Research of strain state and dislocation density in the multiple AlGaN epitaxial layers with high Al content

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In this paper, the p-i-n multiple-layer $Al_xGa_{1-x}N$ sample with high Al ($x > 0.45$) content was measured by the triple-axis X-ray diffraction measurement. The strain state and screw dislocation density of each layer in $Al_xGa_{1-x}N$ epitaxial layers were determined by RSM (reciprocal space map) method. Then, the PV function was used to fit the rock curves separated from the RSM. At last, the strain and the screw dislocation density of each layer were accurately calculated by fitting these rock curves.

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The design and growth of device quality AlGaN thin film with good properties is a topic at the very center of today's nitride research. Despite the remarkable achievements over the past decade in GaN-based blue light emitters, full technology realization of many other potential nitride-based device applications of the $Al_xGa_{1-x}N$ ternary material system, especially those involving layers with large x values, remains beset with formidable materials challenges. Examples include $Al_xGa_{1-x}N$ alloy layer with compositions $0.4 < x < 0.6$ which are potentially useful as optical, solar-blind sensors. In these $Al_xGa_{1-x}N$ materials with high Al content ($x < 0.4 < 0.6$), the dislocation density is so high to about 10^{13} cm^{-3} due to the lattice misfit and the remained strain[1,2], which limit its application in device. As it is well known that strain due to lattice misfit is released by forming the dislocation, so the dislocation is related the strain directly.

$$PV(x) = I_0\left[\eta L(x) + (1-\eta)G(x)\right], \tag{1}$$

$$\varepsilon_\perp = \beta_{2\theta-\omega}[0.184446 + 0.812692(1-0.998497\eta)^{0.5} -0.659603\eta + 0.445542\eta^2]/4\tan\theta, \tag{2}$$

$$\frac{c-c_0}{c_0} = \nu_c\frac{a-a_0}{a_0}, \tag{3}$$

$$\alpha_\Theta = \beta_\omega\left[0.18446 + 0.812692\,(1-0.99849\eta)^{0.5} -0.65960\eta + 0.44554\eta^2\right], \tag{4}$$

$$N_\alpha = \frac{\alpha_\Theta^2}{2\pi\ln 2b^2}. \tag{5}$$

In this paper, the aim is to determine the strain state and the screw dislocation density of the p-i-n multiple-layer $Al_xGa_{1-x}N$ ($0.4 < x < 0.6$) epitaxial material. Because it was used to make the solar-blind photo-detector, so Al content of n-type layer($x = 0.55$) is higher than that of p and i layer ($x = 0.45$). The Bond method was used to measure the strained lattice parameter at first[3,4] and the RSM method was also adopted to analyze the strain state of the multiple epitaxial layers[5]. Then the PV (pseudo-voigt) function was used to fit the curves separated from the RSM[2,6]. The PV function is the convolution of the Lorentz and the Gauss function expressed by Eq. (1). Through the PV function fitting function method, the $\varepsilon_\perp$ can be directly obtained from the fitted results by Eq. (2). Where, I_0 is the intensity of the rock curve, $L(x)$, $G(x)$ indicate the Lorentz function and the Gauss function. The parameter η is the portion of the Lorentz function. Through the $2\theta/\omega$ can mode, the $\varepsilon_\perp$ can be calculated by the integrated width of the rock curve $\beta_{2\theta-\omega}$ and the parameter η by Eq. (2). The $\varepsilon_{//}$ can be determined by Eq. (3) and the Al content x was obtained by the Vegard relation. Then strained lattice c, a parameter of each layer were determined by the Bond method, and the unstrained lattice c_0, a_0 were determined by the Vegard relation. In the other hand, through the ω can, the α_Θ can be obtained by Eq. (4) through fitting the rock curves separated from the RSM and β_ω is the integrated width of rock curve. The screw dislocation density N_α can be calculated by Eq. (5)[2,7].

The sample measured is grown by the MOVCD on c-plane (0001) of sapphire substrate, using trimethylgallium, Trimethylalumimum and NH_3 as the source reagents. A buffer layer of AlN of approximately 50-nm thickness was first deposited at 450 °C, followed by n-type $Al_{0.55}Ga_{0.45}N$ (1.5 μm), indicated as the window layer, and undopped $Al_{0.45}Ga_{0.55}N$ (0.2 μm), indicated as the active layer, the p-type $Al_{0.45}Ga_{0.55}N$ (0.4 μm).

Table 1. The Fitting Parameters and Calculation Results

$2\theta/\omega$ Scan Mode	I_0	η	$\beta_{2\theta-\omega}$	$\varepsilon_\perp$	$\varepsilon_{//}$
$Al_{0.45}Ga_{0.55}N$	85	0.112	4.17×10^{-4}	7.66×10^{-4}	-6.14×10^{-3}
$Al_{0.55}Ga_{0.45}N$	290	0.32	8.72×10^{-5}	2.26×10^{-4}	-3.60×10^{-3}
ω Scan Mode	I_0	η	α_Θ	N_α	
$Al_{0.45}Ga_{0.55}N$	113	0.34	4.99×10^{-3}	2.22×10^{13}	
$Al_{0.55}Ga_{0.45}N$	502	0.16	7.64×10^{-3}	5.18×10^{13}	

The structure information was obtained using a high resolution X-ray diffractometer (Philips) with a front Bartels-type monochromator [4×Ge(220)]. CuK_{a1} characteristic X-rays ($\lambda = 1.540598$) are used to probe samples. In the RSM measurement processes, the scan step length is 0.0004° and the diffraction area of the X-ray is 2×2 (mm).

Figure 1 shows the RSM of the sample. The reciprocal space point of n layer is further from the surface because the lattice parameter of n layer is smaller than that of p and i layers. It can be seen from the RSM that the cross broadening of the n layer is smaller than that of the p and i layers because the strain in the n layer was almost released by its larger thickness[8]. But on the contrary, dislocation density of n is higher due to its larger perpendicular broadening. Through fitting the curves separated from the RSM, the $\varepsilon_\perp$ can be directly obtained by Eq. (2). Figure 2 shows the curves obtained under $2\theta/\omega$ can mode separated from the RSM and the fitting results by the PV function. In addition, the curves under ω can mode and the fitting results were also shown in Fig. 3. These fitting parameters and calculation results were showed in Table 1.

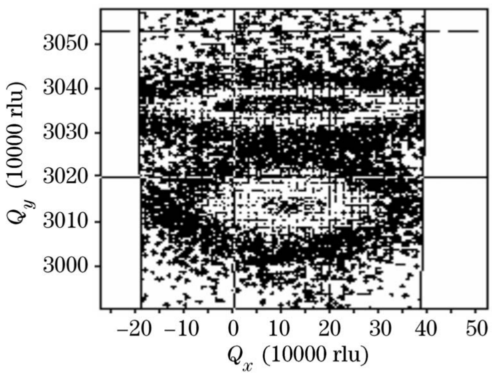

Fig. 1. The RSM of the multiple-layer AlGaN epitaxial materials (the Al content of the upper is 0.55 and the other is 0.45).

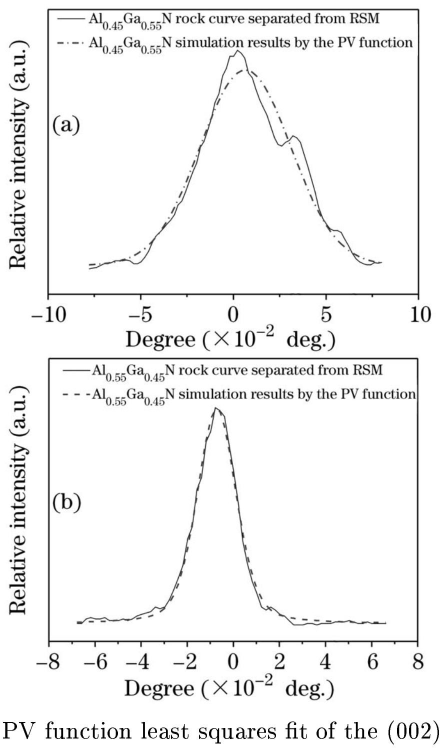

Fig. 2. The PV function least squares fit of the (002) diffraction in triple-axis scan mode: (a) the rock curve and the simulation results of the layer with $x = 0.45$; (b) the rock curve and simulation results of the layer with $x = 0.55$.

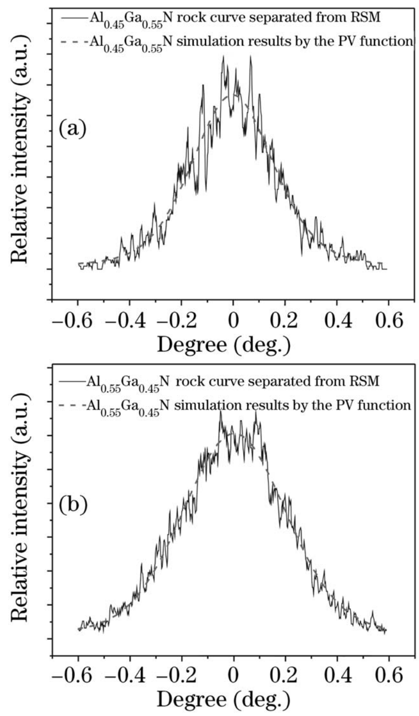

Fig. 3. The PV function least squares fit of the (002) diffraction in triple-axis scan mode: (a) the rock curve and the simulation results of the layer with x=0.45; (b) the rock curve and simulation results of the layer with x=0.55.

In summary, the strain state and the screw dislocation density were obtained by the RSM method, its results is consistent with those determined by the elastic theory and iterative method[9]. These results show that the RSM method is a useful and powerful tool to investigate the strain state of the multiple layer structure epitaxial materials.

References

1. P. F. Fewster, N. L. Andrew, and C. T. Foxon, Crystal Growth **230,** 398 (2001).
2. T. A. Lafford and P. J. Parbrook, Phys. Stat. Sol. C **1,** 542 (2002).
3. W. J. Bartels and W. Nijman, Crystal Growth **44,** 518 (1978).
4. J. Hornstra and W. J. Bartels, Crystal Growth **44,** 513 (1978).
5. T. Metzger, R. hopler, and E. born, Philos. Mag. A **77,** 1013 (1998).
6. J. Domagala, M. Leszczynski, and P. Prystawko, Alloy and Compounds **286,** 284 (1999).
7. J. E. Ayers, Crystal Growth **135,** 71(1994).
8. E. Zielinska-Rohozinska, M. Kowalska, and K. Pakula, Cryst. Res. Technol. **38,** 951 (2003).
9. S. Einfeldt, V. Kirchner, H. Heinke, M. Dieβelberg, S. Figge, K. Vogeler, and D. Hommel, J. Appl. Phys. **88,** 7029 (2000).