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The effect of single AlGaN interlayer on the structural properties of GaN epilayers grown on Si (111) substrates*

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High-quality and nearly crack-free GaN epitaxial layer was obtained by inserting a single AlGaN interlayer between GaN epilayer and high-temperature AlN buffer layer on Si (111) substrate by metalorganic chemical vapor deposition. This paper investigates the effect of AlGaN interlayer on the structural properties of the resulting GaN epilayer. It confirms from the optical microscopy and Raman scattering spectroscopy that the AlGaN interlayer has a remarkable effect on introducing relative compressive strain to the top GaN layer and preventing the formation of cracks. X-ray diffraction and transmission electron microscopy analysis reveal that a significant reduction in both screw and edge threading dislocations is achieved in GaN epilayer by the insertion of AlGaN interlayer. The process of threading dislocation reduction in both AlGaN interlayer and GaN epilayer is demonstrated.

Keywords: GaN, Si (111) substrate, metalorganic chemical vapor deposition, AlGaN interlayer
PACC: 6855, 7280E, 8115H

1. Introduction

The growth of GaN film on Si substrate has attracted extensive attention because of the advantages of Si such as low cost, high crystal quality, large size availability, and good thermal and electrical conductivities.[1,2] In addition, there may be a possibility to integrate the GaN-based devices with Si microelectronics. However, for GaN heteroepitaxy on Si substrate, the large lattice mismatch and thermal mismatch between GaN and Si usually lead to high threading dislocation (TD) density and the formation of cracks when cooling down to room temperature from the growth temperature.[3] Up to now, various interlayers (ILs) such as AlN IL,[4−6] AlN/GaN superlattice[7,8] and step-graded or composition-graded AlGaN IL,[9−13] have been introduced into the growth of GaN epilayer to compensate for the large thermal tensile stress and prevent the formation of cracks. Among these ILs, AlN IL reduces the crack density and concurrently introduces extra edge-type TDs in the top GaN films, AlN/GaN superlattice or step-graded AlGaN IL growth needs a precise control of layer parameters and is very much dependent on the experimental system. However, the growth of a single AlGaN IL could not only reduce crack density and improve the crystal quality of GaN epilayer, but also can be less dependent on the experimental system, becoming an efficient and practical choice to realise the lattice-mismatched growth of GaN on Si.

In this study, we present the high-quality and nearly crack-free GaN epitaxy on Si (111) substrate by inserting a single AlGaN IL between GaN epilayer and high-temperature AlN buffer layer. The effect of AlGaN IL on the surface morphology, strain status

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and microstructure evolution of GaN epilayer was investigated by comparing two GaN samples with and without AlGaN IL, which will give us a further understanding of the role of AlGaN IL in the growth of GaN epilayer on Si substrate.

2. Experimental

Two samples were prepared by using low pressure metalorganic chemical vapor deposition (MOCVD). Trimethylgallium (TMGa), trimethylaluminum (TMAl) and ammonia (NH_3) were used as Ga, Al and N precursors in H_2 carrier gas. The 2-inch Si (111) substrates were etched in a 5% HF solution for 1 min before being loaded into the reactor. Sample A was firstly grown with a 330-nm AlN buffer layer at 1080 °C, followed by an $Al_{0.37}Ga_{0.63}N$ IL for a thickness of about 630 nm. Lastly, a 1.5-μm GaN epilayer was grown on top at 1040 °C. For comparison, sample B was prepared by depositing GaN epilayer directly on AlN buffer layer without AlGaN IL.

The surface morphology of GaN epilayers was characterised by optical microscopy. The crystalline quality and microstructure of the GaN epilayers were studied by high-resolution x-ray diffraction (HRXRD) and transmission electron microscopy (TEM). The TEM specimen was thinned by conventional polishing and then by Ar-ion milling. The cross-section TEM images were performed by using JEM-2010 operated at 200 kV. The strain status at room temperature was measured by micro-Raman scattering spectroscopy. For the micro-Raman scattering measurements, a 532-nm laser was employed as the excitation source with a spatial resolution of 1 μm in a backscattering geometry.

3. Results and discussion

The cracks in GaN epilayers were studied by optical microscopy. In the case of sample B which has no AlGaN IL, a lot of cracks are observed due to the large thermal tensile stress during the cooling down to room temperature from growth temperature. However, by inserting one AlGaN IL between GaN epilayer and AlN buffer layer, the crack density in sample A is significantly reduced, as shown in Fig.1(a). In fact, no cracks are observed in a circular area with a diameter of about 3 cm near the central region of sample A. Although cracks are still observed near the edge part, the overall crack density of sample A is substantially reduced. The decrease of crack density can be attributed to a reduction of tensile strain with the insertion of AlGaN IL, which provides a compressive strain for the subsequent GaN layer and consequently compensates the large thermal tensile strain during the cooling process.

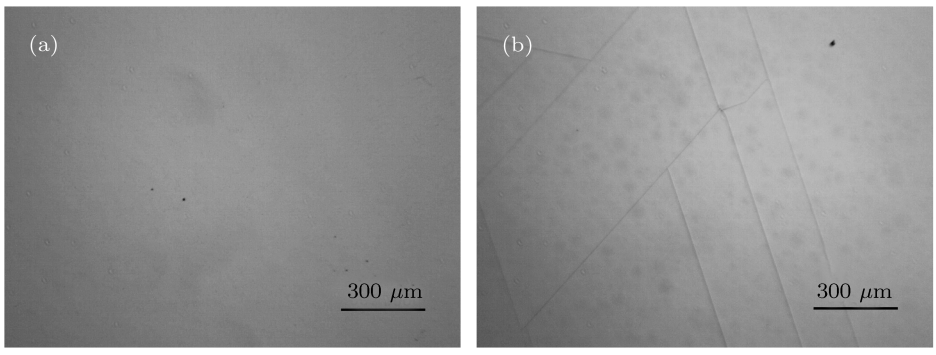


Fig.1. Optical microscopy images of two GaN epilayers: (a) sample A ; (b) sample B.

Figure 2 shows the XRD (0002) triple-axis 2θ–ω scan plots of the two investigated GaN samples. The Bragg angle of GaN (0002) has been corrected considering zero setting of instrumental alignment according to the method proposed by Zheng *et al.*[14] One can clearly observe an intense peak of GaN (0002) and a

weak AlN (0002) diffraction peak for both samples A and B. An additional peak of AlGaN (0002) is found for sample A. It is worth while noting that the (0002) peak of GaN is located at $2\theta = 34.592°$ and 34.598° for samples A and B respectively. It shows an obvious shift to the lower angle for sample A. For symmetric GaN (0002) plane Bragg reflection, the shift of the peak is caused by the variation of strain in the GaN layer. This result indicates that the GaN epilayer with AlGaN IL is compressively strained in comparison with the GaN without IL, which confirms that the AlGaN IL has a remarkable effect in introducing relative compressive strain in the top GaN layer.

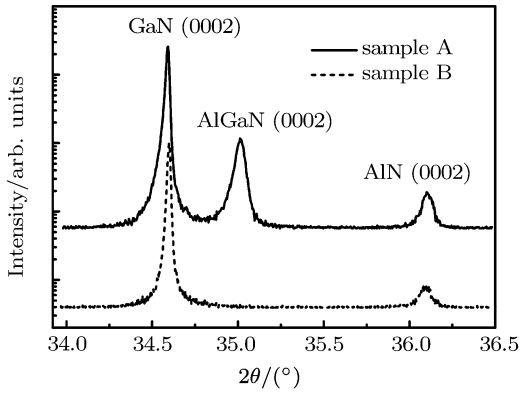


Fig.2. X-ray 2θ–ω scan plots of the symmetric (0002) diffraction for sample A and sample B.

Such a compressive strain introduction in the GaN epilayer is further checked by the micro-Raman scattering spectroscopy at room temperature as shown in Fig.3. According to the Raman selection rules, only the phonon modes of E_2 and A_1 (LO) can be observed in the Z $(X,\ X)$ $\bar{Z}$ backscattering geometry with Z along the growth direction $\langle 0001 \rangle$. Three prominent Raman scattering peaks are observed in the range of 530–900 cm^{-1}. The strongest peaks at 565.8 cm^{-1} and 564.3 cm^{-1} for sample A and sample B, respectively, are related to the E_2 (high) mode for the GaN epilayers. The weak peak at about 649.0 cm^{-1} corresponds to the E_2 (high) mode of the AlN buffer layer. The moderate peak at about 733 cm^{-1} is associated with the A_1 (LO) mode of the GaN epilayer. The E_2 (high) phonon mode is usually used to evaluate the strain status because it is particularly sensitive to the biaxial strain and usually gives the strongest signal in the Raman spectra. The blue shift of the E_2 (high) mode of about 1.5 cm^{-1} for sample A compared with sample B indicates that GaN epilayer grown with AlGaN IL is compressively strained compared with that of grown without AlGaN IL. It can be concluded that the AlGaN IL provides a compressive strain to the top GaN layer, which partially compensates the thermal tensile strain between GaN and Si. It is in good agreement with the conclusions obtained from XRD and optical microscopy. In addition, it is found that the shift of the E_2 (high) mode of about 8.4 cm^{-1} towards low frequency for the AlN buffer layers of sample A and sample B compared with the unstrained AlN (657.4 cm^{-1})[15] indicates the existence of a large biaxial tensile strain in the AlN buffer layer due to the large lattice mismatch between AlN and Si.

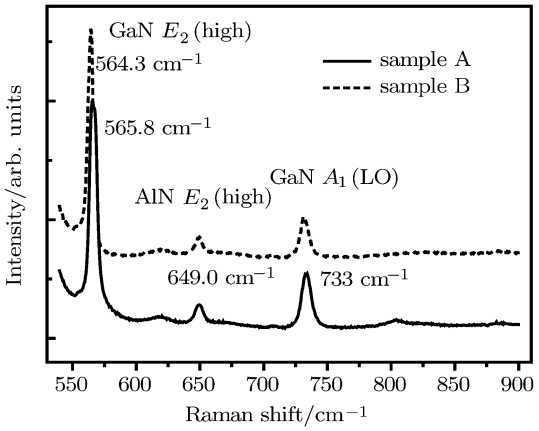


Fig.3. A comparison of Raman scattering spectra of sample A and sample B.

The x-ray ω-scan measurements for two GaN sampls A and B were carried out with both symmetric (0002) and skew (10–12) reflections. The full width at half maximum (FWHM) of rocking curve peaks are listed in Table 1. It is clearly seen that the FWHM of both reflections are much decreased for sample A by the insertion of AlGaN IL. The FWHM values of the GaN (0002) and GaN (10–12) ω-scan for sample A are 493 and 994 arc sec, respectively, being much smaller in comparison with 558 and 1300 arc sec for sample B. These values are comparable to or even better than the ones recently reported for GaN grown on silicon.[13] As is well known, the symmetric (0002) reflection is affected by dislocations consisting of screw components in screw and mixed type TDs, while the skew (10–12) reflection is sensitive to all screw, mixed and edge type TDs. The TD density (TDD) of the two GaN epilayers can be calculated from the equations[16]

$$\beta^2_{10\bar{1}2} = \beta^2_{\mathrm{s}} + \beta^2_{\mathrm{e}}, \tag{1}$$

$$D_{\mathrm{s}} = \frac{\beta^2_{0002}}{4.35 b^2_{\mathrm{s}}} = \frac{\beta^2_{\mathrm{s}}}{4.35(b_{\mathrm{s}} \cos\alpha)^2},$$

$$D_{\mathrm{e}} = \frac{\beta^2_{\mathrm{e}}}{4.35(b_{\mathrm{e}} \sin\alpha)^2} \quad (\alpha = 43.19°), \tag{2}$$

where D_s is the screw TDD, D_e is the edge TDD, β is the FWHM measured by XRD rocking curve and b is the Burger vector length ($b_s = 0.5185$ nm, $b_e = 0.3189$ nm). Here, screw TD refers to the sum of pure screw type and screw component of mixed type dislocations and the edge TD represents the sum of pure edge type and edge component of mixed type dislocations. As seen in Table 1, both TDs in sample A, especially edge TDs, have been substantially reduced by the insertion of AlGaN IL. Thus, we can state that the insertion of AlGaN IL has significantly improved the crystalline quality of GaN epilayers.

Table 1. FWHM of (0002), (10–12) ω-scan and TDD for the two GaN samples deduced from the XRD measurements.

sample	FWHM of (0002) ω-scan/(arc sec)	FWHM of (10–12) ω-scan/(arc sec)	screw TDD (10^8 cm^{-2})	edge TDD (10^9 cm^{-2})
A	493	994	4.9	9.7
B	558	1300	6.3	17.3

As a further proof of the advantage of AlGaN IL to crystalline quality of GaN epilayers, the cross-section TEM measurements are performed on sample A under two beam diffraction conditions with $\boldsymbol{g}$=[11–20] and $\boldsymbol{g}$ = [0002]. According to the invisibility criterion of $\boldsymbol{g}\cdot\boldsymbol{b} = 0$ ($\boldsymbol{b}$ is Burgers vector), screw and mixed type TDs are observable with $\boldsymbol{g}$ = [0002], while the edge and mixed type TDs are observable with $\boldsymbol{g}$=[11–20]. One can clearly see that a larger number of edge component TDs than screw ones is observed in the AlGaN IL and GaN epilayer, which is consistent with the results of XRD. There is a high density of TDs in AlN buffer layer, while most of these TDs are decreased substantially in the GaN epilayer by inserting AlGaN IL between GaN epilayer and AlN buffer layer. Significant TD reduction firstly occurs at the interface between AlGaN IL and GaN epilayer, where many of TDs are terminated and bent into the growth plane as shown by the dashed circles in Figs.4(a) and 4(b). Moreover, few TDs are produced at this interface. It is noted that a second TD reduction takes place in the first 200 nm GaN epilayer above the AlGaN IL where many TDs are inclined away from the growth direction, whose driving force is the compressive strain derived from the lattice mismatch between AlGaN IL and GaN epilayer. These inclined TDs interact with the TDs with opposite Burger vector and finally are annihilated (shown by the arrows in Figs.4(a) and 4(b)), leading to the reduction of most TDs in GaN epilayer and the compressive strain relaxation.[17] The above-mentioned TD's behaviors all contribute to an efficient reduction of the total TD density in the GaN epialyer.

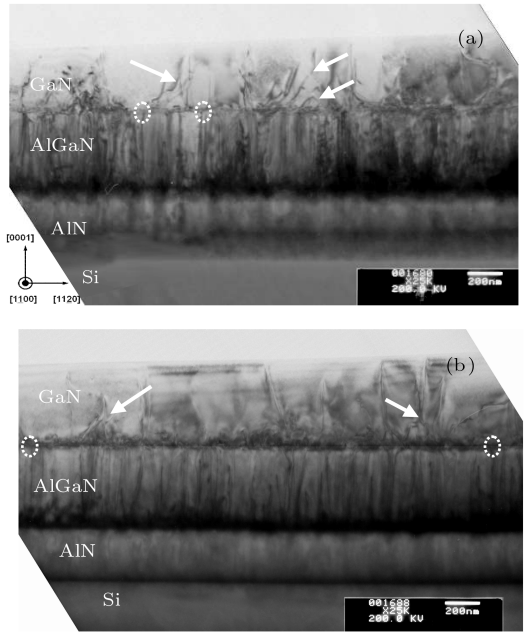


Fig.4. Cross-section bright field TEM images of sample A taken under two-beam diffraction condition with $\boldsymbol{g}$=[11–20] (a) and $\boldsymbol{g}$ = [0002] (b). The dashed circles indicate the termination of TDs at the interface between AlGaN IL and GaN epilayer, and the arrows show the inclination and interaction of TDs.

4. Conclusions

In conclusion of this paper, we have studied the growth and structural characterization of GaN epi-

layers grown on Si (111) substrate with and without AlGaN IL. Nearly crack-free GaN films have been obtained by inserting AlGaN IL between GaN epilayer and AlN buffer layer, which introduces a compressive strain in top GaN epilayer, substantially decreasing the in-plane tensile strain in GaN epilayer and significantly reducing screw and edge TD density. The obtained results show that AlGaN IL can greatly improve the structural properties of GaN epilayers grown on Si substrate and is very helpful for a better understanding of the role of AlGaN IL in the growth of GaN on Si.

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