Microscopic Structure of Al$_{0.15}$In$_{0.01}$Ga$_{0.84}$N/In$_{0.2}$Ga$_{0.8}$N and In$_{0.2}$Ga$_{0.8}$N/GaN of GaN-based Quantum-well

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Abstract GaN-based quantum wells are the core structure of optoelectronic devices such as light-emitting diodes, laser diodes. Our experiments show that, In$_{0.2}$Ga$_{0.8}$N/GaN ternary alloys quantum wells and Al$_{0.15}$In$_{0.01}$Ga$_{0.84}$N/In$_{0.2}$Ga$_{0.8}$N quaternary alloy quantum wells, two different quantum well structures for laser diode, have significant differences about the electrical properties and luminous efficiency. In this paper, we study on microscopic characteristics of these two different quantum well structure. Through high-resolution X-ray diffraction, we got the satellite peaks of these two different alloys quantum wells by $\omega/2\theta$ scanning. Using X-ray diffraction, we got the rocking curves by ω scanning of two kinds of MQW's symmetry face (002) and asymmetric face (101), (102), (103), (104), (105) and (201). Through atomic force microscope, photoluminescence spectra and high resolution X-ray diffraction, it revealed the different nature of the macro factors of the In$_{0.2}$Ga$_{0.8}$N/GaN ternary alloys and Al$_{0.15}$In$_{0.01}$Ga$_{0.84}$N/In$_{0.2}$Ga$_{0.8}$N quaternary alloys.

Key words: AlInGaN; InGaN; MQWs; XRD; AFM

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1 Introduction

In recent years, because great potential of quaternary alloy in semiconductor photoelectronic devices, more and more attentions are focused on it, especially in the short wavelength GaN-based light emitting diode (LED) and GaN-based blue-violet laser diode (LD) in the development[1~3]. In the traditional short-wavelength GaN-based quantum-well laser diode, InGaN is as well layer and GaN is as barrier layer. However, because the problem of lattice mismatch between GaN and InGaN material, it will leads to piezoelectric field, triggered quantum field Stark effect (QCSE) and lower luminous intensity of the device[4,5]. Recently, quaternary alloys materials are used to overcome those problems. Because of the better match of lattice constant[6], a multi-storey structure of the device using quaternary AlInGaN materials will greatly reduce the dislocation density. At the same time, it can reduce the stress and piezoelectric field. However, few documents detailly report AlInGaN/InGaN quantum wells microstructure.

Therefore, in this paper we study on the micro-architecture of Al$_{0.15}$In$_{0.01}$Ga$_{0.84}$N/In$_{0.2}$Ga$_{0.8}$N quantum-well and traditional In$_{0.2}$Ga$_{0.8}$N/GaN MQW in detail.

2 Theory

AlInGaN/InGaN MQWs can be by taking the

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AlInGaN layer as a well layer[7,8]. By varying the flow rates of the Al and Ga metal organic sources, the lattice constant and the energy gap can be controlled[9~11]. The AlInGaN / InGaN MQWs can have better carrier confinement due to the higher band gap energy of AlInGaN compared to GaN without increasing the built in piezoelectric field effect than traditional InGaN /GaN MQWs[8,12]. It was reported that the electroluminescence properties of the AlInGaN / InGaN MQWs can be enhanced, compared to that of InGaN /GaN MQWs due to the better carrier confinement effect by the AlInGaN layers[13].

The introduction of indium into the barrier layers can affect the MQW properties via three different mechanisms[7]. First, the indium molar fraction might have a very pronounced effect on the overall strain and on the strain in the quantum wells. According to the first order theory of elasticity, thin multiquantum well layers simply adjust to the lattice constants of the buffer layer. In this case, the introduction of indium into the barrier layers would only change strain in these layers, and not in the quantum wells, assuming that the structure is fully strained. Therefore, the magnitude of strain in the barrier layers might directly affect the dislocation density and the materials quality of the quantum wells. Second, the magnitude of the built-in fields induced by the spontaneous polarization should be affected. The introduction of quaternary barriers should allow us to independently control both spontaneous polarization and strain. Finally, the introduction of indium improves the materials quality and surface morphology. The improvement in materials quality with the introduction of indium is the dominant factor responsible for the observed differences in photoluminescence spectra.

3 Experiment

The $Al_{0.15}In_{0.01}Ga_{0.84}N$ /GaN quaternary MQW samples were grown using metal organic chemical vapor deposition (MOCVD). In order to reduce the dislocation density in the samples, firstly, heterostructure lateral epitaxial technology was used to grow the GaN layer on sapphire substrates, then a Si-doped n-type GaN was grown on the GaN layer. After that, the $Al_{0.15}In_{0.01}Ga_{0.84}N$ / $In_{0.2}Ga_{0.8}N$ MQWs were grown with five periods. The thickness of well/barrier layers are 2 nm and 8 nm, respectively. In order to compare $Al_{0.15}In_{0.01}Ga_{0.84}N$ / $In_{0.2}Ga_{0.8}N$ MQW with the traditional $In_{0.2}Ga_{0.8}N$ / GaN MQW, the same method was employed to fabricate the $In_{0.2}Ga_{0.8}N$ /GaN MQW ternary samples with five periods.

In order to analyze the quantum well crystal quality, we use X-ray diffraction (XRD, Philips X'Pert 3-axis) to characterize the two MQWs. In addition, we also use AFM and photoluminescence spectra to investigate the two different components of quantum well structures.

4 Experimental Results and Discussion

4.1 Atomic Force Microscope (AFM) Scanning

Fig. 1(a) and Fig. 1(b) show the atomic force microscope (AFM) images of $In_{0.2}Ga_{0.8}N$ /GaN ternary quantum-well (001) surface and $Al_{0.15}In_{0.01}$-$Ga_{0.84}N$ / $In_{0.2}Ga_{0.8}N$ quaternary quantum wells (001)

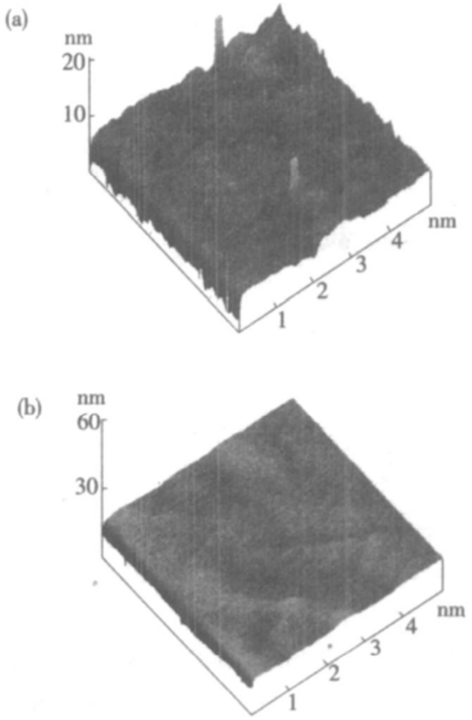

Fig. 1 (a) AFM scanning of $In_{0.2}Ga_{0.8}N$ /GaN ternary quantum-well (001) surface; (b) AFM scanning of $Al_{0.15}In_{0.01}Ga_{0.84}N$ / $In_{0.2}Ga_{0.8}N$ quaternary quantum wells (001) surface.

surface, respectively. We can see that there are some of tiny terraces as well as some micro-pits on the quaternary quantum wells (001) surface and ternary quantum wells (001). However, by comparing we found that the pits on quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum wells (001) surface significantly less than that on the traditional ternary $In_{0.2}Ga_{0.8}N/GaN$ quantum-well (001) surface. From the AFM diagrams, we can see that the quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum wells (001) surface smoother than that of ternary $In_{0.2}Ga_{0.8}N/GaN$ quantum-well (001) surface, significantly. It means that quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum well crystal quality was significantly better than that of traditional ternary $In_{0.2}Ga_{0.8}N/GaN$ MQW.

Table 1 Full width at half maximum (FWHM) data of XRD peaks for symmetrical face and asymmetric face of ternary and quaternary quantum well using high-resolution XRD ω scanning

Planes	(0002)	(1011)	(1012)	(1013)	(1014)	(1015)	(2021)
Angle of inclination	0°	61.96°	43.19°	32.0475°	25.151°	20.58°	75.09°
Sample 1: $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ MQWs							
f	0.420 23	0.274 1	0.543 54	0.728 91	0.513 23	0.519 24	0.295 45
FWHM (°)	0.092 8	0.138 8	0.120 8	0.104 6	0.09 82	0.105 0	0.187
Sample 2: $In_{0.2}Ga_{0.8}N/GaN$ MQWs							
f	0.350 33	0.162 54	0.597 05	0.463 43	0.327 57	0.329 98	0.088
FWHM (°)	0.097 7	0.160 1	0.145 7	0.117 2	0.108 8	0.110 3	0.191 8

4.2 ω Scanning by XRD

Table 1 shows full width at half maximum (FWHM) dates of XRD peaks for symmetrical face and asymmetric face of ternary and quaternary quantum well using high-resolution XRD ω scanning. Then, in order to compare them clearly and more conveniently, selecting two different data and by linear fitting we obtained Fig. 2. From Fig. 2 we can see that the FWHM of rocking curve of $Al_{0.15}In_{0.01}Ga_{0.04}N/In_{0.2}Ga_{0.8}N$ quantum well are narrower than that of ternary $In_{0.2}Ga_{0.8}N/GaN$ quantum well, either for the symmetry (002) of ternary alloys, or the non-symmetrical face (101), (102), (103), (104), (105), (201) of quaternary alloys. Generally, the narrower crystal rocking curves, the better crystal quality. Therefore, by contrasting we can judge that, the crystal quality of quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum well is superior to ternary $In_{0.2}Ga_{0.8}N/GaN$ quantum well crystal quality. These conclusions are consistent with the above conclusions got by AFM scanning.

In order to prove this conclusion, we followly processed ω/2θ scanning by using the high-resolution X-ray diffraction.

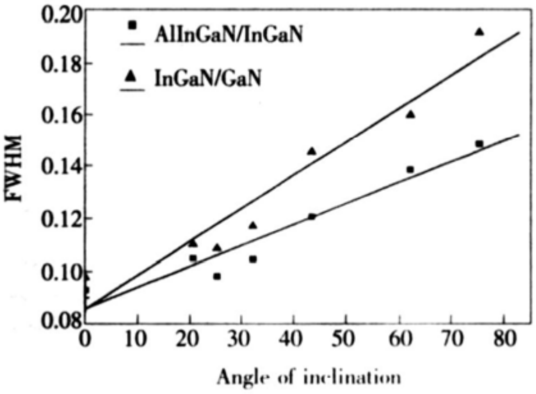

Fig. 2 Contrast of FWHM of rocking curvers for ternary $In_{0.2}Ga_{0.8}N/GaN$ MQW and quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ MQW, (001) symmetrical face and (101), (102), (103), (104), (105), (201) asymmetric faces

4.3 ω/2θ Scanning by XRD

Fig. 3 showed the XRD satellite peaks of two samples got by ω/2θ scanning. The gray curve represented $In_{0.2}Ga_{0.8}N/GaN$ ternary MQW and below the rocking curves, the black curve represented $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quaternary alloys. In order to enhance contrast levels, we enlaged the satellite peaks from 14° to 17.3°. By contrast Fig. 3 (b) we can find, quaternary QW satellite peaks are sharper than that of ternary quantum well. This indicates that the quaternary QW has better periodic structure than that of ternary QW and the interface quality between well and barrier are higher than that of ternary quantum wells noticeably. We also calculated the screw dislocation density of these two kinds of samples by their satellite peak. The result is 0.43×10^{8} cm^{-2} for $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quaternary alloys and 0.844×10^{8} cm^{-2} for $In_{0.2}Ga_{0.8}N/GaN$ ternary alloys. So, the qualities of quaternary alloys are better than that of ternary alloys.

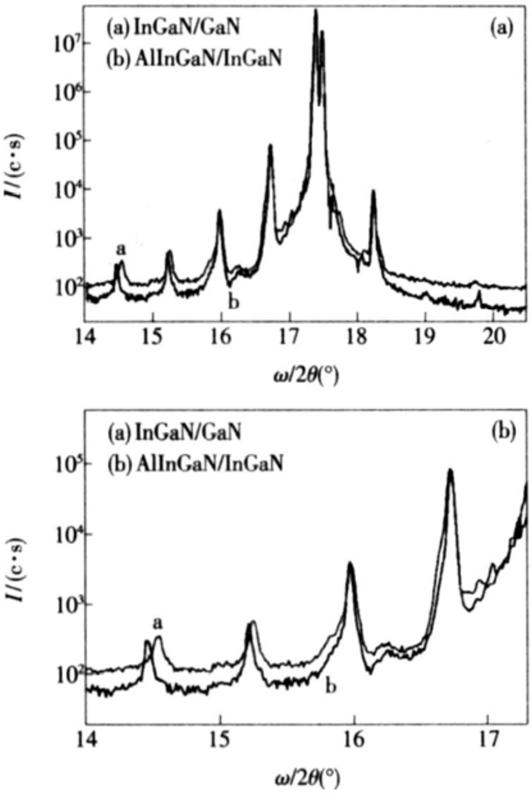

Fig. 3 (a) comparison of the XRD satellite peaks of ternary $In_{0.2}Ga_{0.8}N/GaN$ quantum wells and quaternary alloys $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum wells; (b) comparison of the left part of satellite peaks of ternary $In_{0.2}Ga_{0.8}N/GaN$ quantum wells and quaternary alloys $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum wells

4.4 Photoluminescence Spectrum

Fig. 4 showed the photoluminescence (PL) spectra of the quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ QW and ternary $In_{0.2}Ga_{0.8}N/GaN$ QW. By comparison we found that main PL peak intensity of the quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ QW is more intense than that of ternary $In_{0.2}Ga_{0.8}N/GaN$ QW. This shows that the optical properties of the quaternary MQWs are better than that of ternary MQWs. There can be several possible mechanisms for the increased PL intensity for the quaternary MQWs structure. Firstly, quaternary MQWs have better MQW quality resulting in a reduction of the band tail states. Secondly, stronger carrier confinement due to a larger band gap offset resulting from the use of AlInGaN layers. Thirdly, possible reduction in the polarization charge. At the same time, from the PL spectrum, we found that the yellow peak of the quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum wells was lower than the yellow peak of ternary $In_{0.2}Ga_{0.8}N/GaN$ MQW in PL spectra. And there is some blue shift. Ponce F. A *et al.* thought that the yellow peak of PL spectrum is due to MOCVD growth in the process and caused by the angle grain boundaries at the end of the dislocation[14]. T. Ogino, *et al.* thought it is due to the screw dislocation and mixed dislocations in GaN materials[15]. But one point is recognized: that is due to crystal defects caused by the structure. Therefore, by Fig. 4, we can got another conclusion: the defects in quaternary QW obviously less than that in ternary QW and the crystal quality of quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum well better than that of ternary $In_{0.2}Ga_{0.8}N/GaN$ quantum well, and its optical performance also is superior to ternary quantum wells.

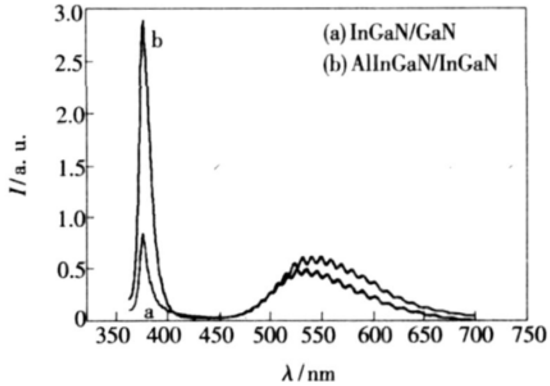

Fig. 4 Micro area photoluminescence spectra of quaternary $Al_{0.15}In_{0.01}Ga_{0.84}N/In_{0.2}Ga_{0.8}N$ quantum wells and ternary $In_{0.2}Ga_{0.8}N/GaN$ quantum wells at room temperature

5 Conclusion

In this paper, we investigated the quaternary

$Al_{0.15}In_{0.01}Ga_{0.84}N / In_{0.2}Ga_{0.8}N$ quantum well and ternary $In_{0.2}Ga_{0.8}N / GaN$ quantum well by using of atomic force microscopy (AFM), X-ray diffraction (XRD) and photoluminescence spectra (PL) measurement. Using X-ray diffraction study we found that the period of quaternary MQWs is better than $In_{0.2}Ga_{0.8}N / GaN$ MQWs ternary, and the interfaces between the well layers and the barrier layer are more uniform. Through the AFM and PL spectra analysis we concludes that the defects in quaternary alloys obviously less than ternary alloys in the quantum well, also, its crystal quality is better than ternary quantum wells.

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三元系和四元系 GaN基量子阱结构的显微结构

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摘要: GaN基量子阱是光电子器件如发光二极管、激光二极管的核心结构。实验表明,采用 InGaN/GaN三元和 AlInGaN/GaN四元两种不同量子阱结构的激光二极管的发光性质和发光效率有明显差别,研究了这两种不同量子阱结构的显微特征。利用原子力显微镜表征了样品的(001)面;通过高分辨 X射线衍射对两种量子阱结构的(002)面作 ω/2θ扫描测得其卫星峰并分析了两种不同量子阱结构的界面质量;利用 X射线衍射对 InGaN/GaN和 AlInGaN/GaN这两种量子阱的(002)、(101)、(102)、(103)、(104)、(105)和(201)面做 ω扫描,进而得到其摇摆曲线。最后利用 PL谱研究了它们的光学性能。通过这些显微结构的分析和研究,揭示了 InGaN/GaN三元和 AlInGaN/GaN四元两种不同量子阱结构宏观性质不同的结构因素。

关 键 词: AlInGaN; InGaN; 量子阱; 原子力显微镜

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