Growth and electrical properties of high-quality Mg-doped p-type $Al_{0.2}Ga_{0.8}N$ films*

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Abstract: The growth of high-performance Mg-doped p-type $Al_xGa_{1-x}N$ (x = 0.2) using metal-organic chemical vapor deposition is reported. The influence of growth conditions (growth temperature, magnesium flow, and thermal annealing temperature) on the electrical properties of Mg-doped p-type $Al_xGa_{1-x}N$ (x = 0.2) has been investigated. Using the optimized conditions, we obtained a minimum p-type resistivity of 0.71 Ω·cm for p-type AlGaN with 20% Al fraction.

Key words: p-type AlGaN; thermal annealing; resistivity
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1. Introduction

UV devices based on AlGaN alloys have gained a lot of interest in recent years[1]. AlGaN systems are especially suitable for these applications since they cover wavelengths from 200 to 364 nm. However, it is rather difficult to develop high conductivity n-type and p-type AlGaN alloys with high Al fraction, which are indispensable for achieving high performance in UV devices[2, 3]. Several groups have used different methods for the Si doping of n-type AlGaN and made great progress[4–7]. But, it is still a significant challenge to achieve good conductivity for p-type AlGaN. On the one hand, the activation energy of the Mg acceptors increases when increasing the Al fraction of AlGaN[2]; on the other hand, high density defects, which can compensate for the dopants, come into being when increasing the Al fraction[8]. For Mg-doped p-type GaN, resistivities lower than 1 Ω·cm have been obtained[9, 10]. For p-AlGaN, Yu *et al.*[11] have achieved a resistivity of 3.5 Ω·cm for p-type AlGaN with 0.35 Al fraction. Jeon *et al.*[12] have reported a resistivity of 10 Ω·cm for p-type $Al_xGa_{1-x}N$ (x = 0.5). For p-AlGaN, resistivities lower than 1 Ω·cm have not been reported.

In this paper, we demonstrate the MOCVD growth conditions suitable for the fabrication of Mg-doped $Al_xGa_{1-x}N$ (x = 0.2). The influence of the growth temperature on the electrical properties of Mg-doped AlGaN is examined. The Mg molar flow rate to the grow chamber is optimized. In addition, the effects of the thermal annealing temperature are investigated. Under optimized growth conditions, a minimum p-type resistivity of 0.71 Ω·cm is obtained. This is the lowest resistivity ever measured for the uniform p-type AlGaN with 20% Al fraction.

2. Experiments

Mg-doped AlGaN epitaxial layers were grown in a low pressure MOCVD reactor, using triethylgallium (TEG), trimethylaluminum (TMAl), ammonia, and biscyclopentadienylmagnesium (Cp_2Mg) as Ga, Al, N, and Mg precursors, respectively. H_2 was used as a carrier gas. The buffer structure included: a 10 nm thick, low temperature (600 °C) AlN nucleation layer, 100 nm high temperature (1070 °C) AlN，10 period $Al_{0.4}Ga_{0.6}N$(12 nm)/AlN(8 nm) superlattices, and 0.6 μm undoped $Al_{0.4}Ga_{0.6}N$ layers. After the deposition of these layers, 150 nm Mg-doped $Al_{0.2}Ga_{0.8}N$ layers were grown using different parameters. The cross-sectional view of the sample structure is shown in Fig. 1.

Thermal activation experiments were performed in nitrogen atmosphere. The annealing temperatures were varied to obtain the optimal annealing conditions for the samples grown at different conditions.

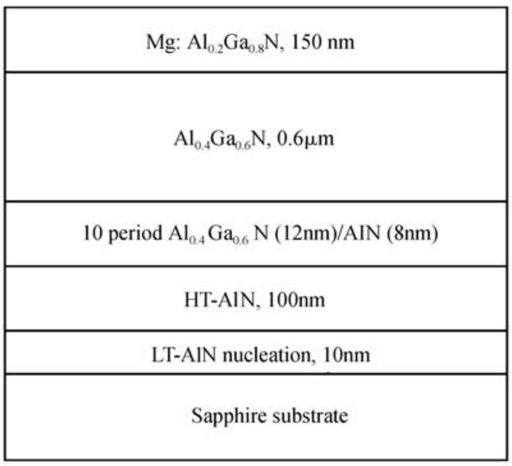

Fig. 1. Cross-sectional view of the sample structure.

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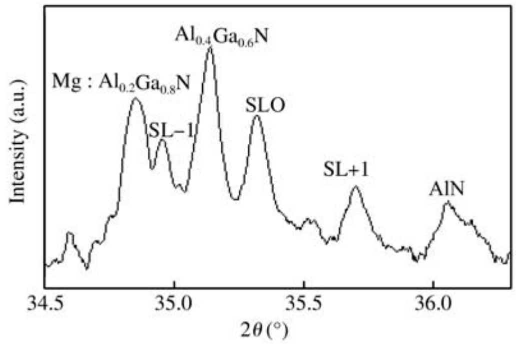

Fig. 2. 2θ–ω scans result of the epitaxy layer.

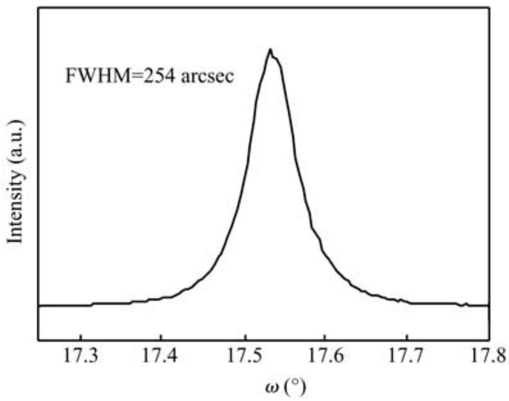

Fig. 3. XRD rocking curve of undoped $Al_{0.4}Ga_{0.6}N$.

The Van der Pauw method was used in room temperature Hall measurements. Indium solder was used to fabricate ohmic contacts for the electrical measurements. A Bruker D8 high resolution X-ray diffraction (HRXRD) system was used to characterize the quality of the materials, and atomic force microscope (AFM) was used to characterize the surface morphology.

3. Results and discussions

Before the deposition of the AlGaN layer, high quality HT-AlN templates were grown using the pulsed atomic layer epitaxy (PALE) method, which was proved to be very useful in suppressing gas phase reactions via a separate supply of group III and group V sources[13]. X-ray diffraction reveals that the AlN layer has a narrow full width at half maximum (FWHM) of the rocking curve: 43 arcsec for (0002) scans and 236 arcsec for $(10\bar{1}2)$ scans, respectively. $Al_{0.4}Ga_{0.6}N$/AlN superlattices are also optimized to control the strain and to reduce the defect density. Figure 2 is the XRD (0002) 2θ–ω scan of the epitaxy layer. The peaks are assigned to the AlN template, the $Al_{0.4}Ga_{0.6}N$/AlN SLs satellites, the undoped $Al_{0.4}Ga_{0.6}N$, and the top Mg-doped $Al_{0.2}Ga_{0.8}N$ layer, respectively. These sharp peaks show that the layers have fine boundaries and a high quality. Using the Vegard law, we obtained the Al mole fraction of all layers from XRD 2θ–ω scan.

Figure 3 is the (0002) rocking curve of undoped $Al_{0.4}Ga_{0.6}N$. Despite of the Al content being high, the FWHM is only 254 arcsec. This value is close to the common value of GaN, which is about 200 arcsec[14]. A high quality undoped $Al_{0.4}Ga_{0.6}N$ film is key to improve the electrical properties of the subsequent Mg-doped AlGaN layers, because it is very useful to reduce the defects existed in Mg-doped AlGaN layers. The surface morphology of the Mg-doped AlGaN layer was characterized by AFM, as shown in Fig. 4. The scan area is $5 \times 5\ \mu m^2$. A smooth surface is observed. The root mean square (RMS) is only 0.443 nm, which is close to the height of one atomic layer. All the above results show that the obtained layers have good quality.

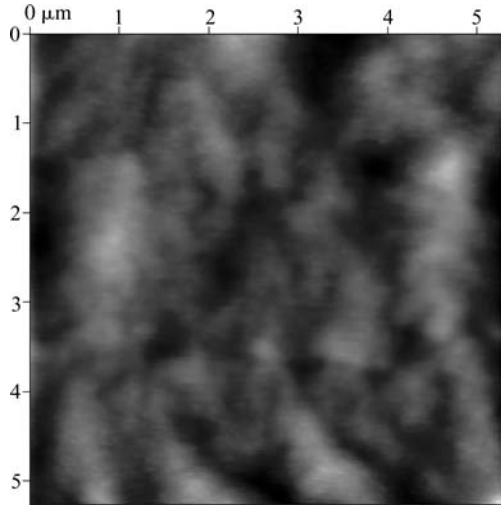

Fig. 4. AFM image of Mg-doped AlGaN.

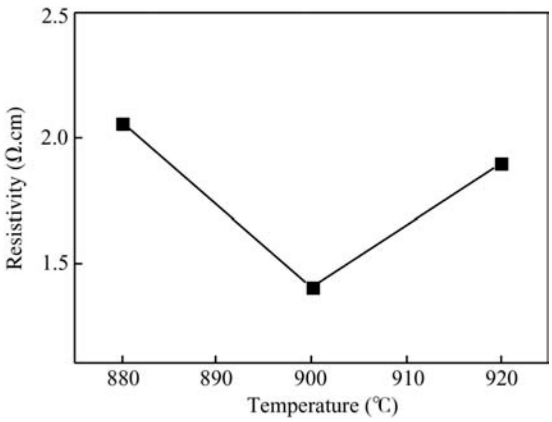

Fig. 5. Resistivity of Mg-doped $Al_{0.2}Ga_{0.8}N$ as a function of growth temperature.

With the purpose of exploring the influence of the growth conditions on the electrical properties of Mg-doped $Al_{0.2}Ga_{0.8}N$, samples were grown at five different temperatures: 1000, 950, 920, 900, and 880 °C, respectively. Other conditions remained unchanged. After growth, samples were annealed at 850 °C in N_2 ambient for 10 min to achieve p-type conduction. Hall measurements were used to characterize the electrical properties. The resistivity of Mg-doped AlGaN with an Al fraction 0.2 as a function of growth temperature is shown in Fig. 5. The resistivity of p-AlGaN decreases from 2.06 to 1.4 Ω·cm when the growth temperature increases from 880 to 900 °C, and then increases to 1.9 Ω·cm at 920 °C. It should be pointed out that Mg-doped AlGaN grown at

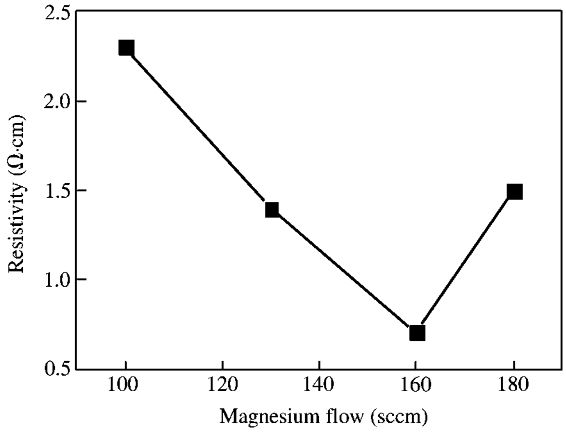

Fig. 6. Resistivity of Mg-doped $Al_{0.2}Ga_{0.8}N$ as a function of magnesium flow.

1000 and 950 °C have high resistivity, but we did not obtain accurate values. This can be explained as follows: when the growth temperature increases, the quality of p-type AlGaN is improved and the density of defects, which can compensate the acceptor dopants, is reduced, thus, enhancing p-type conduction. But increasing the temperature will limit the incorporation of Mg atoms[15]. So, the acceptor density reduces and the resistivity is increased. The results show that the most suitable growth temperature for the p-AlGaN with 0.2 Al fraction is 900 °C.

The influence of the magnesium flow on the resistivity of p-$Al_{0.2}Ga_{0.8}N$ is shown in Fig. 6. Samples were grown with different magnesium flows, but the TMA and the TEG flow were kept constant. The growth temperature was 900 °C and the pressure was 100 Torr. The annealing temperature was 850 °C in N_2 ambient for 10 min. The results show that the resistivity values first decrease with when increasing the magnesium flow from 100 to 160 sccm and then increase to 1.5 Ω·cm. An optimal value of 0.71 Ω·cm is obtained when the magnesium flow was 160 sccm (the mole ratio Cp_2Mg / (TMA + TEG) = 1.6×10^{-2}). This is because adding Mg dopants increases the acceptor concentration and enhances the p-type conduction. But when excessive Mg-doping is used, the quality of the AlGaN films is reduced. Therefore, the resistivity increases when the magnesium flow exceeds 160 sccm.

All the as-grown samples were highly resistive, and post growth rapid thermal annealing was done to activate the Mg acceptors. The dependence of the resistivity of Mg-doped $Al_{0.2}Ga_{0.8}N$ on the thermal annealing temperature is examined in our study. Samples were grown under the same conditions. The annealing time was 10 min in N_2 ambient. The results are shown in Fig. 7. The minimum resistivity value is obtained when the sample was annealed at 850 °C. When the annealing temperature is lower or higher than 850 °C, the resistivity increases. The optimal annealing temperature of Mg-doped $Al_{0.2}Ga_{0.8}N$ is higher than that of Mg-doped p-GaN, which is annealed at 550 °C. This can be explained by first-principle calculations[16]. The activation energy of p-$Al_xGa_{1-x}N$ increases when increasing the index

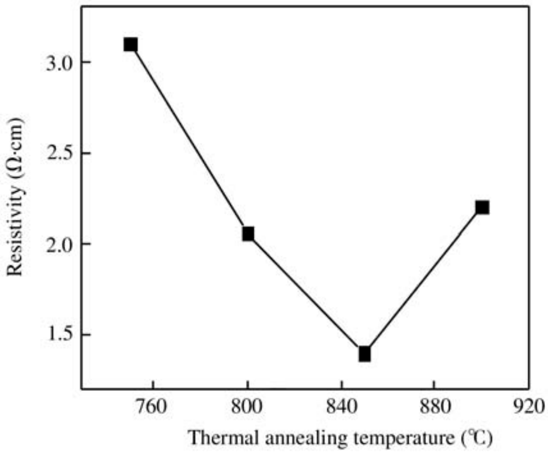

Fig. 7. Resistivity of Mg-doped $Al_{0.2}Ga_{0.8}N$ after thermal annealing at different temperatures.

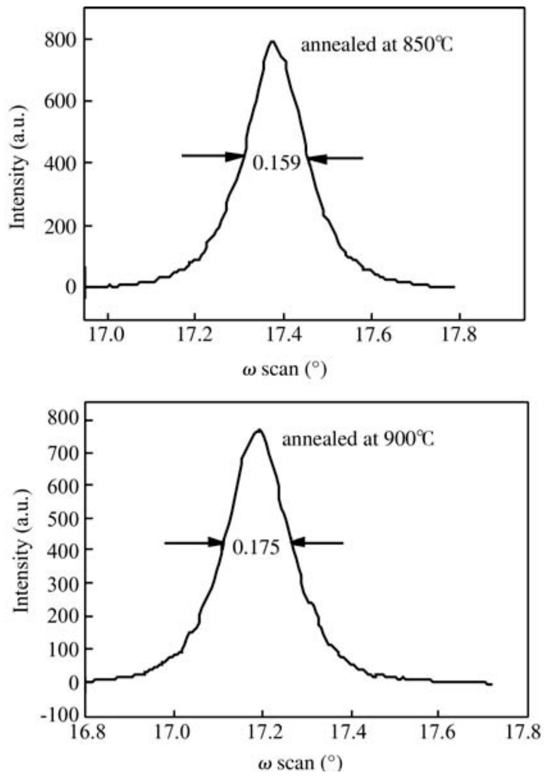

Fig. 8. XRD rocking curve of Mg-doped $Al_{0.2}Ga_{0.8}N$ annealed at 850 and 900 °C.

x. When the temperature is too low, the energy is not high enough to activate the Mg-acceptors completely. When the temperature is too high, the quality of the films can be reduced and the conductivity is decreased. This can be proven by XRD rocking curves of the (002) plane, as shown in Fig. 8. The FWHM of samples annealed at 850 °C is 0.159 °, but when samples were annealed at 900 °C, the value of the FWHM increases to 0.175°.

To measure the concentration of Mg and impurity atoms (C, H, and O), SIMS depth profiles were recorded after annealing. As shown in Fig. 9, the Mg concentration in the p-type AlGaN layer is approximately 3×10^{19} atoms/cm^3. This is a very high doping concentration. Van de Walle *et al.*[2] reported that when increasing the Al fraction, the doping efficiency of

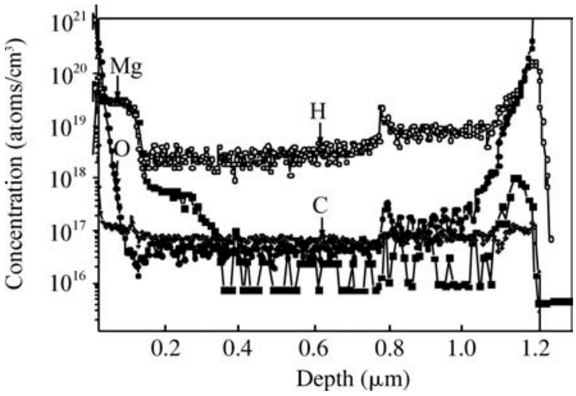

Fig. 9. SIMS profile of Mg and impurity atoms (H, C, and O) in the layer.

Mg will decreased. This is because the nitrogen vacancy has a low energy and can successfully inhibit p-type doping of AlGaN. So, the high Mg-doping concentration can ascribe to the high quality of the epitaxy layers. It is noticed that the H concentration is close to the Mg concentration in p-type AlGaN. In MOCVD growth, the main source of H is the carrier gas and the decomposition of the reactant. H can deactivate Mg by the formation of an Mg–H complex in p-AlGaN; a similar process can take place in p-GaN [17]. So, rapid thermal annealing is necessary to break the Mg–H bonds. From Fig. 9, we can find that the C concentration has slightly increased, while the O concentration obviously increases in Mg-doped p-type AlGaN. It is commonly believed that the O contamination is mainly due to ammonia, and C atoms originate from the decomposition of metal-organic compounds. The SIMS results show that the concentration of the impurities H, C, and O in Mg-doped p-type AlGaN layer is higher in other layers. This can be ascribed to the growth conditions of p-type AlGaN, which have a low growth temperature and a high growth pressure.

4. Conclusion

In summary, the influence of the growth conditions (growth temperature, magnesium flow, and thermal annealing temperature) on the electrical properties of Mg-doped p-type $Al_xGa_{1-x}N$ ($x = 0.2$) have been investigated. It is found that an improvement of the AlGaN crystal quality and an optimization of the Mg-doped AlGaN growth conditions are key to improve the electrical characteristics of p-type $Al_xGa_{1-x}N$ (x = 0.2). By optimizing the growth conditions, a p-type resistivity of 0.71 Ω·cm for p-type $Al_{0.2}Ga_{0.8}N$ have been obtained, which is the lowest resistivity ever measured for AlGaN with a 20% Al fraction.

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