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Influence of dislocations in the GaN layer on the electrical properties of an AlGaN/GaN heterostructure*

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This paper reports on a comparative study of the spatial distributions of the electrical, optical, and structural properties in an AlGaN/GaN heterostructure. Edge dislocation density in the GaN template layer is shown to decrease in the regions of the wafer where the heterostructure sheet resistance increases and the GaN photoluminescence band-edge energy peak shifts to a high wavelength. This phenomenon is found to be attributed to the local compressive strain surrounding edge dislocation, which will generate a local piezoelectric polarization field in the GaN layer in the opposite direction to the piezoelectric polarization field in the AlGaN layer and thus help to increase the two-dimensional electron gas concentration.

Keywords: GaN, edge dislocation, piezoelectric polarization, two-dimensional electron gas
PACC: 6170G, 7280E, 7320D, 7760

1. Introduction

Despite the impressive achievements of the III–V nitride heterostructure technology, which has led to the realization of high-temperature and high-power electronic devices,[1] there are still substantial physical properties that need to be fully understood. One of them concerns the electrical activity associated with dislocations which are commonly observed in GaN epitaxial films.[2] To date, most studies have focused on their impacts on the electrical properties of the GaN layer.[3,4] Dislocation is taken as a kind of acceptor-like state that affects carrier scattering and doping distribution in the GaN layer.[5] However, the influences of dislocations in the GaN layer on the electrical properties of an AlGaN/GaN heterostructure have not been studied in detail, especially experimentally.

One of the difficulties lies in the fact that the impact of dislocations cannot be easily separated from that of the other factors which work on the two-dimensional electron gas (2DEG) formation, since it is difficult to change dislocation densities in a GaN template without causing any other structure variations. For example, even grown under the same conditions, one cannot make sure that the thicknesses and compositions of AlGaN layers and the n type background carrier concentrations of GaN layers are exactly the same for different samples, whose slight variations, rather than dislocations, might significantly influence 2DEG in the heterostructure. Hence the effects of dislocations cannot be observed at all or can be confused with the other effects.

In the present work, a simple but effective experimental method is used to correlate the structural properties with the physical properties of an AlGaN/GaN heterostructure. Our experimental results reveal that edge dislocation density in the GaN template layer decreases in the regions of the wafer where sheet resistance of the heterostructure increases and the GaN photoluminescence (PL) band-edge energy peak shifts to a high wavelength. A model concerning the local strain and piezoelectric polarization around dislocations has been proposed to interpret this phenomenon.

2. Experiments

The AlGaN/GaN heterostructures analysed here were grown by metalorganic chemical vapour phase deposition on *c*-plane sapphire (α-Al_2O_3) substrate. Triethylgallium, trimethylaluminium, and ammonia were used as precursors, with H_2 as a carrier gas. The sample has the following structure starting from the

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substrate: an initial low temperature AlN nucleation layer, followed by an unintentionally doped GaN base layer of 1614 nm thickness, and finally, an AlGaN barrier layer. Hall effect measurements have revealed that the sheet carrier concentration and Hall mobility at room temperature of the sample are 2.39×10^{13} cm^{-2} and 975 cm^2/(V·s), respectively.

We use the nondestructive testing method to investigate the local distributions of material properties within the wafer, in order to eliminate uncertainties brought in during growth and processing between different lots of samples and hence concentrate on the effect of dislocations. The sheet resistance distribution of the heterostructure was studied by a Lehighton sheet resistance mapper (LEI 1500). The PL mapping was performed at room temperature with an Accent Opto RPM 4000 PL mapper. The excitation source was a HeCd laser (λ = 325 nm) with a maximum power of 5 mW on a sample spot of 50 μm. High resolution x-ray diffraction (XRD) measurements were performed at three specific positions within the wafer, i.e. (0, 0), (11, 11), (13, –9), employing a Bruker D8 Discover system with a 1 mm×1 mm aperture at source exit to define the irradiated area.

3. Results and discussion

Figure 1 shows the sheet resistance mapping of the 2-inch (50.8 cm) $Al_{0.29}Ga_{0.71}N$/GaN heterostructure sample. Resistances at the bottom right (11, 11) and top right (13, –9) of the wafer are much higher than those at any other regions. Figure 2 shows the room temperature PL mapping of the sample, which represents the band-edge emission distribution of the GaN template layer, because the AlGaN band-edge peak cannot appear in the wavelength range of 357.7nm to 371.7 nm,[6] and the 2DEG PL emission will not show up at room temperature.[7] The GaN band-edge peak shifts to a high wavelength in the abovementioned two regions with the highest sheet resistance. This red shift is related with a shrinkage of the GaN bandgap,[8] which results from lattice expansion, indicating that either a decreasing compressive strain[9,10] or an increasing tensile strain[11] is present in these regions. What causes this lattice expansion, and how does it affect the electrical properties of the AlGaN/GaN heterostructure? To answer these questions, three positions on the wafer with significant variations of electrical and optical properties, i.e. the centre (0, 0), the top right (11, 11), and the bottom right (13, –9), are selected for structural analysis.

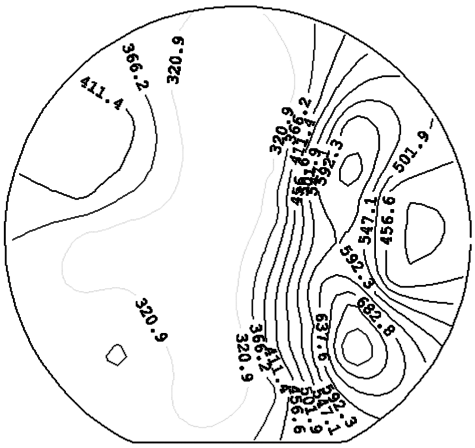


Fig.1. Sheet resistance mapping of the 2-inch $Al_{0.29}Ga_{0.71}N$/GaN heterostructure. The average sheet resistance is 400.7 Ω/□ with maximum resistance of 841.2 Ω/□ and minimum value of 280.7 Ω/□.

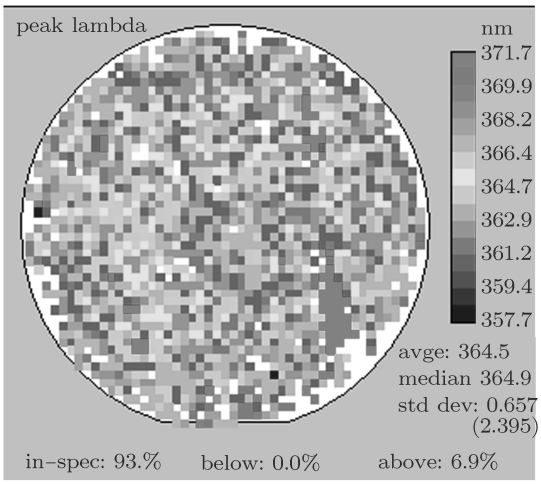


Fig.2. PL mapping of the GaN base layer showing the band edge peak position distribution in an AlGaN/GaN heterostructure wafer at room temperature.

The strains in the GaN base layer, $\Delta c/c_0 = (c-c_0)/c_0$, as well as the aluminium compositions, x, and the degree of relaxations, r, in the AlGaN layer are calculated from the lattice constants a and c of GaN and AlGaN determined[12] by means of the reciprocal space map (RSM) of the (104) reflection of the AlGaN/GaN heterostructure(see Fig.3). Analysis of the $\omega-2\theta$-scan FWHM of AlGaN allows the determination of the aluminium thickness, t, since the broadening of the $\omega-2\theta$-scan of the symmetric reflection (0002) of the AlGaN layer is caused by the limited thickness t and a heterogeneous strain along the c-axis.[13,14] Analysis of the ω-scan FWHMs of

the GaN (0002) and (30-32) reflections allows the determination of dislocation densities, since the (0002) diffraction peak broadening is related to the mean tilt angle of the mosaic structure induced by screw dislocations,[15] and the (30-32) peak broadening can be taken as an appropriate figure of merit for the twist induced by edge dislocations.[16] All of the calculated values are summarized in Table 1.

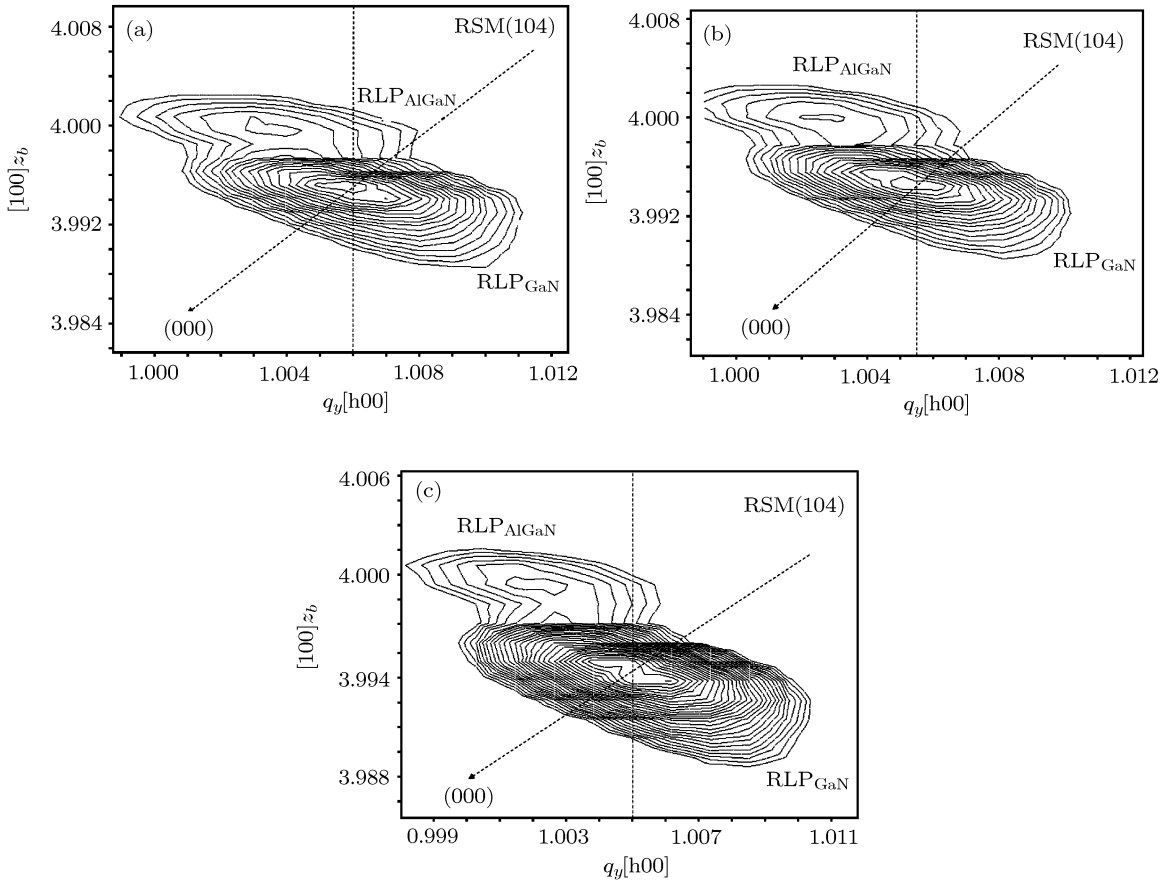


Fig.3. Reciprocal space mapping of asymmetric reflection (10-14) for the AlGaN/GaN heterostructure at three positions (a) (0, 0), (b) (11, 11), (c) (13, –9). The dotted line points to the origin of the reciprocal lattice, and the broken line is parallel to the surface normal across the reciprocal lattice point (RLP) of GaN.

Table 1. XRD measurement data and calculation results for three positions with different sheet resistances.

position	sheet resistance	FWHM of ω-scan/(arc sec)		screw	edge	Al composition	Al thickness	relaxation	strain in GaN
	/ (Ω/□)	(0002)	(30-32)	/10^8 cm^{-2}	/10^9 cm^{-2}	x	/nm	$r/10^{-3}$	$\Delta c/c_0/10^{-3}$
(0, 0)	280.7	493	1830	1.22	4.44	0.277	21.64	2.65	1.3
(11, 11)	592.3	502	1782	1.26	4.21	0.277	22.23	2.68	1.2
(13, –9)	841.2	502	1771	1.26	4.16	0.277	22.19	2.62	1.1

Both the thickness and aluminium composition of the AlGaN layer at these three positions are almost the same, due to the small required thickness of this layer and the identically equal growth condition. As a result, the effects of the AlGaN layer on the electrical properties of the AlGaN/GaN heterostructure can be ignored here, and the only impact factor comes from the GaN layer. With increasing

sheet resistance of the heterostructure, the density of screw dislocation of GaN increases slightly, while the density of edge dislocation shows a clear decrease of 2×10^8 cm^{-2}. Therefore, the edge dislocations rather than screw ones in the GaN layer are the dominant structural feature responsible for the electrical properties of the heterostructure. The XRD results also reveal that a compressive in-plane strain perpendicular to the c-axis exists in all of the measured regions, which decreases with increasing sheet resistance of the AlGaN/GaN heterostructure and with decreasing edge dislocation density in the GaN layer. This is consistent with the PL result and demonstrates that the red shift of the PL band-edge peak results from the reduction of compressive strain.

The reduced compressive strain should not be a biaxial component, but a hydrostatic component. It is reported that two strain components coexist in GaN, biaxial and hydrostatic stress field.[17] Their origins are physically different. The biaxial residual compressive strain is expected to occur on cooling due to the difference in thermal expansion coefficients between GaN and sapphire,[18,19] and in most cases, it will be reduced by generating a large number of edge dislocations.[19] However, here, the reduction of compressive strain is accompanied by a decreased density of edge dislocation instead of an increased one. Therefore, the reduced amount of strain in GaN layer should not be the biaxial component. Hydrostatic strain is generated through free electron expansion of the lattice of GaN.[18,20] Free electrons increase the total energy of a crystal. To decrease the energy, the level of the conduction band becomes lower, which is related to a change of volume of the crystal.[20] Hence a reduced free electron concentration will result in a reduced compressive strain. But why do free electrons reduce in some specific regions of the wafer?

Notice that compressive strain is eliminated in the area where edge dislocation density reduces. Since edge dislocations introduce acceptor centres along the dislocation line which capture electrons from the conduction band in an n-type semiconductor,[4,5] the free electron concentration decreases significantly in the vicinity of edge dislocations.[21,22] Consequently, the lattice expansion caused by free electrons will be suppressed around the edge dislocation line. This means that the lattice constant in the vicinity of the edge dislocation line is smaller than that in the dislocation free regions, or in other words, there is a compressive hydrostatic strain associated with edge dislocation. Therefore, a reduction of the edge dislocation density in GaN will result in a decreased compressive strain, and hence a shrinkage of the GaN bandgap. A simple calculation will demonstrate this: suppose that one unit cell contains one dangling bond and captures one free electron;[23] the increased free electron concentration n resulting from the reduced edge dislocation density is up to $e^{-1}/(c\times\rho)$, where e^{-1} is electronic charge, c the c-axis lattice constant, ρ is the reduced edge dislocation density and equals 2×10^8 cm^{-2} here. In addition, the PL peak energy depends on the carrier concentration n according to[24] $E_{\rm g} = E_{\rm g}(0) - An^{1/3}$, where A is the proportionality constant. The calculated bandgap reduction is approximately in agreement with the experimental result of 0.13 eV.

The compressive strain in the vicinity of edge dislocation will then give rise to a local piezoelectric polarization. As schematically illustrated in Fig.4, suppose that strain is relaxed in the dislocation free region in the GaN layer; however, in the vicinity of edge dislocations, the band gap will be increased due to the hydrostatic compressive strain, and the conduction band is raised in comparison with that in the dislocation free region. The resulting piezoelectric polarization field in the GaN layer possesses an opposite direction to that in the AlGaN layer, which enhances the piezoelectric polarization field in the interface of the heterostructure. The slope of the conduction band edge from the bulk GaN to the AlGaN/GaN interface becomes sharper where edge dislocations gather in the corresponding GaN layer, and hence helps to localize 2DEG and increase the 2DEG concentration. On the other hand, previous work has demonstrated that the room temperature 2DEG mobility cannot be influenced by dislocations in GaN significantly.[25] Therefore, the overall effect reduces the sheet resistance of the heterostructure. As shown in our mapping results, where edge dislocation density decreases, the compressive strain is reduced and the GaN band-edge peak shifts to a high wavelength. This reduction of compressive strain will then suppress the piezoelectric polarization and increase the local sheet resistance of the heterostructure. As a result, a nonuniform distribution of edge dislocation in the GaN layer during growth will result in a nonuniform distribution of the electrical property of the heterostructure.

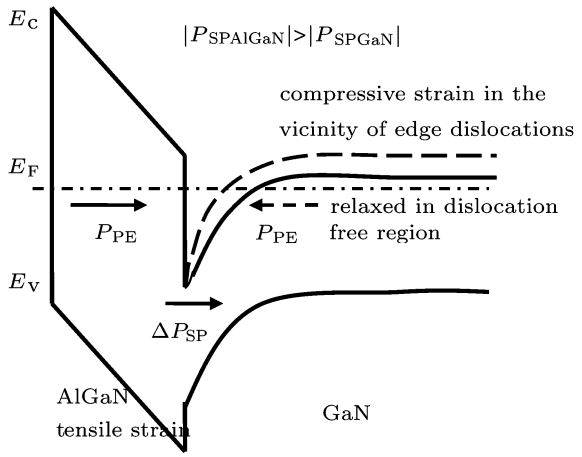


Fig.4. Schematic representation of an AlGaN/GaN heterostructure. The local piezoelectric polarization field in the vicinity of edge dislocations, denoted by the dotted arrow, makes the potential, denoted by the dotted line, slope down from the bulk GaN towards the AlGaN/GaN interface and helps to localize 2DEG.

It should be pointed out that the edge dislocations we talk about here are in the GaN layer, not at the AlGaN/GaN interface, so they can reduce the electron concentration in the GaN layer while increasing the electron concentration at the heterostructure interface. The hydrostatic strain will always associate with edge dislocation unless there is no n type background carrier in GaN. As it is hard to reduce the background electron concentration to zero by using the present growth methods of GaN, the local piezoelectric polarization enhancement caused by edge dislocations will always show up. Since the n type background carrier concentration of the sample investigated by us here is high, the nonuniform distribution of piezoelectric polarization caused by the nonuniform distribution of dislocations is very prominent here. Hence it provides us with a great opportunity to investigate the physical nature of edge dislocations.

Previous work shows that edge dislocation in high resistive GaN helps to suppress the parasitic parallel conductivity through the compensation effect,[26] and hence increases the total mobility of the AlGaN/GaN heterostructure. Although the local piezoelectric polarization effect associated with edge dislocations essentially results from the deficiency of free electron concentration in the vicinity of dislocation, it is another important mechanism different from the compensation effect that could influence the electrical properties of the AlGaN/GaN heterostructure. This is because, with the present testing method, the parallel conduction channel in GaN cannot play its role in influencing the measured total resistance, but resistance still shows itself to be influenced by edge dislocation density. This indicates that another mechanism needs to be taken into account. Hence it can be concluded that edge dislocation in the GaN layer not only suppresses the parallel conductivity through the compensation effect, but also increases the 2DEG concentration through the local piezoelectric polarization effect.

However, this result does not mean that we should promote edge dislocation density in order to improve the electrical properties of the AlGaN/GaN heterostructure. It is interesting that GaN based devices can operate despite dislocation densities far in excess of conventional III–V semiconductor material,[27] such as GaAs, which implies that dislocation, as a kind of defect, is not always a disadvantage in a GaN material system. The biggest difference between GaN and other wide bandgap semiconductor materials lies in the characteristic of the piezoelectric effect in GaN. Our research here can interpret this intriguing behaviour of GaN to some extent. A nearly perfect crystal structure is indeed ideal for every kind of semiconductor device, but as long as the dislocation density in GaN cannot be reduced as low as in silicon, at least up to now, simply concentrating on dislocation densities cannot get improved device performance. Tolerance of dislocations to some extent is not always that bad for a GaN material system.

4. Conclusion

In summary, the influence of threading dislocations in the GaN layer on the electrical properties of an AlGaN/GaN heterostructure has been studied by means of investigating the local distributions of material properties within the wafer. A compressive hydrostatic stress field is found to associate with the edge dislocations in GaN. This will then give rise to a local piezoelectric polarization field and help to increase the 2DEG concentration. In addition to the compensation effect, edge dislocation in GaN could play a role in influencing the electrical properties of an AlGaN/GaN heterostructure through the piezoelectric polarization effect.

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