber is too low to complete the epitaxy process on the substrate surface. When the growth temperature is high ($T_1 > 320$ °C), the increase in thermal stress introduces misfit dislocations, which corresponds to the analysis in Fig. 4.

When the first growth temperature T_1 is 320 °C, the mobility of samples increases from 2600 $cm^2/V{\cdot}s$ to 3600 $cm^2/V{\cdot}s$ as the second growth temperature T_2 increases from 450 °C to 520 °C, and it decreases from 3600 $cm^2/V{\cdot}s$ to 3040 $cm^2/V{\cdot}s$ as the second growth temperature T_2 increases from 520 °C to 540 °C. It is known that the growth temperature can provide a migration power for the surface atoms in the surface-diffusion process during growth and play an important role in the transition of growth mode. When the growth temperatures are high, such as 540 °C, the surface atom has such high energy to migrate that the three-dimensional (3D) growth is enhanced and the residual strain is relaxed by the introduction of misfit dislocations. The misfit dislocations in the InAs films lead to the reduction of the electron mobility.

However, when the growth temperature decreases, the surface atoms diffusion is restricted and the 3D growth mode is delayed. Therefore, the misfit dislocations in the InAs film layer are decreased by optimizing the second growth temperature. It can also be seen that the overall trend of T_1 is not changed in T_2 at 520 °C, but the mobility is improved. As can be seen from Fig. 4, T_1 at 320 °C is the optimum growth temperature for nucleation layer, and the lower misfit dislocations in T_2 at 520 °C lead to the higher mobility compared with T_2 at 450 °C.

It is obvious that the changes in electron mobility are related to the growth temperature of InAs. In the InAs film layer, the misfit dislocations in the film layer act as scattering centers and reduce the electron mobility. Thus, it is implied that there is the smallest density of misfit dislocations in the InAs film layer of the sample grown at T_1 of 320 °C and T_2 of 520 °C, leading to the highest electron mobility (3600 $cm^2/V{\cdot}s$).

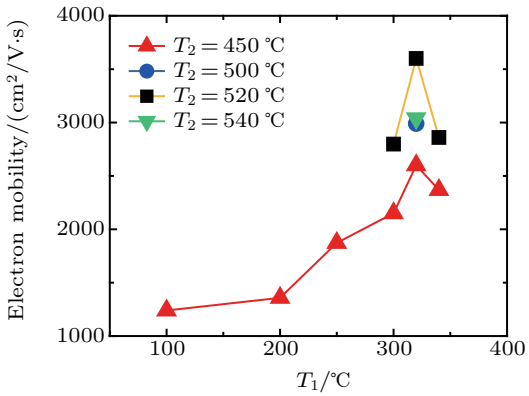


Fig. 5. The electron mobility versus growth temperature.

As shown in Fig. 5, comparing the mobilities of the samples grown at T_1 of 320 °C and T_2 from 450 °C to 540 °C, there is a big difference in the electron mobility, indicating that the growth temperature of the second InAs layer has a greater impact on the overall quality of the material. This may be because the process of heating up to the growth temperature T_2 is an annealing process for the first InAs layer, which reduces the misfit dislocations introduced by the lattice mismatch in the first InAs layer on the Si substrate and provides a good surface morphology for the growth of the second InAs layer. Based on this presumption, an annealing step in the growth process is proposed to verify this conjecture, in which the growth of the nucleation layer is performed at a low temperature of 320 °C followed by ramping up to the annealing temperatures of 400 °C, 560 °C, and 580 °C, while the nucleation layer is annealed for 15 min and the second layer growth temperature is 520 °C. The results show that as annealing step is added, the electron mobility is increased as listed in Table 1. A sharp increase in mobility can be acquired for the annealing temperature at 560 °C. The *in situ* thermal annealing can further improve the efficacy of filtering defects due to the increase of the migration of the defects, leading to their annihilation before the subsequent growth. This indicates that the two-step growth method with the in-situ thermal annealing inserted is helpful for improving the surface morphology and electron mobility of the InAs film layer if an appropriate growth temperature is adopted. The highest electron mobility is 4640 $cm^2/V{\cdot}s$ when the 10-nm InAs nucleation layer is grown at a low temperature of 320 °C followed by ramping up to 560 °C, in which the nucleation layer is annealed for 15 min and a second layer growth is 520 °C. It should be mentioned that the electron mobility of this paper is obtained with a 1000-nm thick InAs layer, which is higher than that in Refs. [10] and [11]. The growth of InAs film directly on the Si substrate provides an important technical reference for the application of InAs/Si TFET.

Table 1. The electron mobilities of samples grown at different annealing temperatures.

Sample	Annealing temperature/°C	Electron mobility /($cm^2/V{\cdot}s$)
D1	400	3350
D2	560	4640
D3	580	4385

3.2. InAs film layer grown on Si substrate with a metamorphic buffer inserted

The InAs surface morphology has been analyzed by AFM characterization. Figure 6 displays the images of a 10 μm× 10 μm surface scan of samples A and B with an RMS roughness of 3.6 nm and 12.4 nm, respectively. It shows that sample A has a smoother surface than the sample B.

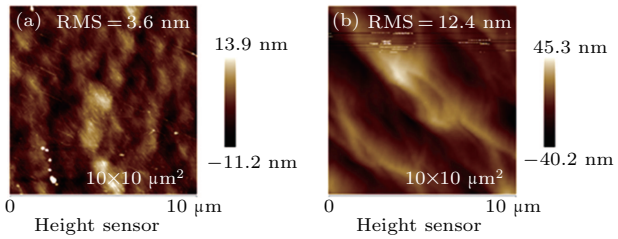


Fig. 6. AFM images of InAs surface: (a) sample A and (b) sample B.

The electrical characterization of various structures has been examined for determining the Hall properties, as shown in Table 2. Hall measurements are performed on 1 cm× 1 cm pieces at 300 K to obtain the electron mobility. The Hall electron mobilities of sample A and sample B are 7648 $cm^2/V{\cdot}s$ and 9222 $cm^2/V{\cdot}s$, respectively. It should be mentioned that there are a few reports on the InAs growth on GaAs (100) to have an electron mobility larger than 10000 $cm^2/V{\cdot}s$.[16] Also, it has not been found yet for the experimental result on the successful growth of InAs on Si (100) to have an electron mobility of 9222 $cm^2/V{\cdot}s$.

Table 2. Hall measurements on the samples.

Sample	Ohm /(Ω/cm)	Electron mobility /(cm^2/V·s)	Carrier concentration/cm^{-3}
A	6.31×10^{-2}	7648	5.1×10^{16}
B	1.36×10^{-2}	9222	4.99×10^{16}

It can be seen from Table 2 that sample B with a 2.5-μm-thick InGaAlAs metamorphic buffer layer has a higher electron mobility than the sample A, because the electron mobility is very sensitive to the strain.[17,18] The III–V material can provide greater flexibility for strain design by adjusting the lattice mismatch between materials. In order to characterize the strain and crystalline quality of InAs layers elaborated on different templates, the samples are then studied by x-ray diffraction (XRD) with CuKα1 radiation ($\lambda = 1.5406$ Å). Figure 7 shows the HRXRD measurement results around symmetric 004 reflections and asymmetric 115 reflections of InAs for samples A and B. In all the samples, the diffraction peaks originated from InAs, GaAs, and Si are clearly observed as shown in Fig. 7. Typically, the 004 and 115 peak positions for a fully relaxed InAs crystal are located at 30.58° and 41.35°, respectively. The InAs peak position varies with the nature of the sublayers. In our case, experimental 004 peak positions are located at 30.67° and 30.36°, and the 115 peaks positions are located at 41.12° and 40.94° for samples A and B, respectively.

Next, the lattice constant is calculated by the Bragg equation to investigate strain relaxation in the InAs. Bragg angle analysis suggests that the lattice constants are along the out-of-plane ($a_\perp$) and in-plane ($a_\parallel$) direction. The peak positions of the symmetric 004 scanning indicate the relationship between the lattice constants of each epitaxial material along the out-of-plane direction, while the asymmetric 115 scanning shows the lattice constants along in-plane direction. As can be seen in Table 3, a compressive in-plane strained InAs layers of the samples A and B are emphasized by the slight shift toward the lower θ_B values. The lattice constant of the InAs layer is given by

$$a = \frac{2\nu}{1+\nu}a_\parallel + \frac{1-\nu}{1+\nu}a_\perp, \tag{1}$$

where ν is the Poisson coefficient of the InAs layer ($\nu = 0.35$). Table 3 shows the calculation results of lattice constant for sample A and sample B. There are different strains in the InAs layer due to the various buffer layer structures. The value of strain ε is deduced from the following relation:

$$\varepsilon_\parallel = \frac{a_\parallel - a_s}{a_s}, \tag{2}$$

$$\varepsilon_\perp = \frac{a_\perp - a_s}{a_s}, \tag{3}$$

where a_s is the lattice parameter of sublayer. A large strain of the InAs films grown on the Si substrate with a 2.5-μm-thick InGaAlAs metamorphic buffer layer is confirmed by the estimated strain of 8%, as shown in Table 3. For samples A and B, the difference of strains is about 1%, and the electron mobility in sample B is 30% higher than that in sample A. Therefore, the observed values indicate that the strain is accumulated in the InAs layer along the out-of-plane ($a_\perp$) and in-plane ($a_\parallel$) direction. Thus, it can be seen that the addition of InGaAlAs metamorphic buffer layer can significantly improve the electron mobility.

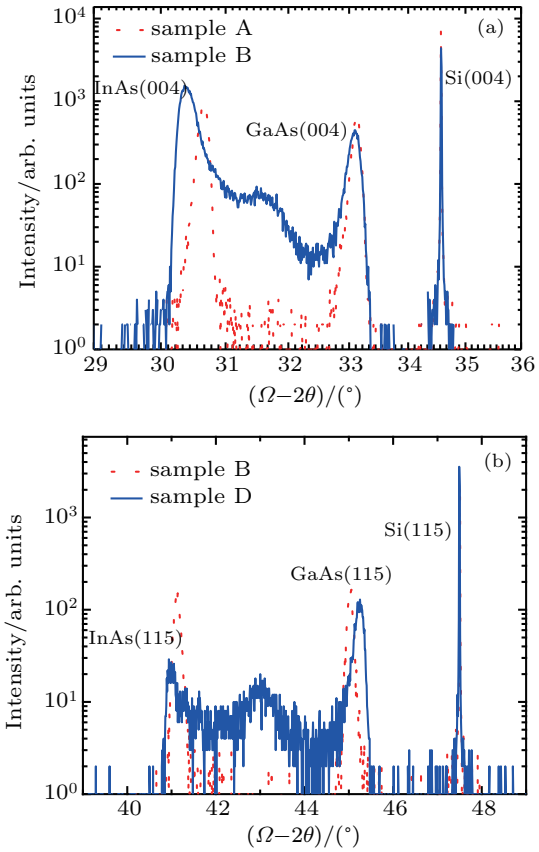


Fig. 7. HRXRD spectra of (a) (004) peak and (b) (115) peak for the samples.

Table 3. Peak positions with associated lattice parameter and strain of samples A and B.

Sample	(004) scanning			(115) scanning			a/Å
	Bragg angle/(°)	$a_\perp$/Å	$\varepsilon_\perp$/%	Bragg angle/(°)	$a_\parallel$/Å	$\varepsilon_\parallel$/%	
A	30.67	6.041	7	41.12	6.086	7.5	6.062
B	30.36	6.096	8	40.94	6.108	8.3	6.101

4. Conclusion

In conclusion, a series of samples formed by two-step procedure to directly grow the InAs film on the Si substrate deflected from the plane (100) at 4° towards (110) by molecular beam epitaxy have been used to investigate the effect of the growth and annealing temperature on the electron mobility and surface topography. The results indicate that the growth of InAs at appropriate growth and annealing temperature is essential because it can reduce misfit dislocations as the scattering center in the InAs film layer, resulting in the improvement of electron mobility. The results show that the highest electron mobility is 4640 $cm^2/V{\cdot}s$ in the 10-nm InAs nucleation layer grown at a low temperature of 320 °C followed by ramping up to 560 °C, in which the nucleation layer is annealed for 15 min and the second layer of InAs is grown at 520 °C. The influence of different metamorphic buffer layers on the electron mobility in the samples have also been investigated, which shows the highest electron mobility of 9222 $cm^2/V{\cdot}s$ at 300 K has been found in a sample grown on a thick, linearly graded InGaAlAs buffer layer deposited at 420 °C. Inserting an InGaAlAs metamorphic buffer layer between the InAs and GaAs buffer layer can significantly improve the electron mobility due to the fact that the electron mobility is very sensitive to the strain. The results of this study could be helpful for the applications in electronic devices with high electron mobility.

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