Heterostructures with two-dimensional electron gas based on GaN with InAlN/AlGaN barrier

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The possibility of obtaining GaN-based heterostructures with composite InAlN/AlGaN barrier with a sheet resistance of $\sim 220-230\,\Omega$/sq. at room temperature by metalorganic vapor phase epitaxy, which is comparable to commercial structures with InAlN barriers, was experimentally demonstrated. Based on numerical calculations, it was shown that a significant reduction of the 2DEG mobility was due to alloy disorder potential scattering in the AlGaN layers.

Keywords: gallium nitride, transistor, InAlN.

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1. Introduction

Field-effect transistors based on III-N alloys are of great interest for high power and high frequency applications. Currently, such transistors are mainly fabricated based on AlGaN/GaN heterostructures with aluminum mole fraction generally not exceeding 30%. In these structures, a two-dimensional electron gas (2DEG) is formed on the heterointerface due to the difference in spontaneous and piezoelectric polarizations between AlGaN and GaN layers, with concentration $N_{2D} \sim 1 \cdot 10^{13}\,\mathrm{cm}^{-2}$ and mobility $\mu_{2D} \sim 2000\,\mathrm{cm}^2/(\mathrm{V}^{-1} \cdot \mathrm{s}^{-1})$. Typically, the sheet resistance of such structures exceeds $300\,\Omega$/sq. Increase in Al mole fraction in the barrier layer ensures concentrations of two-dimensional electron gas to $6 \cdot 10^{13}\,\mathrm{cm}^{-2}$ for pure AlN [1]. However, the large strain arising from the lattice mismatch between GaN and AlN significantly limits the critical thickness of the AlN barrier layer and negatively affects the reliability of the final device. At the same time, the growth of pure AlN by metal-organic vapor-phase epitaxy (MOVPE), the main industrial growth method of III-N structures, is practically impossible due to the unintentional incorporation of Ga atoms [2].

InAlN can serve as an alternative barrier layer material, enabling the production of a two-dimensional electron gas with a concentration $\sim (2.0-3.5) \cdot 10^{13}\,\mathrm{cm}^{-2}$ [3]. However, InAlN requires growth at significantly lower temperatures, which negatively affects its crystalline perfection and the quality of the heterointerface. This, along with the larger alloy scattering potential, results in low mobility values, making the final value of R_S comparable to or even higher than that of standard AlGaN/GaN structures. The use of a thin $1-2\,\mathrm{nm}$ AlN layer between InAlN and GaN generally enhances mobility, despite the ongoing issues of increased heterointerface roughness and unintentional Ga incorporation during MOVPE.

An interesting approach is the use of heterostructures with a thin composite InAlN/AlGaN barrier layer, which theoretically can achieve 2DEG concentrations comparable to those in InAlN-barrier heterostructures while maintaining mobilities similar to AlGaN-barrier structures. This paper presents the results of experimental studies and modeling of such structures.

2. Structures and experimental procedure

The studied structures were grown by MOVPE in the Dragon-125 epitaxial system on sapphire substrates. The structures consisted of a GaN:Fe-buffer layer and an undoped channel layer with a thickness of $\sim 1\,\mu$m [4,5], on top of which the barrier layers were grown: 1 nm nominally binary AlN, a $1-2\,\mathrm{nm}$ AlGaN-spacer, and an InAlN barrier of varying thickness. The electrical properties were studied through Hall effect measurements using the Van der Pauw method.

3. Results and discussion

Figure 1 presents the results of the study of the structure with the AlN/AlGaN/InAlN (1/2/4 nm) barrier conducted via scanning transmission electron microscopy with a high-angle annular dark-field detector (STEM-HAADF). Figure 1, *a* clearly shows the GaN, AlGaN, and InAlN layers with relatively smooth heterointerfaces between them;

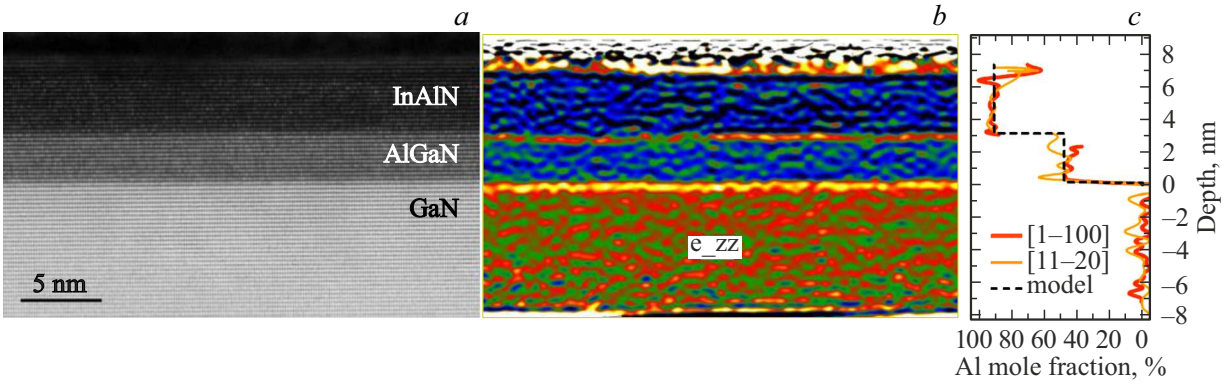

Figure 1. *a* — STEM-HAADF image of the structure; *b* —crystal lattice strain map relative to unstrained GaN; *c* — Aluminum mole fraction distribution through the depth of the structure.

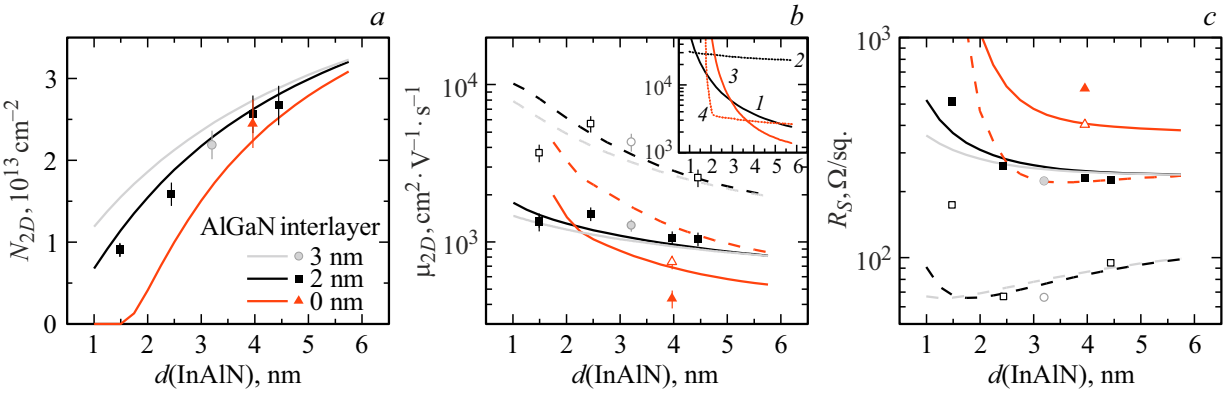

Figure 2. Concentration (*a*), mobility (*b*) and sheet resistance (*c*) vs. thickness of InAlN layer. Lines — calculation, symbols — experiment. Solid lines and filled symbols correspond to room temperature; dashed lines and open symbols — 77 K. In insert: *1, 2* — mobilities limited by scattering on alloy potential and interface roughness in the structure with 2-nanometer AlGaN-spacer; *3, 4* — same in structure without AlGaN-spacer.

however, no distinct nominally binary AlN layer is observed. A 1-nm-thick oxide layer is detected on the sample surface. A similar layer was also observed on the as-deposited sample in Ref. [6], which suggests that deposition of *in situ* passivating layers, such as Si_3N_4, is preferable. In the Al mole fraction distribution plots (Figure 1, *c*), obtained from the crystal lattice strain map (Figure 1, *b*), no AlN layer is observed, indicating unintentional incorporation of Ga atoms.

The measured values of concentration, mobility and sheet resistance of the 2DEG as a function of InAlN thickness are shown by symbols in Figure 2. It can be seen that increasing the barrier layer thickness results in a higher concentration of the 2DEG. At the same time, a decrease in the 2DEG mobility is observed, and the room temperature (295 K) sheet resistance decreases to $\sim 220-230\,\Omega$/sq. as the InAlN thickness increases to ~ 3 nm and remains constant with further thickness increase. The R_S value at low temperature has a minimum $\sim 67\,\Omega$/sq. at an InAlN thickness of 2.5 nm, with higher values for both thinner and thicker barrier layers. For comparison, a structure without an AlGaN spacer with a 4 nm InAlN barrier layer was also grown (marked with a triangle in Figure 2). The concentration of the 2DEG in this structure is slightly lower than in similar structures with an AlGaN spacer, but the mobility dramatically decreased to 435 and 745 $\mathrm{cm^2 \cdot V^{-1} \cdot s^{-1}}$) at 295 and 77 K, respectively, with corresponding R_S values of 587 and 400 Ω/sq.

To analyze the dependencies, numerical calculations were performed. The dependence of the concentration on the InAlN thickness was calculated by self-consistent solution of the Poisson and Schrödinger equations [7], and the expressions for scattering by acoustic and optical phonons, dislocations, heterointerface roughness and alloy disorder from the Refs. [3,8] were used to calculate the mobility. The choice of the alloy disorder scattering potential is critical in this calculation. In Ref. [9], it was shown through first-principles calculations that the value of the alloy disorder potential scattering U_0 for AlGaN of a given composition agrees well with $\partial E_c/\partial x$, where E_c — the conduction band edge energy. In our paper, the band offset $\Delta E_c/\Delta E_v = 0.7/0.3$ was adopted for AlGaN and InAlN in

the entire composition range, and the dependence $E_c(x)$ was calculated accordingly. Besides, the bowing parameter of the InAlN band gap dependence, unlike AlGaN, itself significantly depends on composition [10], which was also considered. So, the used values U_0 are 1.782 and 6.305 eV for AlGaN and InAlN, respectively. The average root-mean-square interface roughness values of 0.3 and 0.9 nm are used for AlGaN/GaN and InAlN/GaN, respectively, based on experimental data from Ref. [3]. In the calculations, a typical dislocations density value of $N_{\text{disl}} = 10^9\,\text{cm}^{-2}$ for GaN on sapphire was accepted, with a filling factor $f = 1$ [5,11].

The obtained dependences N_{2D}, μ_{2D} and R_S are presented in Figure 2 as lines. Since the expressions used to calculate scattering rates are valid only for a degenerated 2DEG, structures without AlGaN spacer with InAlN thickness of < 1.75 nm were excluded from calculations μ_{2D} and R_S. It is evident that the model effectively describes the observed dependences for structures with AlGaN spacer. The values of the mobilities limited by scattering by alloy disorder and interface roughness for structures with and without the AlGaN spacer are shown in the inset of Figure 2, *b*. It is evident that the contribution of alloy scattering in the structure without the AlGaN-spacer at the barrier thickness of > 3 nm is much higher than in the structure with the spacer. At the same time, the interface roughness scattering rate in the structures without the spacer is comparable to the alloy scattering in terms of its contribution. The discrepancy between the calculated and experimental values for the structure without the AlGaN spacer may be due to simplifications of this model when calculating the scattering rates (all electrons are assumed to occupy the ground state in the quantum well), unintentional incorporation of gallium into the barrier layer (which leads to higher alloy disorder scattering) or even greater roughness of the interface. But for correspondence of calculated values to the experimental values the roughness value > 1.5 nm is necessary, we think this is somewhat overestimated. We also can not rule out the combination of the abovementioned factors, and additional studies are required for unambiguous conclusions, both experimental and theoretical.

4. Conclusion

In conclusion, in this work, we experimentally demonstrated the fabrication of GaN-based heterostructures with a composite InAlN/AlGaN barrier with a sheet resistance $\sim 220-230\,\Omega$/sq. at room temperature via MOVPE, which is comparable to the commercial structures with InAlN-barriers [12]. It was shown that alloy disorder scattering in the AlGaN layers contributes significantly to the mobility reduction of the 2DEG.

Conflict of interest

The authors declare that they have no conflict of interest.

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