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The effects of vicinal sapphire substrates on the properties of AlGaN/GaN heterostructures*

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AlGaN/GaN heterostructures on vicinal sapphire substrates and just-oriented sapphire substrates (0001) are grown by the metalorganic chemical vapor deposition method. Samples are studied by high-resolution x-ray diffraction, atomic force microscopy, capacitance–voltage measurement and the Van der Pauw Hall-effect technique. The investigation reveals that better crystal quality and surface morphology of the sample are obtained on the vicinal substrate. Furthermore, the electrical properties are also improved when the sample is grown on the vicinal substrate. This is due to the fact that the use of vicinal substrate can promote the step-flow mode of crystal growth, so many macro-steps are formed during crystal growth, which causes a reduction of threading dislocations in the crystal and an improvement in the electrical properties of the AlGaN/GaN heterostructure.

Keywords: GaN, AlGaN/GaN heterostructures, vicinal substrate

PACC: 7280E, 7340L, 7360L

1. Introduction

As a wide band-gap semiconductor material, gallium nitride (GaN) has attracted more and more interest due to its excellent properties. Compared to many conventional semiconductor materials (such as silicon or gallium arsenic), GaN possesses many advantages such as wide band-gap, high saturated electron drift velocity, high breakdown field strength, high radiation resistance properties and good chemical stability. A two-dimensional electron gas (2DEG) with high density and high mobility can be formed in the AlGaN/GaN hetero-interface owing to the large band gap offset between AlGaN and GaN, as well as their high spontaneous and piezoelectric polarizations. GaN and its associated compound semiconductors will play a significant role in the future development of high temperature, high power and high frequency electronic devices.[1−4] However, it is still difficult to obtain bulk GaN of high quality and large size: common GaN film is usually heteroepitaxially grown on c-face sapphire substrate or SiC substrate. It is rather well known that III−V nitrides are generally grown on sapphire substrates for their low cost and stability at high temperature, in comparison with SiC substrates. However, their lattice parameters and thermal expansion coefficients are not well matched. The large mismatch leads to a high density of threading dislocations in the grown GaN layer. Even though incorporating a GaN or AlN nucleation layer can improve the crystal quality, the available dislocation density is always in the range of 10^8–$10^{10}/\mathrm{cm}^2$.

Several techniques, for example, epitaxial lateral overgrowth (ELOG),[5−7] have been proposed to reduce the dislocation density. Unfortunately, this technique cannot uniformly reduce the threading dislocations and will complicate the fabrication technology. However, some researchers have reported superior material properties of GaN layer grown on vicinal c-plane sapphire substrate.[8] Grudowski *et al*[9] first reported that a higher photoluminescence (PL) intensity could be obtained when a GaN layer was formed on vicinal sapphire substrate. Later, Fatemi *et al*[10] found better crystal quality and electrical properties of GaN film when it was grown on vicinal substrate. However, up to now, there have been few reports on the effects of small miscut angles of c-plane sapphire substrates on the properties of AlGaN/GaN heterostructures prepared by the metalorganic chemical vapor deposition (MOCVD) method. It has been proposed that the optimal vicinal angle to obtain high-quality GaN film was about 0.5° in previ-

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ous research.[11] Based on the previous research, in this paper, we propose that a small misorientation of substrate from the c-face about 0.5° will considerably improve the morphology and the electrical properties of the AlGaN/GaN heterostructure, and a better crystal quality will also be obtained on the vicinal substrate.

2. Experimental details

Our samples in this study were grown by the cold-wall low-pressure MOCVD system using a conventional two-step growth method. Triethylgallium, trimethylaluminum, and ammonia (NH_3) were used as the Ga, Al and N precursors, respectively, and high purified hydrogen (H_2) as the carrier gas. The vicinal sapphire substrate (0001) used in our study was inclined toward the ⟨11–20⟩ direction with a vicinal angle of 0.4°. A low-temperature AlN nucleation layer with a thickness of 15 nm was first grown at ∼620 °C,

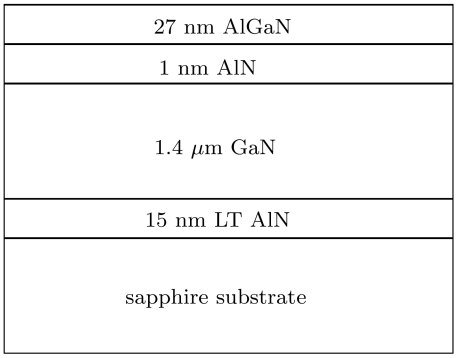


Fig.1. Schematic structure of the samples.

then an unintentionally doped GaN layer was grown at about 1000 °C; the growth time was set to yield about a 1.4-μm-thick GaN layer. Finally, a 1-nm AlN spacer layer and a 27-nm AlGaN barrier layer were grown. The total thickness of the structure is 1450 nm according to the transmission spectrum analyzer measurement.[12] Figure 1 depicts the schematic structure of the sample used in our study. For comparison, an identical heterostructure was prepared on a just-oriented c-plane sapphire substrate under the same conditions. In the following discussion, the sample grown on the vicinal substrate is labeled as sample A, while the other one is labeled as sample B. To check the structural qualities of the layers grown on these substrates, the samples have been examined by high-resolution x-ray diffraction (HRXRD). For the characterization of the surface morphologies of the layers, we used atomic force microscopy (AFM). The electrical properties of the AlGaN/GaN structures were measured by capacitance–voltage (C–V) measurement and the Van der Pauw Hall-effect technique.

3. Results and discussion

To determine the crystal qualities of the layers, we first performed x-ray rocking curve measurements of symmetric (0002) and asymmetric (10–12) diffraction. Figure 2 shows the measured rocking curves of the samples. From Fig.2, it is found that the full width at half maximum (FWHM) of symmetric (0002) XRD rocking curves of samples A and B are 455 arcsec and 576 arcsec, respectively, while the FWHM of asymmetric (10–12) XRD rocking curves of samples A and B are 750 arcsec and 863 arcsec, respectively. It is well known that the FWHM of symmetric (0002) and asymmetric (10–12) XRD spectra are associated with the screw dislocation and the edge dislocation of a layer, respectively. Compared to sample B, both the FWHM of symmetric (0002) and asymmetric (10–12) XRD spectra of sample A are slightly smaller, which indicates the better crystal quality of sample A. The dislocation densities of materials can be calculated by using the following equation[13]

$$D_{\rm dis} = \frac{\beta^2}{9b^2},$$

where $D_{\rm dis}$ is the dislocation density, β is the FWHM of (0002) or (10–12) XRD spectra and b represents the Burgers vector of a given XRD peak (b is equal to 0.5185 nm and 0.3189 nm for the screw dislocation and the edge dislocation, respectively). From the equation, it is found that the screw dislocation densities of samples A and B are $2\times10^8/\mathrm{cm}^2$ and $3.2\times10^8/\mathrm{cm}^2$, respectively, and the edge dislocation density is reduced from $1.93\times10^9/\mathrm{cm}^2$ to $1.45\times10^9/\mathrm{cm}^2$ by using the vicinal substrate. Note that both the screw and the edge dislocation density of the layer are reduced when the vicinal substrate is used. It has been clarified that inclined threading dislocations would be formed in layers grown on vicinal substrates.[14] The threading dislocations existing in the as-grown films are all vertical threading dislocations when the samples are grown on just-oriented substrates. However, some of the vertical threading dislocations will be inclined when the samples are grown on vicinal substrates. Thus, a fraction of the vertical threading dislocations will be terminated where they encounter the inclined threading

dislocations, resulting in an obvious reduction of the dislocation density. Furthermore, it is also thought that the vertical threading dislocations will react with the inclined threading dislocations to form dislocation loops, resulting in a further reduction in the dislocation density of the grown layer.

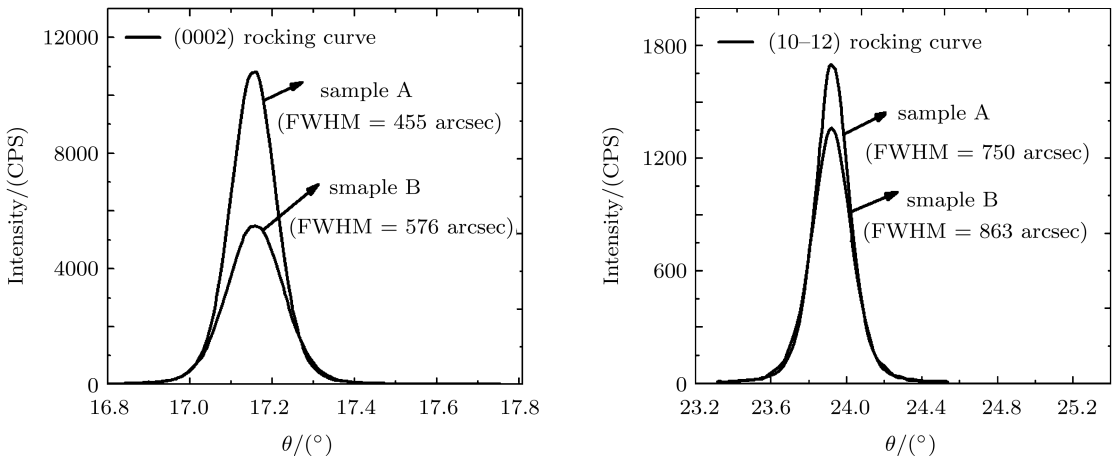


Fig.2. The XRD spectra of the samples.

AFM was used to characterize the morphologies of the samples. Images of the samples are shown in Fig.3. The dark spots in the images are due to threading dislocations in the epitaxial layers. It is readily found that the dark spots in Fig.3(a) are significantly less than those in Fig.3(b), which indicates a great reduction of the dislocation density in the structure grown on the vicinal substrate again. The root-mean-square (RMS) roughness of samples A and B are 0.387 nm and 0.674 nm, respectively. Three-dimensional images of the samples are shown in Fig.4. The images show that the surface of sample A is smooth with few hillocks, while there are lots of hillocks in the surface of sample B. In fact, it is considered that the surface morphology is greatly improved by using the vicinal substrate. Furthermore, it is found that the surface takes on a step-like feature for the structure grown on the vicinal substrate in Fig.3. For the structure prepared on the just-oriented substrate, there are no clear steps which can be observed. This is due to the fact that the use of vicinal substrate can promote the step-flow mode of crystal growth. This mode leads to the formation of macro-steps,[11] and reduces the generation of dislocations when three-dimensional islands coalesce with each other.

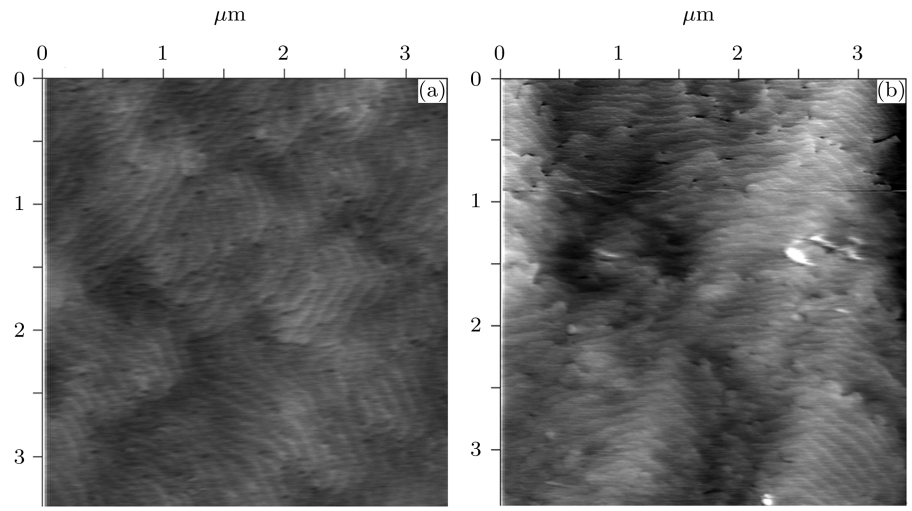


Fig.3. AFM images of the samples (3×3 μm^2). (a) Image of sample A (RMS = 0.387 nm); (b) Image of sample B (RMS = 0.674 nm).

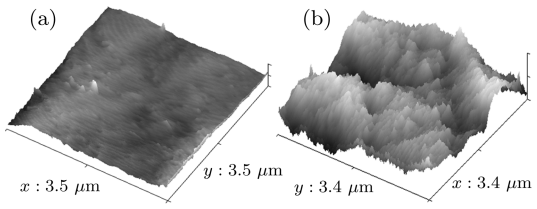


Fig.4. Three-dimensional AFM images of samples A and B. (a) Image of sample A; (b) image of sample B.

The electrical properties of the structures were measured by capacitance–voltage (C–V) measurement and the Hall-effect technique. Figure 5 illustrates the carrier distribution profiles of the two samples. As can be seen from Fig.5, the peak values of the two curves are nearly the same, while the background carrier density in sample B is slightly lower than that in sample A. The results from C–V measurement indicate that there is no obvious difference in the 2DEG densities of the two samples.

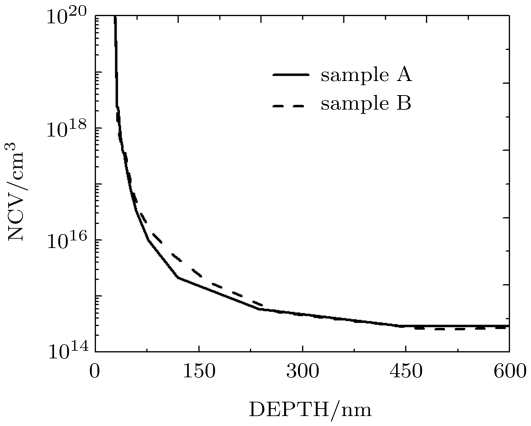


Fig.5. Carrier distribution profiles of the samples.

Figure 6 presents the 2DEG densities and the electron mobilities of the samples as functions of temperature measured by Hall-effect measurement. Focusing on the dependence of the electron mobilities of the samples on temperature, we find that obviously the mobility of sample A is considerably higher than that of sample B. For example, in the case of sample A, the room temperature electron mobility is 1372 cm^2/Vs, while it is 1236 cm^2/Vs in the case of sample B. The difference is even larger when the measuring temperature is 77 K, at which the mobilities of samples A and B are 5741 cm^2/Vs and 4056 cm^2/Vs, respectively. It is clear that a higher carrier mobility of the sample is obtained when it is prepared on the vicinal substrate. From Fig.6, it is also found that the 2DEG densities of the samples are about $1.9\times10^{13}/cm^2$ at room temperature. However, when the temperature is reduced to 77 K, the 2DEG density in sample B is decreased much more than that in sample A. Therefore, the above-mentioned results show that better electrical properties of the heterostructure are obtained by using the vicinal substrate.

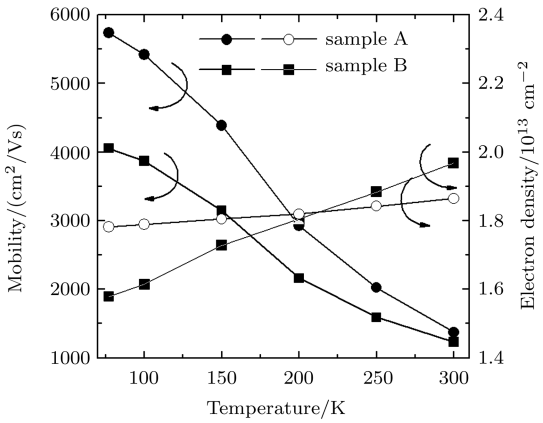


Fig.6. Dependence of 2DEG density and electron mobility on temperature.

In order to understand the electron transport properties of the 2DEG in these two samples, the carrier scattering mechanism is analyzed in details. It is well known that the electron mobilities in AlGaN/GaN heterostructures are restricted by various kinds of scattering processes, such as alloy disorder scattering, interface roughness scattering, dislocation scattering, acoustic deformation-potential scattering and piezoelectric scattering. It was found that the dominant carrier scattering processes in the AlGaN/GaN samples were the alloy disorder scattering process and the interface roughness scattering process at low temperature.[15] In a sample with a high Al-content (where the Al-content is higher than 25%) and a thick AlGaN barrier layer (where the thickness is larger than 20 nm), the interface roughness scattering will significantly restrict the carrier mobility due to the increase of interface roughness, which is caused by the accumulation of stress in the AlGaN barrier layer. As shown above, samples A and B were grown under the same conditions excluding the substrates, so it is thought that the influences of the alloy disorder scattering on the 2DEG carrier mobilities of the samples are nearly the same. The Al-contents in the two samples are about 35% according to the XRD measurement and the barrier layers are both 27 nm thick. The high Al-contents and the thick barrier layers of the samples lead to very high 2DEG densities

of $1.93 \times 10^{13}/\text{cm}^2$, which results in the 2DEG electrons shifting closer to the AlGaN/GaN interface. So it is thought that the determined carrier scattering process at low temperature in our samples is interface roughness scattering. This analysis combining the AFM results shown above indicates that the significant increase of the 2DEG electron mobility at low temperature can be attributed to the great improvement of the AlGaN/GaN interface roughness by using the vicinal substrate. Furthermore, a GaN layer with a lower dislocation density was obtained by using the vicinal substrate, which further improved the carrier mobility in sample A.

All the results we have obtained are summarized in Table 1. From the table, it is proposed that the use of vicinal sapphire substrate with a small miscut angle can significantly improve the morphology of the heterostructure, and the electron mobility in the conducting channel can be much higher than that of a sample prepared on the conventional c-face sapphire substrate while having nearly the same 2DEG densities. It is also clear that the crystal quality of the layer is slightly improved when the vicinal substrate is used.

Table 1. Results measured by various techniques.

sample	(0002) FWHM (arcsec)	(10–12) FWHM (arcsec)	RMS roughness (nm)	mobility at 300 K (cm^2/Vs)	mobility at 77 K (cm^2/Vs)	2DEG at 300 K ($\times 10^{13}/\text{cm}^2$)	2DEG at 77 K ($\times 10^{13}/\text{cm}^2$)
A	455	750	0.387	1372	5741	1.87	1.78
B	576	863	0.674	1236	4056	1.96	1.57

4. Conclusion

Based on the previous research, this paper presents the influence of a vicinal sapphire substrate with a small vicinal angle of 0.4° on the properties of an AlGaN/GaN heterostructure. For the structure grown on the vicinal substrate, the surface morphology was greatly improved and the threading dislocation density was reduced due to the step-flow mode growth of the layer. It is thought that the use of the vicinal substrate can promote the formation of inclined threading dislocations, which prevent conventional vertical dislocations threading to the surface. By C–V and Hall-effect measurements, it was found that a higher carrier mobility was obtained by using the vicinal substrate while having nearly the same 2DEG densities. The electrical properties of the structure grown on the vicinal substrate were much better than those on the substrate without vicinal angle when the samples were measured at 77 K.

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