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Two dimensional electron gas in a hybrid GaN/InGaN/ZnO heterostructure with ultrathin InGaN channel layer

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HIGHLIGHTS

- We calculated 2DEG properties for hybrid GaN/$In_xGa_{1-x}N$/ZnO HEMT structures.
- This paper shows that 2DEG density of these structures can reach over 1×10^{13} cm^{-2}.
- We investigated effects of ultrathin InGaN channel layer on 2DEG of these structures.
- We propose an optimized device structure to reduced short channel effects.

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ABSTRACT

We investigated the influence of an ultrathin InGaN channel layer on two-dimensional electron gas (2DEG) properties in a newly proposed hybrid GaN/$In_xGa_{1-x}N$/ZnO heterostructure using numerical methods. We found that 2DEG carriers were confined at InGaN/ZnO and GaN/InGaN interfaces. Our calculations show that the probability densities of 2DEG carriers at these interfaces are highly influenced by the In mole fraction of the InGaN channel layer. Therefore, 2DEG carrier confinement can be adjustable by using the In mole fraction of the InGaN channel layer. The influence of an ultrathin InGaN channel layer on 2DEG carrier mobility is also discussed. Usage of an ultrathin InGaN channel layer with a low indium mole fraction in these heterostructures can help to reduce the short-channel effects by improvements such as providing 2DEG with higher sheet carrier density which is close to the surface and has better carrier confinement.

1. Introduction

In recent years, III–V and II–VI group semiconductor material systems have been studied as hybrid heterostructures for light-emitting diodes (LEDs) applications [1–3]. In addition to widely studied AlGaN/GaN, InGaN/GaN systems, hybrid ZnO/InGaN/GaN [4], InGaN/MgZnO [5], InGaN/CdZnO [6], p-GaN/InGaN/ZnO [7] heterostructures for LED applications and hybrid n-ZnO/i-InGaN/p-GaN [8] heterostructures for solar cell applications have been also studied in a number of studies. In 2010, dc characteristics of GaN/InGaN/ZnO npn heterojunction bipolar transistors were also examined by K. Hsueh et al. [9]. Furthermore, without any doping, GaN and ZnO based hybrid heterostructures may be an alternative material system for high electron mobility transistor (HEMT) applications due to their spontaneous and piezoelectric polarization properties. Strong piezoelectric polarization (P^{PE}) and spontaneous polarization (P^{SP}) between GaN and ZnO ($P^{SP}_{GaN} = -0.034$ C/m^2, $P^{SP}_{ZnO} = -0.050$ C/m^2) can lead to high induced sheet carrier densities within two-dimensional electron gas (2DEG) at an interface of the related hybrid heterostructure [10–12]. On the other hand, similar material properties of GaN and ZnO such as room temperature band gaps, electron drift velocities and wurtzite crystal structures are promising for building up GaN and ZnO based hybrid transistor heterostructures [4,12,13]. For GaN epitaxial layers grows, ZnO substrates can be a successor to widely used sapphire substrates. ZnO has a common stacking order with GaN, and there is low lattice mismatch between ZnO and GaN (about 2%) [14,15], which also very low when compared with the lattice mismatch between sapphire and GaN (about %14). ZnO can be grown at low temperatures compared with GaN growth [8]. This is important due to the stability problems of indium atoms at high temperatures in InGaN epitaxial layer growths [8,16]. The development of GaN epitaxial layer growth using a ZnO buffer offers a significant advantage for future studies of hybrid GaN and ZnO based heterostructures [15].

In a GaN-based transistor heterostructure, the 2DEG channel

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must be close to the surface to reduce short-channel effects [17]. However, this is a problem for traditional AlGaN/GaN heterostructures. With the decreasing AlGaN barrier thickness on a GaN buffer, the sheet carrier density tends to decrease, and when the 2DEG channel is close to the surface, current collapse may occur as a result of surface traps. One way to solve this problem is to insert an InGaN channel layer [17]. Since heterostructures with an InGaN channel layer exhibit better carrier confinement compared with traditional AlGaN/GaN heterostructures, the current collapse possibility is decreased [17,18]. Despite these important features, 2DEG carrier mobility is affected negatively by the alloy disorder scattering mechanism in these heterostructures due to the use of an alloy InGaN channel layer. In addition to this alloy disorder scattering mechanism, 2DEG carrier mobility is significantly affected by the interface roughness of the AlGaN/InGaN interface [17,19]. In addition, when InGaN is introduced to enhance the carrier confinement, the crystal quality of AlGaN/GaN heterostructures is degraded due to high number of produced dislocations [20]. Without an AlGaN barrier layer, GaN/$In_xGa_{1-x}N$/ZnO transistor heterostructures, which provide similar sheet carrier densities to traditional AlGaN/GaN heterostructures, can be suggested for transistor device applications. The short channel effects on these hybrid heterostructures with an ultrathin InGaN channel layer can be suppressed because of the possible advantages, such as providing large sheet 2DEG carrier density which is close to the device surface.

In this paper, we focused on hybrid GaN/$In_xGa_{1-x}N$/ZnO heterostructures that are suitable for transistor device applications. For this purpose, we investigated the influence of an InGaN channel layer on 2DEG properties in proposed hybrid GaN/$In_xGa_{1-x}N$/ZnO heterostructures with an ultrathin InGaN channel layer. Numerical investigation of hybrid GaN/$In_xGa_{1-x}N$/ZnO transistor heterostructures was carried out by the solutions of one-dimensional (1D) self-consistent Schrödinger–Poisson equations including the strain, polarization induced charges and band structures of wurtzite semiconductors [21]. The effects of different In mole fractions and thicknesses of an InGaN channel layer on 2DEG properties were investigated. This paper shows that sheet carrier densities of hybrid GaN/$In_xGa_{1-x}N$/ZnO heterostructures can be reached over 1×10^{13} cm^{-2}. It was also found that 2DEG carrier confinement is strongly affected by In mole fraction of $In_xGa_{1-x}N$ channel layer in these heterostructures.

2. Computational methods

Conduction band diagrams, carrier densities, electron probability densities and polarization charges have been calculated for different In mole fractions and thicknesses of the InGaN channel layer using numerical methods which included the solutions of 1D self-consistent Schrödinger–Poisson equations [21]. Numerical calculations have been performed on the self-consistent solution of the mutually coupled equations of the Poisson model for carrier transport as implemented in the TiberCAD simulation software [22]. In the numerical methods, the Poisson model for carrier transport given by

$$-\nabla(\varepsilon\nabla\varphi - P) = -e\left(n - p - N_d^+ + N_a^-\right) \tag{1}$$

where ε is permittivity, φ is electric potential; P is the electric polarization due to, for example, piezoelectric effects; n and p are electron and hole densities; and N_d^+ and N_a^- are the densities of ionized donors and acceptors respectively.

The carrier statistics were provided by Fermi–Dirac statistics, assuming local equilibrium. The conduction band edges and effective masses were obtained from **k•p** calculations. Quantum mechanical models based on the envelope function approximation (EFA) were used for the calculation of the eigenstates of confined particles in heterostructures [23,24]. In this way, an approximation of numerical methods was developed in order to solve a single particle Schrödinger equation for electrons and holes in a semiconductor crystal. This problem is an eigenvalue problem which was treated as a generalized complex eigenvalue problem

$$H\psi = ES\psi \tag{2}$$

where H and S are the Hamiltonian and S-matrix respectively. The solution of the eigenvalue problems resulting from the EFA model provides the electron densities and probability densities. The electron densities and probability densities were calculated by populating the electron states according to the expectation value of the corresponding electrochemical potential. The electron densities and probability densities were then fed back to the Poisson model for self-consistent Schrödinger/Poisson calculations [24].

Piezoelectric polarization at each interface was calculated by

$$P^{PE} = 2\varepsilon_1\left\{e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right\}\left(C/m^2\right). \tag{3}$$

Here, e_{31} and e_{33} are piezoelectric constants, and ε_1 is in-plane strain [25]. The parameters of GaN, InN and ZnO materials are given in Table 1 [26–28]. The material parameters of $In_xGa_{1-x}N$ were obtained by using the parameters given in Table 1 with Vegard's law.

$$P^{SP}_{InGaN}(x) = xP^{SP}_{InN} + (1-x)P^{SP}_{GaN} + bx(1-x). \tag{4}$$

Here, b is the bowing parameter (b=0.037 for InGaN) [29].

The calculation of the possible strain relaxation due to lattice mismatch has a significant importance. Strain relaxation limits can be calculated by a simple critical thickness calculation approach [30] which is given as

$$t_{cr} \cong \frac{b_e}{2\varepsilon_{xx}} \tag{5}$$

where b_e is Burger's vector with a value of b_e=0.3250 nm; ε_{xx} is one of the diagonal strain components for the [0001] growth axis wurtzite structure and was calculated by

$$\varepsilon_{xx} = \frac{a_{Bottom} - a_{Upper}}{a_{Upper}}. \tag{6}$$

Here, a_{Bottom} and a_{Upper} are the lattice parameters of the bottom and upper layers respectively.

Fig. 1 shows the calculated critical thickness of a pseudomorphically grown $In_xGa_{1-x}N$ layer on a ZnO substrate for different In mole fractions using Eqs. (5) and (6). In hybrid InGaN/ZnO heterostructures, when the In mole fraction of a $In_xGa_{1-x}N$ channel layer is x=0.17, the lattice match between the InGaN layer and the ZnO layer is revealed. In this case, strain is minimized. This value of the In mole fraction was calculated by implementing Vegard's law using the lattice parameter values of GaN, InN and ZnO listed

Table 1
Lattice parameters, spontaneous polarization, piezoelectric and elastic constant values of GaN, InN and ZnO materials [26–28].

	GaN	InN	ZnO
a (nm)	0.3189	0.3545	0.3250
e_{31} (C/m^2)	−0.39	−0.57	−0.57
e_{33} (C/m^2)	0.67	0.97	1.34
C_{13}(GPa)	103	92	90
C_{33}(GPa)	405	224	196
P^{SP}(C/m^2)	−0.034	−0.042	−0.050