Effects of the strain relaxation of an AlGaN barrier layer induced by various cap layers on the transport properties in AlGaN/GaN heterostructures*

Liu Zi-Yang(刘子扬), Zhang Jin-Cheng(张进成)†, Duan Huan-Tao(段焕涛), Xue Jun-Shuai(薛军帅), Lin Zhi-Yu(林志宇), Ma Jun-Cai(马俊彩), Xue Xiao-Yong(薛晓咏), and Hao Yue(郝 跃)

School of Microelectronics, and State Key Discipline Laboratory of Wide Band Gap Semiconductor Technology, Xidian University, Xi'an 710071, *China*

(Received 19 January 2011; revised manuscript received 25 April 2011)

The strain relaxation of an AlGaN barrier layer may be influenced by a thin cap layer above, and affects the transport properties of AlGaN/GaN heterostructures. Compared with the slight strain relaxation found in AlGaN barrier layer without cap layer, it is found that a thin cap layer can induce considerable changes of strain state in the AlGaN barrier layer. The degree of relaxation of the AlGaN layer significantly influences the transport properties of the two-dimensional electron gas (2DEG) in AlGaN/GaN heterostructures. It is observed that electron mobility decreases with the increasing degree of relaxation of the AlGaN barrier, which is believed to be the main cause of the deterioration of crystalline quality and morphology on the AlGaN/GaN interface. On the other hand, both GaN and AlN cap layers lead to a decrease in 2DEG density. The reduction of 2DEG caused by the GaN cap layer may be attributed to the additional negative polarization charges formed at the interface between GaN and AlGaN, while the reduction of the piezoelectric effect in the AlGaN layer results in the decrease of 2DEG density in the case of AlN cap layer.

Keywords: cap layer, strain relaxation, AlGaN/GaN, transport properties

PACS: 77.65.Ly, 72.10.Fk, 72.80.Ey **DOI:** 10.1088/1674-1056/20/9/097701

1. Introduction

Research on GaN-based high electron mobility transistors (HEMTs) has been carried out intensively over recent decades due to their high temperature, high power, and high frequency electronic properties.[1−3] The two-dimensional electron gas (2DEG) formed near the interface of AlGaN/GaN heterostructures is induced by spontaneous and piezoelectric polarization, and the increase of Al content in the AlGaN barrier layer can improve the electronic properties of 2DEG.[4] However, due to the large lattice mismatch between the binary nitrides AlN and GaN (about 2.5%),[5] the increase of Al content may lead to undesired strain relaxation of the AlGaN barrier layer, which causes crystal deformation and decreases the piezoelectric polarization effects.

Cap layers are commonly used to realize various goals in GaN-based electrical and optical devices. Some have proposed that an InGaN cap on GaN or a GaN cap on AlGaN could reduce the resistance of Ohmic contacts.[6] A GaN cap was also utilized to increase the Schottky barrier height of AlGaN/GaN heterostructures, by which gate leakage current was significantly reduced.[7] In addition, it was suggested that a low-temperature AlN cap could act as a good gate insulator and a passivation layer for both AlGaN/GaN HEMTs and GaN-based ultraviolet photodiodes.[8,9] The influence of strain state in modulation-doped AlGaN on the 2DEG transport properties has been analysed by changing the thickness of the AlGaN layer.[10] In addition, it was reported that a GaN cap could improve 2DEG mobility and reduce 2DEG density.[11,12] However, even though the cap layers are extensive used in GaN-based devices, there is a lack of research into the relationship between strain variation in AlGaN induced by different kinds of cap layers and the electrical properties of AlGaN/GaN heterostructures, especially with a relative high Al content.

In this study, the variation of the strain state of the AlGaN barrier layer in AlGaN/GaN heterostructures is studied with different kinds of thin cap lay-

*Project supported by the National Science and Technology Major Project of the Ministry of Science and Technology of China (Grant No. 2008ZX01002-002) and the Major Program and the Key Program of National Natural Science Foundation of China (Grant Nos. 60890191 and 60736033).

†Corresponding author. E-mail: jchzhang@xidian.edu.cn

© 2011 Chinese Physical Society and IOP Publishing Ltd

ers. The morphology and dislocation density of the AlGaN barrier layer are studied using an atomic force microscope (AFM) and high-resolution X-ray diffraction (HRXRD), respectively. They are believed to be relevant to the 2DEG electronic properties characterized by Hall-effect measurements.

2. Experimental procedure

Samples were grown on (0001) sapphire in a metal-organic chemical-vapour deposition (MOCVD) system. Hydrogen was used as the carrier gas and triethylgallium, trimethylaluminium and ammonia (NH_3) were used as source compounds. The heterostructures were grown on high-temperature AlN buffer layers. The growth conditions of the AlGaN/GaN layers were as follows: the growth temperature was 1060°C, the total pressure was 40 Torr (1 Torr = 133.322 Pa) and the growth rate was 14 nm/min. The thin (2 nm) GaN and AlN cap layers were grown under the same conditions as given above.

Two heterostructures were prepared and, in each sample, the cap structure was different. One consists of a single $Al_{0.37}Ga_{0.63}N$ (22 nm)/GaN (1.5 μm) heterostructure with a thin GaN cap layer (2 nm) on top of the AlGaN barrier layer (sample A), the other has an AlN cap layer (2 nm) (sample B); the same AlGaN/GaN heterostructure without a cap layer (sample C) was also investigated for comparison.

HRXRD analysis was carried out using a Bruker D8 Discover diffractometer with a mirror and a four-bounce asymmetric Ge (220) monochromator (Cu $K\alpha_1$ radiation of wavelength 1.5406 Å was used). Room temperature Hall-effect measurements were performed in the van der Pauw geometry using indium contacts to characterize the electrical properties of 2DEG. The surface morphology was analysed by AFM.

3. Results and discussion

Figure 1 shows the reciprocal space mappings (RSMs) around a (105) reflection of $Al_{0.37}Ga_{0.63}N$/GaN heterostructures in three samples. The dashed lines indicate the position of the completely strained AlGaN layer with different Al contents. In sample C, the AlGaN barrier layer displays a slight relaxation due to its approaching the critical thickness for relaxation with a relative high Al content.[13,14] By introducing a GaN cap layer (sample A), the AlGaN layer is fully strained; while an AlN cap causes a severe relaxation of the AlGaN barrier layer compared with the two other samples. Since the in-plane lattice parameter of GaN is larger than that of AlGaN, and the AlGaN barrier layer is under a tensile strain, the GaN cap layer can stretch the AlGaN barrier below so that the latter can better fit the underlying GaN buffer layer. In contrast, due to a relatively small in-plane lattice parameter of AlN, the AlGaN layer is compressed by the AlN cap and the misfit between the barrier and buffer becomes more severe, leading to a highly relaxed AlGaN layer. Therefore, in sample B the AlGaN layer displays the most severe relaxation.

The lattice parameters for completely relaxed GaN and AlN are $a_0^{\mathrm{GaN}} = 3.1896$ Å, $c_0^{\mathrm{GaN}} = 5.1855$ Å, and $a_0^{\mathrm{AlN}} = 3.111$ Å, $c_0^{\mathrm{AlN}} = 4.98$ Å, respectively.[15,16] R is defined as the degree of relaxation of the AlGaN layer on GaN expressed by the following equation:

$$R = [a(L) - a_0(S)]/[a_0(L) - a_0(S)],$$

where $a_0(S)$ is the in-plane lattice parameter of a completely relaxed substrate, and $a(L)$ and $a_0(L)$ are the measured and completely relaxed in-plane lattice parameters of a layer with given contents, respectively.

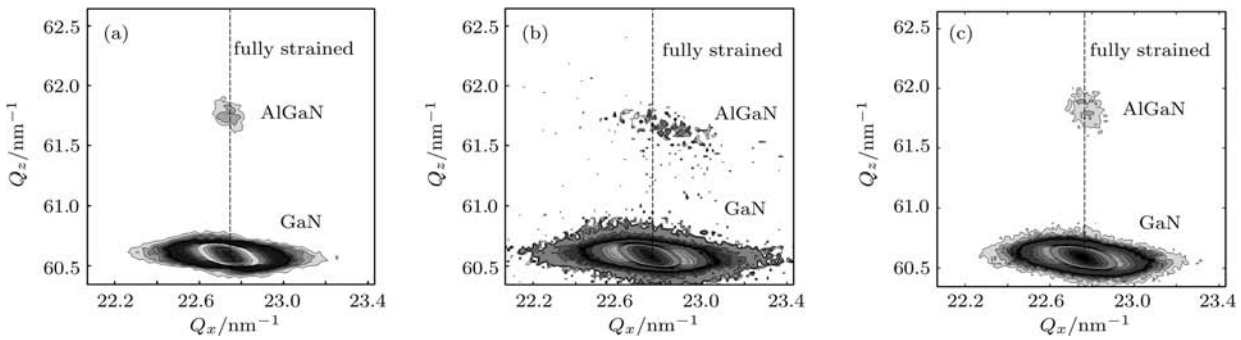


Fig. 1. Reciprocal space maps for the asymmetric (105) reflections of AlGaN/GaN layers with (a) GaN, (b) AlN, and (c) no cap layer on top. The dashed line indicates the completely strained state of AlGaN layer with different Al contents.

Poisson ratios are chosen to be $v_{GaN} = 0.183$ and $v_{AlN} = 0.203$.[17,18] For samples A, B and C, assuming a biaxial in-plane strain, R is 0%, 33% and 6.5%, respectively.

Misfit dislocations (MDs) can be formed at the AlGaN/GaN interface, accompanied with strain relaxation. Its Burgers vector was determined to be $b = a + c$.[13] Symmetric (00l) rocking curves are related to screw or mixed dislocations, whose Burgers vector is c or $a + c$, while rocking curves on an asymmetric or skew-symmetric (hkl) plane with either h or k nonzero will be broadened by edge dislocations, whose Burgers vector is a.[19,20] Both MD and threading dislocation (TD) densities can be revealed by HRXRD ω-scan (rocking curve) of symmetric (002) reflection for AlGaN barrier layer. The result is shown in Fig. 2(a). It suggests that sample A has the smallest full width at half maximum (FWHM) while sample B has the largest. Therefore, the dislocation density in the AlGaN layer is highest in sample B and lowest in sample A. For the purpose of ruling out the possibility that the 2DEG could be influenced by the crystalline quality of the GaN buffer layer, as well as separating the effects of TD and MD on the FWHM of AlGaN (002) rocking curves, both the symmetric (002) and skew symmetric (102) reflections have also been measured for the GaN buffer layers in the three samples. The results are shown in Figs. 2(b) and 2(c), respectively. Neither of the reflections displays notable differences in the three samples. Therefore, the TD densities in the three samples are of the same level, and the order of MD density from the smallest to the largest is sample A, sample C and sample B.

We examined the surface morphology of the three samples with a 5 μm × 5 μm scan area of AFM images, as shown in Fig. 3. Sample A has the smoothest surface owing to the absence of relaxation in the barrier layer. For sample B, however, the relatively severe relaxation creates a rough surface. According to Ref. [21], for the relatively thin AlGaN barrier layer (∼22 nm), the surface roughness of the AlGaN layer inherits that of the underlying GaN buffer layer; and the X-ray reflectivity (XRR) results show that the roughnesses of the AlGaN/GaN interface and the former two are in the same range. The simulation of XRR data for our samples (not shown here) also shows a similar result. Therefore, one can deduce that the interface of AlGaN/GaN is also better in sample A, in which the interface scattering for 2DEG mobility can be reduced in comparison with the two other samples. In addition, recently reported work suggests that a remote surface roughness scattering effect arising from the fluctuation of the barrier width should be considered.[22] Therefore, the contribution of this effect on the decline of mobility should be taken into account in rough-surfaced samples such as sample B.

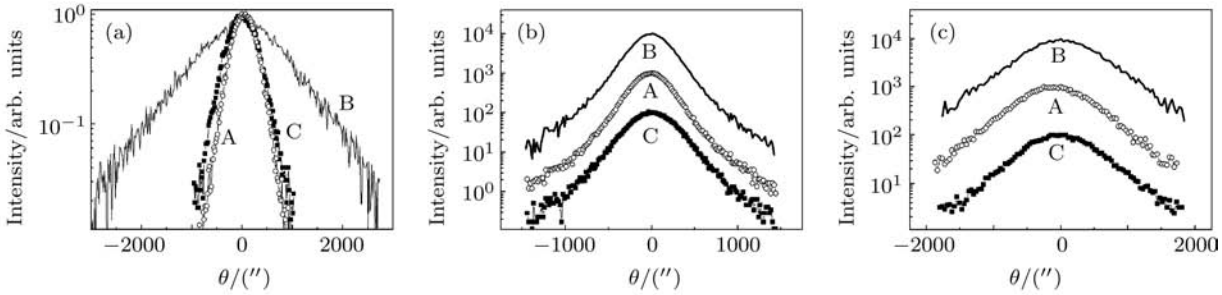


Fig. 2. Rocking curves of (a) (002) reflection for AlGaN layer, (b) (002), and (c) (102) reflection for GaN layer.

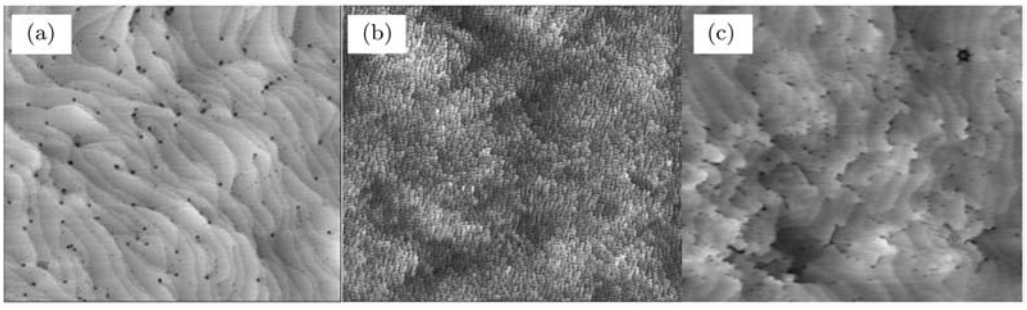


Fig. 3. 5 μm × 5 μm AFM images of (a) sample A, (b) sample B, and (c) sample C.

Table 1. Sheet carrier density (N_s), mobility (μ) and their product (μN_s) for three samples.

Sample structure	$N_s/10^{13}\mathrm{cm}^{-2}$	$\mu/\mathrm{cm}^2\cdot\mathrm{V}^{-1}\cdot\mathrm{s}^{-1}$	$\mu N_s/10^{16}\cdot\mathrm{V}^{-1}\cdot\mathrm{s}^{-1}$
GaN/AlGaN/GaN (A)	1.36	1557	2.12
AlN/AlGaN/GaN (B)	1.32	922	1.22
AlGaN/GaN (C)	1.62	1193	1.93

The results of the Hall-effect measurement are listed in Table 1. Although displaying a lower 2DEG sheet density than sample C does, sample A has a better performance in both 2DEG mobility and the product of mobility and sheet density. Sample B shows the lowest mobility and sheet carrier density. Figure 4 shows the variations of 2DEG mobility and sheet carrier density with R. Mobility decreases monotonically with increasing R (i.e., the aggravation of strain relaxation), while sheet carrier density shows less obvious correlation with the strain state of the AlGaN barrier layers. The strain relaxation of the AlGaN layer causes the decrease of the piezoelectric polarization effect, thus causing a reduced 2DEG density in sample B. On the other hand, for sample A, though the relaxation of the AlGaN layer is suppressed, the GaN cap layer results in negative polarization charges at the interface of cap-GaN/AlGaN, which enhances the electric field in the AlGaN barrier layer and lowers the 2DEG density.[23] Figure 5 shows the schematic diagram of the energy band diagram and electron distribution for samples with and without a GaN cap layer, which provides strong support for the discussion above.

TDs can penetrate through 2DEG and act as scattering centres. The effect of TD on the electrical properties of an AlGaN/GaN heterostructure has been studied.[24] Based on the model in which TD is treated as a line of charges, TD scattering has been analysed.[25] However, as TD densities are almost the same in the buffer layers of all of the samples, their impact cannot and need not be discriminated. It should be noted that as the result of strain relaxation, misfit dislocations can be formed near the interface, and the localized strain state can be changed. The latter may in turn change the localized electric field, leading to a nonuniform piezoelectric field. The deformation of the electric field breaks up the periodic field in crystals and effectively reduces electron mobility by enhancing scattering. Furthermore, as a trap, MD can be charged and may have a remote coulomb scattering effect on 2DEG. Therefore, the main reason for the reduction of 2DEG mobility in strain-relaxed samples (samples B and C) is the deterioration of the surface (or interface) morphology and the formation of misfit dislocations at the interface of AlGaN/GaN.

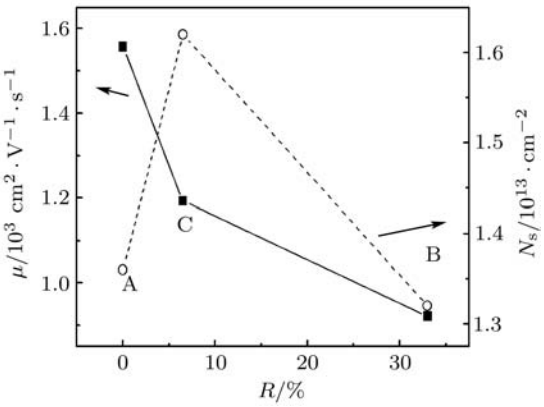


Fig. 4. Hall mobility (solid squares) and sheet carrier density (open circles) versus the degree of relaxation. The solid and dashed lines connecting the data points are guides for the eye.

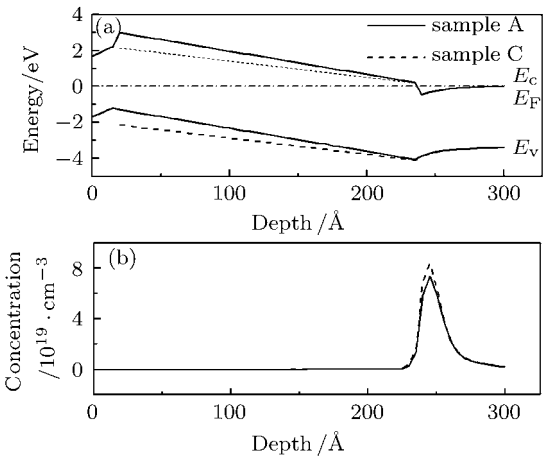


Fig. 5. The schematic diagram of (a) energy band diagram and (b) electron distribution of sample A and sample C. E_c and E_v represent the conduction band and valence band edges, respectively; and E_F represents the Fermi level.

Since 2DEG mobility can be more readily influenced by interface roughness scattering and alloy disorder scattering when the 2DEG is at a high concentration, the improvement of mobility in sample A in comparison with sample C may be partially due to its lower 2DEG concentration. However, in sample B, whose 2DEG concentration is almost the same as that in sample A, we can safely draw the conclusion that the significant decrease of carrier mobility in sample B is mainly caused by the strain relaxation of its barrier layer.

4. Conclusions

In conclusion, for $Al_xGa_{1-x}N$/GaN heterostructures with a relative high Al content ($x = 0.37$), three heterostructures with differently strained AlGaN barrier layers were derived by introducing different kinds of thin cap layers (or without a cap layer). The relationship between the transport properties of 2DEG and the strain state of the barrier layer was studied. The mobility of 2DEG decreases with strain relaxation. The degeneration of surface morphology and the increase of dislocation density near the AlGaN/GaN interface, both accompanied by strain relaxation, are the main causes of the deterioration of 2DEG mobility. However, the concentration of 2DEG displays a subtle trend with the increase of the degree of relaxation, which can be attributed to the reduction of polarization charges at the AlGaN/GaN interface and the additional polarization charges formed at the cap/barrier interface. This research is beneficial for understanding strain-related phenomenon in the application of cap layer structures on AlGaN/GaN-heterostructure based devices.

References

[1] Özgür A, Kim W, Fan Z, Botchkarev A, Salvador A, Mohammad S N, Sverdlov B and Morkoç H 1995 *Electron. Lett.* **31** 1389

[2] Lei S Y, Shen B and Zhang G Y 2008 *Acta Phys. Sin.* **57** 2386 (in Chinese)

[3] Zhang J F, Zhang J C and Hao Y 2004 *Chin. Phys.* **13** 1334

[4] Ambacher O, Smart J, Shealy J R, Weimann N G, Chu K, Murphy M, Schaff W J, Eastman L F, Dimitrov R, Wittmer L, Stutzmann M, Rieger W and Hilsenbeck J 1999 *J. Appl. Phys.* **85** 3222

[5] Wright A F and Nelson J S 1995 *Phys. Rev.* B **51** 7866

[6] Gessmann T, Graff J W, Li Y L, Waldron E L and Schubert E F 2002 *J. Appl. Phys.* **92** 3740

[7] Yu E T, Dang X Z, Yu L S, Qiao D, Asbeck P M, Lau S S, Sullivan G J, Boutros K S and Redwing J M 1998 *Appl. Phys. Lett.* **73** 1880

[8] Selvaraj S L, Ito T, Terada Y and Egawa T 2007 *Appl. Phys. Lett.* **90** 173506

[9] Chang P C, Yu C L, Chang S J, Lin Y C and Wu S L 2007 *IEEE Sens. J.* **7** 1289

[10] Shen B, Someya T and Arakwa Y 2000 *Appl. Phys. Lett.* **76** 2746

[11] Feng Z H, Zhou Y G, Cai S J and Lau K M 2004 *Appl. Phys. Lett.* **85** 5248

[12] Smorchkova I P, Chen L, Mates T, Shen L, Heikman S, Moran B, Keller S, DenBaars S P, Speck J S and Mishra U K 2001 *J. Appl. Phys.* **90** 5196

[13] Floro J A, Follstaedt D M, Provencio P, Hearne S J and Lee S R 2004 *J. Appl. Phys.* **96** 7087

[14] Lee S R, Koleske D D, Cross K C, Floro J A, Waldrip K E, Wise A T and Mahajan S 2004 *Appl. Phys. Lett.* **85** 6164

[15] Deguchi T, Ichiryu D, Toshikawa K, Sekiguchi K, Sota T, Matsuo R, Azuhata T, Yamaguchi M, Yagi T, Chichibu S and Nakamura S 1999 *J. Appl. Phys.* **86** 1860

[16] Tanaka M, Nakahata S, Sogabe K, Nakata H and Tabioka M 1997 *Jpn. J. Appl. Phys.* Part 2 **36** 1062

[17] Moram M A, Barber Z H and Humphreys C J 2007 *J. Appl. Phys.* **102** 023505

[18] Wright A F 1997 *J. Appl. Phys.* **82** 2833

[19] Metzger T, Höpler R, Born E, Ambacher O, Stutzmann M, Stömmer R, Schuster M, Göbel H, Christiansen S, Albrecht M and Strunk H P 1998 *Philos. Mag.* A **77** 1013

[20] Heying B, Wu X H, Keller S, Li Y, Kapolnek D, Keller B P, DenBaars S P and Speck J S 1996 *Appl. Phys. Lett.* **68** 643

[21] Aggerstam T, Lourdudoss S, Radamson H H, Sjödin M, Lorenzini P and Look D C 2006 *Thin Solid Films* **515** 705

[22] Liu B, Lu Y W, Jin G R, Zhao Y, Wang X L, Zhu Q S and Wang Z G 2010 *Appl. Phys. Lett.* **97** 262111

[23] Heikman S, Keller S, Wu Y, Speck J S, DenBaars S P and Mishra U K 2003 *J. Appl. Phys.* **93** 10114

[24] Gao Z Y, Hao Y, Zhang J C, Li P X and Gu W P 2009 *Chin. Phys.* B **18** 4970

[25] Xu X Q, Liu X L, Yang S Y, Liu J M, Wei H Y, Zhe Q S and Wang Z G 2009 *Appl. Phys. Lett.* **94** 112102