ON THE COEXISTENCE OF TWO-DIMENSIONAL ELECTRON AND HOLE GASES IN GAN-BASED HETEROSTRUCTURES

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1. Introduction

In microwave AlGaN/GaN HEMTs (high electron mobility transistors), the layer structure of the active device region frequently consists of a metal gate followed by a GaN cap, an AlGaN barrier and a GaN buffer/channel. A characteristic feature of these heterostructrures is the formation of a 2DEG (two-dimensional electron gas) with high sheet density at the interface between AlGaN barrier and GaN channel [1]. It has been predicted by simulations that under certain conditions, in addition to the 2DEG at the AlGaN barrier – GaN channel interface, a 2DHG (two-dimensional hole gas) may form at the GaN cap – AlGaN barrier interface [2]. The simultaneous appearance of 2DEGs and 2DHGs in GaN/AlGaN/GaN structures has recently been confirmed by experiments [3]. Coexisting electron and hole gases are undesirable for HEMT operation, whereas for other applications they may be beneficial. Currently there is an intense interest in electron-hole-pair (exciton) condensation effects that may occur in closely spaced 2DEGs and 2DHGs separated by a thin barrier [4] and an interesting device concept, the BiSFET (bilayer pseudospin field-effect transistor) exploiting these effects has been proposed [5].

In this work, the conditions for the coexistence of electron and hole gases in GaN/AlGaN/GaN hetrostructures are investigated by means of both numerical Schrödinger-Poisson simulations and analytical models. Special emphasis is put on the effects of the layer design and the bias conditions. We focus on wurtzite Ga-face structures which are commonly used in GaN-based devices.

2. Schrödinger-Poisson simulations

Along the growth direction of AlGaN/GaN heterostructures, carriers are confined in deep and narrow quantum wells. This requires a self-consistent solution of the one-dimensional Schrödinger and Poisson equations [6]. We consider a heterostructure that consists (from top to bottom) of a Schottky gate, a GaN cap having a thickness t_{cap}, an $Al_{0.3}Ga_{0.7}N$ barrier with a thickness t_{bar}, and a thick GaN bulk having a grounded back-side contact. The GaN and AlGaN layers are assumed to be unintentionally n-type doped with a homogeneous donor concentration of 10^{16} cm^{-3}. For the relative dielectric constant, energy gap E_G, conduction and valence band offsets, spontaneous and piezoelectric polarization in GaN and AlGaN, the models from [1] have been used. The electron and hole effective masses are taken from [7] and [8] respectively.

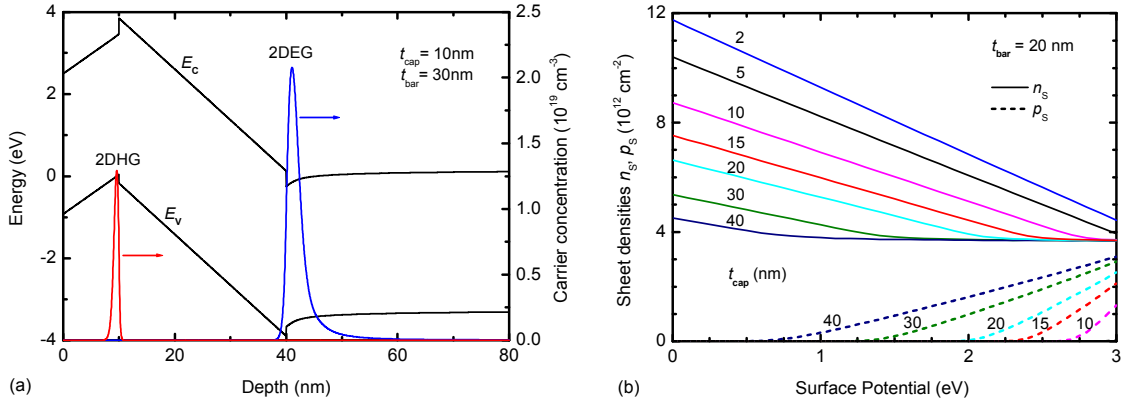

Fig.1: *(a) Band diagram and free carrier distribution in a GaN/$Al_{0.3}Ga_{0.7}N$/GaN heterostructure.(b) 2DEG and 2DHG sheet densities vs. surface potential for different t_{cap}.*

Figure 1(a) shows the calculated band diagram, together with the electron and hole distributions, in a GaN/$Al_{0.3}Ga_{0.7}N$/GaN heterostructure with t_{cap} = 10 nm and t_{bar} = 30 nm for a surface potential E_{C0} (i.e. conduction band edge at the gate contact) of 2.5 eV. According to $V_G = -(E_{C0} - \Phi_B)/q$, such a surface potential corresponds to an applied gate voltage V_G of -1.5 V when assuming a Schottky barrier height Φ_B of 1 eV. As can clearly be seen, under these conditions a 2DEG is formed in the GaN substrate close to the barrier-substrate heterojunction, and additionally a 2DHG appears in the cap close to the cap-barrier interface.

In Fig. 1(b) the calculated 2DEG and 2DHG sheet densities of structures with different cap thicknesses are shown as a function of the surface potential. As can be seen, increasing the cap thickness tends to result in a lower 2DEG density and a higher 2DHG density for a given surface potential. Once a 2DHG starts to form (e.g., at $E_{C0} \approx 0.75$ eV for t_{cap} = 40 nm), a further increase of the surface potential does no longer result in a decreasing

2DEG sheet density n_S. Instead, n_S asymptotically approaches a saturation level while the 2DHG sheet density p_S rises. The 2DHG is located closer to the surface (i.e., to gate) and effectively shields the 2DEG located farther from the gate.

3. Analytical considerations

One can gain further insights into the conditions for the hole gas formation with the help of simple first-order analytical considerations. Assuming the GaN cap and the AlGaN barrier to be fully depleted from mobile carriers and neglecting the unintentional background doping, the potential at the cap/barrier interface φ_{cap} (given in Volts) can be modelled as

$$\varphi_{cap} = \varphi_S \frac{C_1}{C_1 + C_2} - \frac{Q_p}{C_1 + C_2}, \tag{1}$$

where $C_1 = \varepsilon_{cap} / t_{cap}$ and $C_2 = \varepsilon_{bar} / t_{bar}$ are the depletion capacitances of the cap layer and the barrier, respectively, $\varphi_S = -E_{C0} / q$ is the surface potential (given in Volts), and Q_p is the polarization charge. A 2DHG is formed when the valence band edge at the cap/barrier interface touches the Fermi level located at zero energy in Fig. 1(a). In other words, the condition for the formation of a 2DHG is

$$\varphi_{cap} = -E_G^{cap} / q \,. \tag{2}$$

Equating (1) and (2) and assuming identical dielectric constants for GaN and AlGaN, we find an expression for the critical surface potential for the formation of a 2DHG

$$\varphi_S^{crit} = -\frac{E_{C0}^{crit}}{q} = Q_p \frac{t_{cap}}{\varepsilon_{cap}} - \frac{E_G^{cap}}{q} \cdot \frac{t_{cap} + t_{bar}}{t_{bar}}. \tag{3}$$

According to (3), the critical surface potential depends linearly on the cap thickness. This is in excellent agreement with the results from Schrödinger-Poisson simulations, as can be seen in Fig. 2(a). Moreover, Fig. 2(b) shows that the nonlinear dependence on t_{bar} obtained from Schrödinger-Poisson simulations is well reproduced by equation (3) as well.

Our analytical approach also leads to an expression for the minimum barrier thickness t_{bar}^{min}, which is necessary to form a 2DHG and a 2DEG simultaneously,

$$t_{bar}^{min} = \frac{E_G^{cap}}{q} \frac{\varepsilon_{bar}}{Q_p}. \tag{4}$$

In our case $t_{bar}^{min} = 14\,\text{nm}$. Equation (4) can be used to design appropriate heterostructures for certain applications. For instance, if a structure is needed where the saturation of n_S is undesirable, e.g. for HEMTs, the barrier thickness should be smaller than t_{bar}^{min}. In such cases

one could increase $t_{\mathrm{bar}}^{\mathrm{min}}$ by reducing the polarization charge, i.e. by reducing the Al content in the barrier. In BiSFET-like structures, on the other hand, coexisting electron and hole gases separated by a thin barrier (thin enough to allow tunneling) are needed. In that case, a small $t_{\mathrm{bar}}^{\mathrm{min}}$ is necessary that can be achieved either by increasing Q_{p} (by raising the Al content of the barrier) or by moving to another material system with smaller band gaps, such as InN/InGaN.

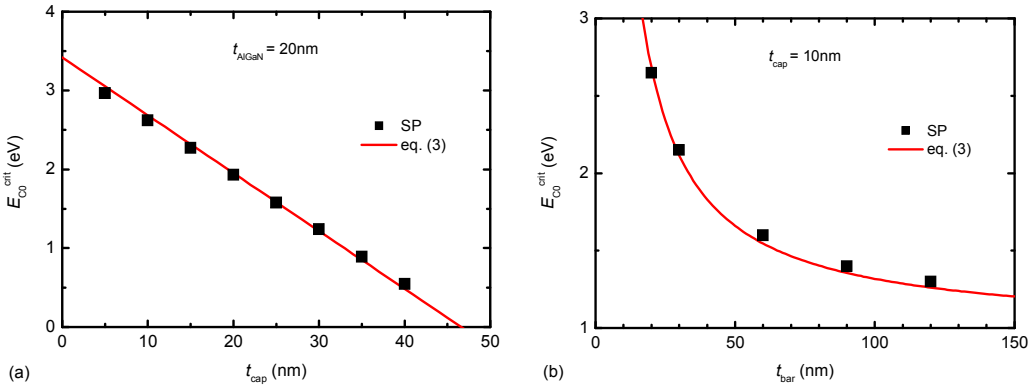

Fig.2: *Critical surface potential for the formation of a 2DHG as function of (a) t_{cap} and (b) t_{bar}. Symbols: Schrödinger-Poisson (SP) results, Line: calculated from Eq.(3).*

4. Conclusion

The conditions for the coexistence of electron and hole gases in GaN/AlGaN/GaN heterostructures have been studied by means of numerical Schrödinger-Poisson simulations and analytical models. When a 2DHG is formed, it effectively shields the 2DEG from the gate field and the electron concentration saturates. The saturation value strongly depends on the AlGaN thickness but is independent of the cap layer thickness. Below a minimum AlGaN thickness it is impossible to form a 2DHG and a 2DEG simultaneously.

Acknowledgement
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