The effects of GaN capping layer thickness on electrical properties of two-dimensional electron gas in GaN/AlGaN/GaN heterostructures

A. Asgari♣, L. Faraone
School of Electrical, Electronic and Computer Engineering, The University of Western Australia, Crawley, WA 6009, Australia

In this article we present a study of the effects of GaN capping layer thickness on the two-dimensional electron gas (2DEG) electrical properties in GaN/AlGaN/GaN heterostructures. The results of our analysis clearly indicate that increasing the GaN capping layer thickness leads to a decrease in the 2DEG density and an increase in the room temperature two-dimensional-electron mobility (2DEM).

1. Introduction

AlGaN/GaN heterostructure field-effect transistors (HFETs) have been the subject of intense research recently, primarily because they have emerged as attractive candidates for high voltage, high-power operation at microwave frequencies.[1] In AlGaN/GaN HFETs with a high 2DEG sheet density, the 2D-electron lie very close to the AlGaN/GaN interface, which makes them very susceptible to any physical processes occurring at the interface such as interface roughness scattering, which is the dominant scattering mechanism at low temperatures. In order to alleviate such affects, the separation between the 2D-carriers and the interface needs to be increased, which can be achieved if the AlGaN/GaN structures are capped with a GaN layer of appropriate thickness. The presence of strong polarization-induced fields in both the AlGaN barrier and the GaN capping layer leads to a very interesting dependence of 2DEG sheet density in GaN/AlGaN/GaN HFETs on GaN capping layer thickness [3]. The purpose of this paper is to present detailed calculations of 2DEG density and mobility versus GaN capping layer thickness using a comprehensive theoretical model combined with precise numerical calculations using Numerov's numerical method [2].

2. Model Derivation

In order to obtain accurate values for the physical parameters needed for 2DEG density and 2DEM, both the Schrödinger and Poisson equations need to be solved self-consistently. In the present study, this has been achieved by solving Schrödinger's equation and simultaneously taking into account the electrostatic potential obtained from Poisson's equation, as well as including the image and exchange-correlation potentials using Numerov's numerical method [2]. A simple electrostatic analysis indicates that the sheet carrier density, N_s, for the GaN/$Al_xGa_{1-x}N$/GaN HEMT structure which takes into account all polarization effects, is given by

$$N_S = \left(1+\frac{\varepsilon_1 d_2}{\varepsilon_2 d_1}\right)\left[\frac{\sigma(x)}{e}-\frac{\varepsilon_1\varepsilon_0}{d_1 e^2}\left(e\Phi_b^{GaN}+E_F-\Delta E_C\right)+\frac{N_1 d_1}{2}+\frac{\varepsilon_1}{\varepsilon_2}\left(N_1 d_2+\frac{N_2 d_2^2}{2 d_1}\right)\right] \quad (1)$$

where $\sigma(x)$ is the $Al_xGa_{1-x}N$/GaN interface polarization sheet charge density (which includes both spontaneous and piezoelectric polarization), d_1 , d_2 , ε_1 and ε_2 are the AlGaN and GaN capping layer thicknesses and the corresponding dielectric constants, N_1 and N_2 are the AlGaN barrier and GaN buffer layer donor doping concentrations, respectively, $e\Phi_b^{GaN}$ is the metal/GaN Schottky barrier height, ΔEc is the conduction-band offset at the AlGaN/GaN interface, and E_F is the Fermi level at

♣ asgari@ee.uwa.edu.au

the AlGaN/GaN interface. Alternatively, the sheet concentration of electrons in the quantum well can be determined by summing over the concentration N_i in each sub-band,

$$N_S = \sum_i N_i = \sum_i^n \frac{m^* k_B T}{\pi \eta^2} \ln\left(1 + \exp\left(\left[E_F - E_i\right]/k_B T\right)\right) \qquad (2)$$

where m^* is the electron effective mass in the GaN channel, k_B and η are the Boltzmann and Plank constants, respectively, and E_i is the i-th sub-band energy in the quantum well. Based on the results of previous studies [2], it is only necessary to take into account occupied and partially occupied sub-bands up to n=5, since higher sub-bands are virtually unoccupied for heterostructure parameters corresponding to practical device structures. The material parameters used in all calculations are kept constant throughout this paper and have been taken from Ref. 2.

By calculating the accurate electron wave-functions, as well as N_S, E_F, and the energy of each sub-band in the AlGaN/GaN hetero-interface quantum well and using these quantities in combination with several important physical mechanisms, such as the effects of polarization fields, the occupancy of individual sub-bands and their corresponding sheet carrier concentrations, and the exact multisub-band coupling coefficients, it is possible to calculate the 2DEM from the combined contributions from each of the individual electron scattering mechanisms. The details of such calculations have been reported in a previous publication [2].

3. Results and Discussion

The results in this paper characterize the 2DEG transport properties of two series of experimental results on GaN capped AlGaN/GaN HFETs that have been published recently [3, 4]. The first series consisted of a GaN/AlN/GaN HFETs with a 35Å thick AlN barrier and a GaN capping layer that varied in thickness from zero to 1000Å. The second series consisted of GaN/$Al_{0.32}Ga_{0.68}N$/GaN HFETs with a 200Å thick $Al_{0.32}Ga_{0.68}N$ barrier and a GaN capping layer that varied in thickness from zero to 2250Å. The 2DEG sheet carrier densities as a function of GaN capping layer thickness have been calculated for the above two series of HFETs, are presented in Fig. 1a and compared with recent published experimental data [3, 4]. The model calculations indicate that the presence of a GaN capping layer results in a monotonic decrease of the sheet carrier density with increasing capping layer thickness. We have assumed that the heterostructures are unintentionally doped and that the doping in GaN layers is negligible. It needs to be emphasized that the only fitting parameter used in calculation was the AlGaN doping concentration, which was $3\times10^{17}\ cm^{-3}$. This value is comparable to previous experimental results [2]. The decrease in 2DEG sheet density with increasing separation between the 2DEG carriers and the AlGaN/GaN interface results in modification of the electron scattering mechanisms and, consequently, on the 2DEM. The calculated 2DEM as a function of GaN capping layer thickness at room temperature is presented in Fig. 1b. At room temperature, with increasing GaN capping layer thickness from 0 (that is, no capping layer) to about 150 Å, the 2DEM increases monotonically; whereas with a further increase in capping layer thickness from 150 Å to 500 Å, the 2DEM decreases slightly and eventually saturates. Also, Fig. 1.b compares calculated results from our model with experimental data published in Ref. 4 for GaN/$Al_{0.32}Ga_{0.68}N$/GaN heterostructures. A detailed study of the dependence of different scattering mechanisms on GaN capping layer thickness indicates that the dominant scattering mechanisms at room temperature are phonon scattering mechanisms, especially polar optical phonon scattering. With increasing GaN capping layer thickness from 0 to 150 Å, the mobility component associated with polar optical phonon scattering increases. This increase is a consequence of the 2DEG sheet density decreasing with increasing GaN capping layer thickness and, in addition, the decrease in the number of fully occupied and partially occupied sub-bands.

Because, with increasing the GaN capping layer thickness from 0 to 150 Å, the second and third sub-bands are rapidly being emptied, so the intrasub-band and intersub-band scattering components related to these sub-bands are reduced as a part of the polar optical scattering mechanisms.

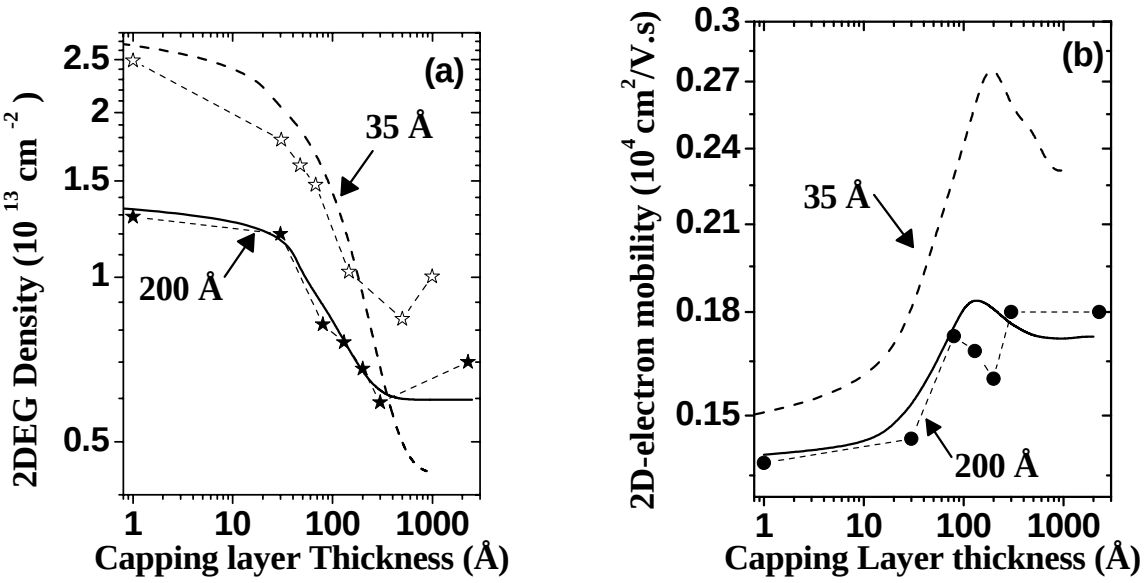

Figure 1. The 2DEG sheet density (a) and the 2DEM (b) at 300K for the GaN/AlGaN/GaN HFETs as a function of GaN capping layer thickness with: the AlN barrier thickness is 35Å; and the $Al_{0.32}Ga_{0.68}N$ barrier thickness is 200Å; the symbols represent experimental data from Ref. 3 and 4, and the lines represent model calculations.

In addition, the 2DEG density is decreasing in this range, which also contributes to the fact that the related mobility increases as capping layer thickness increases from 0 to 150 Å. So, the presence of peak in the 2DEM is the result of carrier-carrier scattering in different fully and partially occupied sub-bands. For GaN capping layer thickness in the range from 150 Å to 500 Å, there is only one occupied sub-band since the difference between the second sub-band energy and the Fermi level is greater than thermal energy at room temperature. Thus, only intrasub-band scattering within the first sub-band is important in the polar optical phonon scattering mechanism. Within this regime, increasing GaN capping layer thickness (that is decreasing 2DEG sheet density) leads to decreasing mobility. This effect can be related to the screening effect of longitudinal optical phonon scattering. At higher capping thickness, the mobility saturates due to the fact that the 2DEG sheet density has saturated. So, the results of this study indicate that the inclusion of a GaN capping layer in AlGaN/GaN heterostructures decreases the 2DEG sheet density and increases the 2DEM. The comparison between published experimental data and our calculated model results (for both 2DEG density and 2DEM) show good agreement.

Reference:

1) Tsung-Hsing Yu and Kevin F. Brennan, J. Appl. Phys. **89**, 3827 (2001).
2) A. Asgari, M. Kalafi, and L. Faraone, J. Appl. Phys. **95**, 1185 (2004)
3) I. P. Smorchkova, L. Chen and T. Mates, L. Shen and S. Heikman, B. Moran, S. Keller, S. P. DenBaars and J. S. Speck, and U. K. Mishra, J. Appl. Phys. **90**, 5196 (2001).
4) Sten Heikman, Stacia Keller, Yuan Wu, James S. Speck, Steven P. DenBaars, and Umesh K. Mishra, J. Appl. Phys. **93**, 10114 (2003).