InGaAs/InAlAs quantum well structures grown on GaAs (001) substrate by molecular beam epitaxy

Hou Xiaobing1,a, Kang Yubin1,b, Tang Jilong1,c, Wang Xiaohua1d, Wei Zhipeng1e*

1School of Science, Changchun University of Science and Technology, Changchun, Jilin, China
aemail: 2020201013@mails.cust.edu.cn, bemail: yubinkangcust@126.com, cemail: jl_tangcust@163.com, demail: biewang2001@126.com
*corresponding author: eemail: zpweicust@126.com

Abstract. A 100 periods In0.53Ga0.47As/In0.52Al0.48As quantum well structure was grown by molecular beam epitaxy (MBE) on GaAs (001) substrate. The XRD results of ternary alloy InGaAs and InAlAs films show that the indium component is similar to the designed structure. In addition, the XRD results show that the In0.53Ga0.47As/In0.52Al0.48As multi-quantum well structure is consistent with the designed structure. The PL spectrum of In0.52Ga0.48As/In0.53Al0.47As quantum well structures is ~1470 nm at room temperature.

1. Introduction
In0.53Ga0.47As films and In0.53Ga0.47As/In0.52Al0.48As multiple quantum wells (MQWs) are widely used in optical fiber communication optoelectronic devices. InGaAs has been extensively explored in many applications for the past several decades due to its high mobility and saturation velocity. Its targeted applications include optoelectronic devices,[1] high-electron mobility transistors (HEMTs),[2] lasers[3] and electro-optic modulators.[4] Currently, the study of InGaAs/InAlAs MQW structures is mainly focused on lattice-matched InP substrates. However, In0.53Ga0.47As/In0.52Al0.48As MQWs grown on other III-V substrates (such as GaAs) is rarely reported due to large lattice mismatch. GaAs substrates have several advantages over InP substrates, which are cheaper, less fragile, have superior crystal quality.[5] Therefore, the InGaAs/InAlAs multi-quantum well structures grown on GaAs (001) substrates may become a trend in the future. Here, we design and grow In0.53Ga0.47As/In0.52Al0.48As multi-quantum well structures on GaAs (001) substrate with a strain-relaxed ternary InAlAs buffer layer (~800 nm) by molecular beam epitaxy.

In this letter, 100 periods lattice-matched In0.53Ga0.47As/In0.52Al0.48As quantum well structures were designed and grown by MBE, which were not on InP substrate but on a strain-relaxed ternary InAlAs buffer (~800 nm) on GaAs (001) substrate. The components of In in the InGaAs and InAlAs films were determined by the XRD Bragg diffraction peaks and the results reached the initial experimental structural design. Moreover, the FWHM of InGaAs and InAlAs films are similar to those of the GaAs (001) substrates, indicating that the grown ternary alloy InGaAs and InAlAs films have high crystalline quality. XRD determined that the periodic thickness of the well and barrier reaches ~ 19.2 nm, consistent with the designed structural periodic thickness of 20 nm. The PL spectra of InGaAs film is ~ 1430 nm, and the PL spectra of In0.53Ga0.47As/In0.52Al0.48As MQWs is ~ 1470 nm.
2. Materials and Methods

2.1. Growth
The In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs were grown on a GaAs (001) substrate using a graded InAlAs buffer layer (~ 800 nm) with increasing In composition by molecular beam epitaxy (MBE) system (DCA-P600). The group-V (As2 and Sb2) sources were supplied by the valved cracker cells. The system is equipped with an infrared pyrometer specified for high temperatures to measure the growth temperature. The layer sequence follows as a ~ 800 nm thick In$_x$Al$_{1-x}$As buffer layer with a linearly increasing of In content ($x = 0–0.52$), and the temperature of the InAlAs buffer layer growth is 520 °C. Then the In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs were grown layer by layer with In$_{0.53}$Ga$_{0.47}$As well layer (12 nm) and In$_{0.52}$Al$_{0.48}$As barrier layer (8 nm) for 100 periods on the InAlAs buffer layer. In$_{0.53}$Ga$_{0.47}$As and In$_{0.52}$Al$_{0.48}$As were grown with the same substrate temperature and In flux of ~500°C and 1.44 × 10$^{-7}$ Torr, respectively. V/III flux ratio of In$_{0.53}$Ga$_{0.47}$As and In$_{0.52}$Al$_{0.48}$As are 15.6 and 15 respectively, corresponding to the Ga and Al beam equivalent pressure of 5.88 × 10$^{-8}$ Torr and 6.72 × 10$^{-8}$ Torr.

2.2. Material Characterization
Crystal structures were determined by collecting XRD, XRD patterns were recorded in the 2θ range of 24-32° with an automated X-ray diffractometer (D8 Discover, Bruker) using Cu Ka radiation ($\lambda = 1.5418$ Å). The optical properties of InGaAs film and In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs were recorded using a HORIBA iHR550 spectrometer with an InGaAs detector. A 655 nm semiconductor diode laser was used as the excitation source.

3. Results & Discussion
Figure 1 shows the schematic diagram of In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs with 100 periods. A 100 periods In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As quantum well structure sandwiched by 800 nm InAlAs buffer layer was grown on a 350 µm thick n-type GaAs substrate by the MBE. And the next 12 nm In$_{0.53}$Ga$_{0.47}$As well and 8 nm In$_{0.52}$Al$_{0.48}$As barrier were grown on the 800 nm InAlAs, and then repeated growth of ninety-nine quantum wells structure. Finally, the growth of MQWs structure was finished under the protection of As flux.

Figure 1. The schematic diagram of In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs with 100 periods. We first grew In$_x$Ga$_{1-x}$As and In$_x$Al$_{1-x}$As films before growing In$_x$Ga$_{1-x}$As/In$_x$Al$_{1-x}$As MQW structures to determine the composition of ternary alloys by XRD. Figure 2a shows the XRD of In$_x$Ga$_{1-x}$As film grown on GaAs (001) substrate. The FWHM of GaAs substrate and In$_x$Ga$_{1-x}$As film are 0.1° and 0.13°, respectively, thus the In$_x$Ga$_{1-x}$As film has high crystalline quality. Moreover, the peak position corresponding to the diffraction peak of the In$_x$Ga$_{1-x}$As film is 31.73°. The lattice constants of InAs and GaAs materials are 0.6058 nm and 0.5633 nm, respectively. The lattice constant of In$_x$Ga$_{1-x}$As film was calculated by Bragg’s formula:[6] 

$$2d \sin \theta = n\lambda$$  

(1)
Here, $\lambda$, $\theta$ and $d$ denote the wavelength of the incident X-rays (0.15418 nm), diffraction angle, and interplanar crystal spacing, respectively. The lattice parameter ($a$) for the In$_x$Ga$_{1-x}$As film was calculated using the formula:\[7\]

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (2)$$

Where, $h$ $k$ $l$ are the Miller indices of the crystal planes and the $a$ is lattice parameter. Therefore, the lattice constant of In$_x$Ga$_{1-x}$As film is 0.5855 nm. The In composition, $x$, of In$_x$Ga$_{1-x}$As film can be calculated by Vegard’s law formula:\[8\]

$$a_{\text{In}_x\text{Ga}_{1-x}\text{As}} = (1-x)a_{\text{GaAs}} + xa_{\text{InAs}} \quad (3)$$

Where, the $a_{\text{GaAs}}$ and $a_{\text{InAs}}$ are lattice constants of GaAs and InAs materials, respectively. Therefore, the In component in In$_x$Ga$_{1-x}$As film is ~ 0.52, which is consistent with the component in our designed InGaAs/InAlAs MQWs structure. We characterized the grown In$_{0.52}$Ga$_{0.48}$As film by photoluminescence (PL) spectra, and the result is shown in Figure 2b. Figure 2b shows that the In$_{0.53}$Ga$_{0.47}$As film has a wide luminescence peak, corresponding to the peak position of ~ 1430 nm.

The In$_x$Al$_{1-x}$As film was grown on GaAs (001) substrate, the result of the corresponding XRD is shown in Figure 3. Figure 3 shows the FWHM of GaAs substrate and In$_x$Al$_{1-x}$As film are 0.11° and 0.15°, respectively. Therefore, the InAs film has high crystalline quality. Moreover, the peak position corresponding to the diffraction peak of the InAlAs film is 31.66°. The lattice constant of AlAs material is 0.5661 nm. Based on the Bragg’s and Vegard’s law formula, the lattice constant of In$_x$Al$_{1-x}$As film is 0.5875 nm. Therefore, the In component in In$_x$Al$_{1-x}$As film is ~ 0.54 based on Vegard’s law, which is consistent with the component in our designed In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs structure.

![Figure 2](image1.png)

**Figure 2.** (a) X-ray diffraction pattern of the In$_x$Ga$_{1-x}$As film grown on GaAs (001) substrate. (b) The PL spectra of the In$_x$Ga$_{1-x}$As film.

![Figure 3](image2.png)

**Figure 3.** X-ray diffraction pattern of the In$_x$Al$_{1-x}$As film grown on GaAs (001) substrate.
On the basis of growing ternary alloy InGaAs and InAlAs films, the In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs structure with 30 periods was grown on the GaAs (001) substrate, the result of XRD is shown in Figure 4. Figure 4 shows the peaks position of the 0-order, -1-order and +1-order diffraction peaks are 31.819°, 31.542 and 32.101, respectively. The Bragg diffraction angle of the two adjacent diffraction peaks is ~0.279°. According to the Bragg diffraction angle of the diffraction peak in Figure 4, the sum of the thickness of InGaAs well $t_w$ and the thickness of InAlAs barrier material $t_b$ can be expressed as equation [9,10]

$$ T = \frac{\lambda}{2\Delta \theta \cos \theta_b} $$

Where $T = t_w + t_b$, $\Delta \theta$ is the difference of the Bragg diffraction angle of the two adjacent diffraction peaks, and $\theta_b$ is the Bragg diffraction angle of the main peak (0 order diffraction peak) of the In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs. Therefore, in the quantum well structure, the periodic thickness of the well and barrier ~18.6 nm, which is close to the designed periodic thickness of 20 nm.

![Figure 4](image1.png)

**Figure 4.** X-ray diffraction pattern of In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs with 30 periods.

![Figure 5](image2.png)

**Figure 5.** (a) X-ray diffraction pattern of the In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs with 100 periods. (b) The PL spectra of the In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs with 100 periods.

Finally, we grew 100 periods In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs structure on GaAs(001) substrates based on successful growth of 30 periods. The XRD pattern of the In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs with 100 periods is shown in Figure 5a. Figure 5a shows the existence of multi-order diffraction peaks, so the multi-quantum well In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As with 100 periods has high crystalline quality. The 0-order, -2-order and +2-order diffraction peaks are 31.824°, 31.259° and 32.352°, respectively. Therefore, the $\Delta \theta \approx 0.273°$ can be obtained. According to formula (4) can be calculated, the periodic thickness of the well and barrier is ~19.2 nm, which is close to the designed periodic thickness of 20 nm. To better understand the optical properties of the 100 periods In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs
structure, the photoluminescence spectra was tested, the result is shown in Figure. 5b. Figure. 5b shows that the In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As MQWs with 100 periods has a narrower luminescence peak, corresponding to the peak position of ~1470 nm, which is very close to the emission peak of the InGaAs film.

4. Conclusions
In conclusion, a 100 periods In$_{0.52}$Ga$_{0.48}$As/In$_{0.53}$Al$_{0.47}$As quantum well structure was designed and grown by molecular beam epitaxy (MBE) on GaAs (001) substrate. The high crystalline quality InGaAs and InAlAs films were grown before the high crystalline quality 100 periods of In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As multi-quantum well structures. XRD results show that the In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As multi-quantum well structure is similar to the designed structure. Finally, the PL spectra of In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As multi-quantum well structure is ~1470 nm.

Acknowledgments
This work was supported by the National Natural Science Foundation of China (61674021, 11674038, 61704011, 61904017, 11804335, 12074045), the Developing Project of Science and Technology of Jilin Province (20200301052RQ), the Project of Education Department of Jilin Province (JJKH20200763KJ) and the Youth Foundation of Changchun University of Science and Technology (XQNJJ-2018-18).

References
[1] Dai, Y.T., Fan, J.C., Chen, Y.F. (1998) Studies of two-subband occupied electron gas in modulation-doped In$_{0.52}$Al$_{0.48}$As/In$_{0.53}$Ga$_{0.47}$As single quantum well by far-infrared modulated photoluminescence. J. Appl. Phys., 83: 2127-2130.
[2] Ajayan, J., Nirmal, D. (2015) A review of InP/InAlAs/InGaAs based transistors for high frequency applications. Superlattices Microstruct., 86: 1-19.
[3] Temkin, H., Alavi, K., Wagner, W.R., et al. (1983) 1.5–1.6 μm Ga$_{0.47}$In$_{0.53}$As/Al$_{0.48}$In$_{0.52}$As multiquantum well lasers grown by molecular beam epitaxy. Appl. Phys. Lett., 42: 845-847.
[4] Gupta, S., Bhattacharya, P.K., Pamulapati, J., et al. (1991) Optical properties of high-quality InGaAs/InAlAs multiple quantum wells. J. Appl. Phys., 69: 3219-3225.
[5] Behet, M., Van der Zanden, K., Borghs, G., et al. (1998) Metamorphic InGaAs/InAlAs quantum well structures grown on GaAs substrates for high electron mobility transistor applications. Appl. Phys. Lett., 73: 2760-2762.
[6] Kumar, P., Misra, A., Kumar, D., et al. (2004) Structural and optical properties of vacuum evaporated Cd$_x$Zn$_{1-x}$ thin films. Opt. Mater., 27: 261-264.
[7] Kurmude, D.V., Barkule, R.S., Raut, A.V., et al. (2014) X-ray diffraction and cation distribution studies in zinc-substituted nickel ferrite nanoparticles. J. Supercond. Nov. Magn., 27: 547-553.
[8] Deki, R., Sasaki, T., Takahasi, M. (2017) Strain relaxation and compositional separation during growth of InGaAs/GaAs (001). J. Cryst. Growth, 468: 241-244.
[9] Vandenberg, J.M., Hamm, R.A., Panish, M.B., Temkin, H. (1987) High-resolution X-ray diffraction studies of InGaAs(P)/InP superlattices grown by gas-source molecular-beam epitaxy. J. Appl. Phys. 62: 1278-1283.
[10] Wen, T.C., Lee, W.I. (2001) Influence of barrier growth temperature on the properties of InGaN/GaN quantum well, Jpn. J. Appl. Phys. 40: 5302.