Effects of GaN cap layer thickness on an AlN/GaN heterostructure*

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In this study, we investigate the effects of GaN cap layer thickness on the two-dimensional electron gas (2DEG) electron density and 2DEG electron mobility of AlN/GaN heterostructures by using the temperature-dependent Hall measurement and theoretical fitting method. The results of our analysis clearly indicate that the GaN cap layer thickness of an AlN/GaN heterostructure has influences on the 2DEG electron density and the electron mobility. For the AlN/GaN heterostructures with a 3-nm AlN barrier layer, the optimized thickness of the GaN cap layer is around 4 nm and the strained *a*-axis lattice constant of the AlN barrier layer is less than that of GaN.

Keywords: AlN/GaN heterostructure, 2DEG, GaN cap layer, *a*-axis lattice constant

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1. Introduction

In the past few years the AlN/GaN heterostructure has attracted much attention due to high power and high frequency applications, for it has a large band gap and polarization effects.[1–4] Despite the excellent material properties, the problems such as surface sensitivity, high leakage current, and easy oxidization have restricted the performances and reliabilities of AlN/GaN devices.[5,6] It is useful to employ a suitable layer to protect the epi-layer in order to solve these problems. To date, it has been reported that GaN cap layer can significantly reduce the leakage current,[7,8] and is widely used as the cap layer in the GaN-based heterostructure. However there are few studies regarding how GaN cap layer thickness affects material properties in AlN/GaN heterostructures. In addition, due to the fact that the AlN barrier layer in AlN/GaN heterostructures is very thin, it is hard to obtain the strained lattice constant information for the AlN barrier layer by measurements. However, the strain of the thin AlN barrier layer is important for the performance of the AlN/GaN heterostructure field effect transistor (AlN/GaN HFET). Thus, it is also urgent to study whether the *a*-axis lattice constant of the thin AlN barrier layer is the same as that of a GaN layer.

In this study, by analyzing the temperature-dependent Hall measurement results for the prepared AlN/GaN heterostructure materials with different GaN cap layer thickness values, both the optimized GaN cap layer thickness and the strained *a*-axis lattice constant for the thin AlN barrier layer are investigated.

2. Experiments

The AlN/GaN heterostucture employed in this study was epitaxially grown on a (0001) sapphire substrate by metal–organic chemical vapor deposition. Figure 1(a) shows

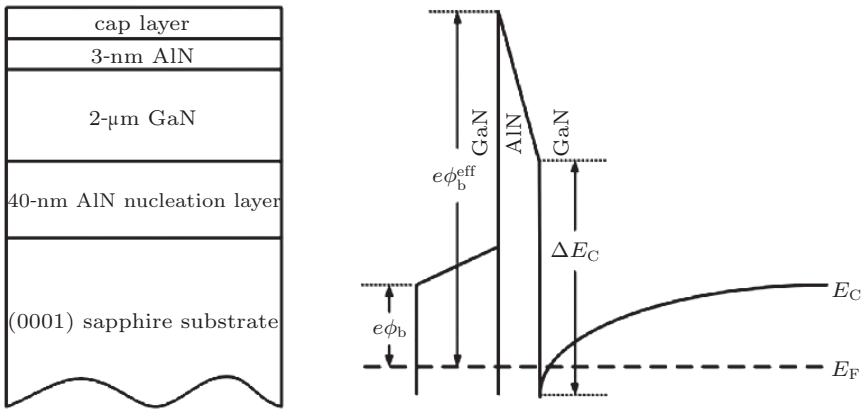


Fig. 1. Schematic (a) and the conduction band diagram at zero bias (b) of the AlN/GaN heterostructure with GaN cap layer.

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the schematic diagram of the AlN/GaN heterostructure with a GaN cap layer. The heterostructure consists of a 40-nm AlN low-temperature nucleation layer, followed sequentially by a 2-μm undoped GaN layer, a 3-nm AlN barrier layer, and a GaN cap layer with different thickness values. Here, the investigated GaN cap layer thickness values are 2 nm, 4 nm, and 8 nm, marked as A, B, and C, respectively.

3. Calculation and analyses

Figure 1(b) shows the conduction band diagram at zero bias of the undoped Ga-face AlN/GaN heterostructure with a GaN cap layer. The two-dimensional electron gas (2DEG) sheet electron concentration n_S can be calculated by using the AlN/GaN interface polarization sheet charge density σ from the following equation[9]

$$n_S = \left(1+\frac{d_{GaN}}{d_{AlN}}\right)^{-1}\left\{\frac{\sigma}{e}-\left(\frac{\varepsilon_0\varepsilon_{AlN}}{d_{AlN}e^2}\right) \times \left[e\phi_b^{eff}+E_F-\Delta E_C\right]\right\}, \quad (1)$$

where d_{AlN} and d_{GaN} are the thickness values of the barrier layer and the cap layer respectively; ε_0 and ε_{AlN} are the vacuum permittivity and the dielectric constant of the AlN barrier layer respectively; σ is the AlN/GaN interface polarization sheet charge density; e is the elementary charge, which has a measured value of approximately 1.602×10^{-19} coulombs; $e\phi_b^{eff}$ is the effective Schottky barrier height of the gate contact on the top of GaN/AlN; E_F is the Fermi level with respect to the GaN conduction-band-edge energy; ΔE_C is the conduction-band offset at the AlN/GaN interface where a 2DEG forms.

Figure 2 shows the temperature-dependent Hall measurements of the AlN/GaN heterostructure material as a function of temperature (10 K–290 K). In Eq. (1), $e\phi_b^{eff}$ is almost not related to the GaN cap layer thickness, and E_F is reduced with the decrease of n_S. Thus, according to Eq. (1), the sheet electron concentration should continuously decrease with the increase of the GaN cap layer thickness. However, for sample A with a 2-nm cap layer, the 2DEG sheet density is at its lowest, which seems to be inconsistent with the theoretical result. In order to explore the causes of this phenomenon, atomic-force microscopy (AFM) is performed on the three samples. Figure 3(a) shows that the surface of the sample with a 2-nm thickness of GaN cap layer is relatively coarse, whose root-mean square (RMS) roughness value is 1.04 nm, and has a lot of sharp pillars and dark pits. As the pits are relatively deep, some parts of the AlN barrier layer may be exposed to the air and partly oxidized, which makes the actual AlN barrier layer thinner, and creates more surface donor states situated below the Fermi level which, as a result, cannot be ionized. This may be the reason why the 2DEG sheet density for sample A decreases and is lower than others. The RMS roughness values of samples B and C are 0.490 nm and 0.651 nm, respectively, and no dark pits are found on the surface. So the GaN cap layers with thickness values of 4 nm and 8 nm can better prevent the barrier from oxidizing than with a thickness of 2 nm.

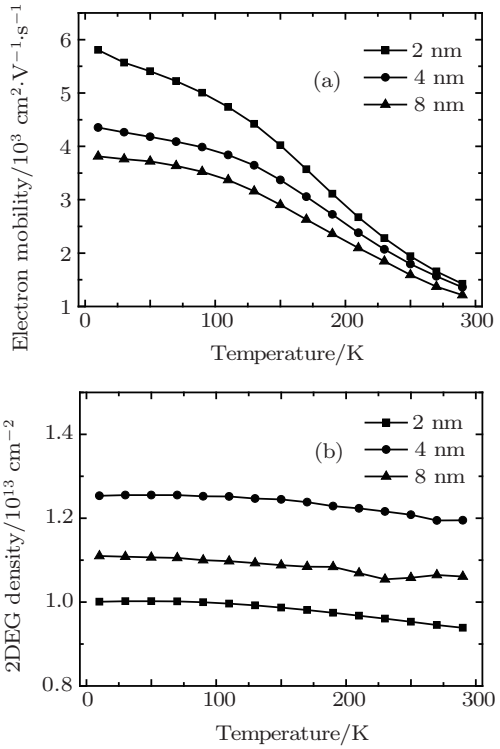


Fig. 2. Dependences of the electron mobility (a) and the 2DEG electron density (b) on temperature for the AlN/GaN heterostructures with different GaN cap layer thickness values.

Scattering mechanisms that affect the 2DEG electron mobility in GaN-based heterostructures have been well described in the literature. Background impurity scattering, alloy disorder scattering, dislocation scattering, interface roughness scattering, and phonon scattering are generally considered to restrict the 2DEG electron mobility (μ).[3] Since our samples are nominally undoped, the alloy disorder scattering and the background impurity scattering can be ignored. According to the accepted theory, polar optical phonon (OP) scattering is inelastic and plays an important role at high temperatures. The OP scattering has an Arrhenius dependence on temperature ($\mu_{OP} \propto \exp(1/T)$).[10,11] Acoustic phonon scattering, including deformation potential (DP) and piezoelectric (PE) scattering, is essentially elastic and has a much weaker contribution at high temperatures. The DP and PE scatterings have been calculated to be proportional to inverse temperature, i.e. $\mu_{AC} \propto 1/T$.[10–12] Dislocation (DIS) and interface roughness (IR) scattering have been calculated to be temperature-independent.[12–14]

The electron mobility affected by the above scattering can be expressed as[14]

$$\frac{1}{\mu_{Total}} = \frac{1}{\mu_{PO}} + \frac{1}{\mu_{AC}} + \frac{1}{\mu_{DIS,IR}}$$

$$= \frac{1}{a\left(\mathrm{e}^{\hbar b/T}-1\right)} + \frac{1}{c/T} + \frac{1}{d}, \qquad (2)$$

where a, b, c, and d are the fitting parameters and can be determined from the fitting of the measured temperature-dependent Hall data set using the total electron mobility expression Eq. (2). As seen from Fig. 4, the fitting curves (solid lines) are well consistent with the Hall measurements. The fitting parameters are listed in Table 1.

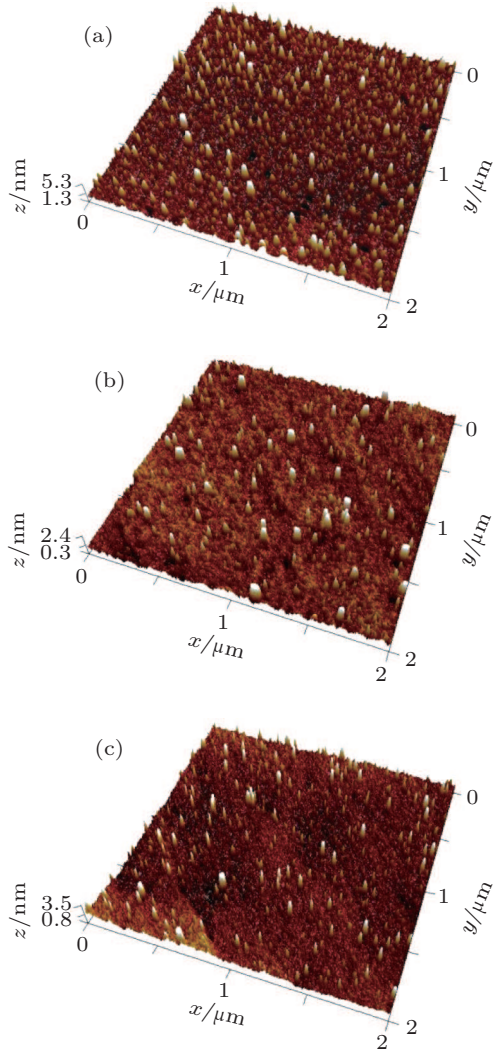


Fig. 3. (color online) 2 μm×2 μm AFM images of the AlN/GaN heterostructures with the GaN cap layer thickness values of (a) 2 nm, (b) 4 nm, and (c) 8 nm.

Table 1. Fitting parameters of the mobility for samples A, B, and C.

Sample	a/(cm^2/V·s)	b/K	c/(K·cm^2/V·s)	d/(cm^2/V·s)
A	123.5	859.2	2.85×10^6	5939.9
B	128.7	846.6	3.6×10^6	4420.0
C	156.3	765.3	3.4×10^6	3892.1

For the samples in this study, the AlN barrier layer thickness is only 3 nm and it is very susceptible to any physical processes occurring on the surface. Since AlN and GaN materials each have a large lattice mismatch and thermal mismatch, the GaN layer and the AlN barrier layer exert forces on each other simultaneously when the AlN barrier layer is grown on the GaN layer. The tensile strain and the compressive strain correspond to the AlN barrier layer and the GaN layer, respectively. It can be seen from the fitted results (Fig. 4) that the dislocation and interface roughness scattering are enhanced as the thickness of the GaN cap layer increases. This means that the lattice mismatch between the AlN barrier layer and the GaN cap layer still exists. The strained a-axis lattice constant of the AlN barrier layer is less than that of GaN. Also, the GaN cap layer and the AlN barrier layer exert a force on each other simultaneously while growing the GaN cap layer. The thicker the GaN cap layer, the larger the compressive strain energy in the GaN cap layer is, and at the same time, the larger the tensile strain energy in the AlN barrier layer is.

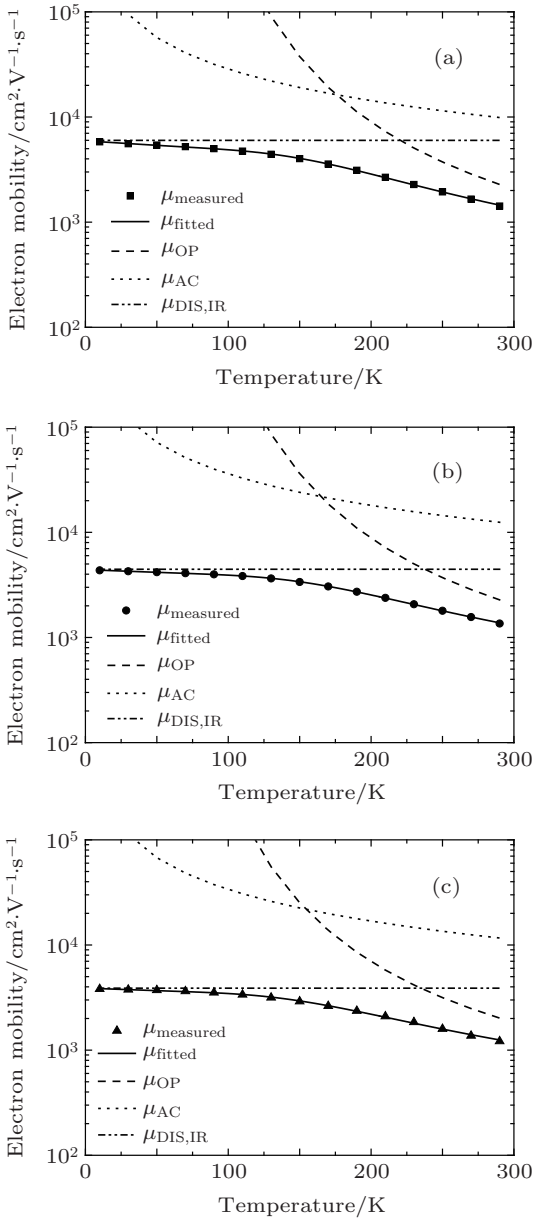


Fig. 4. Plots of measured and calculated (using the measured Hall data) mobility versus temperature of the AlN/GaN heterostructures with the GaN cap layer thickness values of (a) 2 nm, (b) 4 nm, and (c) 8 nm.

As a result, the dislocation density and the interface roughness increase with an increase of the thickness of the GaN cap layer. At room temperature and above, OP scattering dominates the 2DEG electron mobility, which makes the carrier mobilities almost the same for the three samples. In addition, the low temperature mobility of 2DEG in the AlN/GaN heterostructure with 2-nm GaN cap layer appears to be dominated by much stronger acoustic phonon scattering as evidenced by the inverse temperature dependence. With the Hall measurement results, the calculated square resistances for samples A, B, and C at room temperature are 468 Ω/□, 385 Ω/□, and 485 Ω/□, respectively. At this point, the conclusion can be made that the optimized GaN cap layer thickness for a 3-nm AlN barrier layer of AlN/GaN heterostructure is around 4 nm, and the strained *a*-axis lattice constant of the AlN barrier layer is less than that of GaN.

4. Conclusion

In this paper, the GaN cap layer is crucial to the AlN/GaN heterostructure material characteristics by changing the 2DEG electron density and the 2DEG electron mobility. It is found that a very thin GaN cap layer cannot avoid oxidation, while increasing the thickness of the GaN cap layer leads to an increase in dislocation density and interface roughness. The optimized thickness of the GaN cap layer for the AlN/GaN heterostructure with a 3-nm AlN barrier layer is around 4 nm. It is also found that the strained *a*-axis lattice constant of the AlN barrier layer is less than that of GaN for the AlN/GaN heterostructure with 3-nm AlN barrier layer.

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