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Optimization of AlGaN/GaN heterostructures for high-electron mobility transistors

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Abstract. We theoretically study AlGaN/AlN/GaN heterostructures aimed at optimizing the AlGaN barrier for GaN-based high-electron-mobility transistors (HEMTs). Self-consistent Poisson—Schrödinger calculations combined with semi-empirical transport modeling are used to evaluate the two-dimensional electron gas (2DEG) concentration, sheet resistance, and saturation drain current as functions of barrier thickness and aluminum mole fraction. Technologically relevant constraints, including unintentional Ga incorporation, 2DEG-density-dependent mobility and saturation velocity, and the critical thickness of AlGaN coherently strained to GaN, are taken into account. Well-defined optimal barrier thicknesses minimize the sheet resistance to R_S ~ 250 Ω/□, while the saturation drain current increases with barrier thickness and Al content, limited by strain-induced cracking. The results provide practical guidance for barrier design in GaN-based HEMTs.

Keywords: GaN, AlGaN, HEMT, two-dimensional electron gas, Poisson–Schrödinger equations, sheet resistance, critical thickness

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Оптимизация гетероструктур AlGaN/GaN для транзисторов с высокой подвижностью электронов

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Аннотация. В работе теоретически исследуются гетероструктуры AlGaN/AlN/GaN с целью оптимизации барьерного слоя AlGaN для транзисторов с высокой подвижностью электронов на основе GaN. Для оценки концентрации двумерного электронного газа (2ДЭГ), слоевого сопротивления и насыщенного тока стока в зависимости от толщины барьера и мольной доли алюминия применялось численное решение самосогласованной системы уравнений Пуассона–Шрёдингера в сочетании с полуэмпирическим моделированием транспорта. Учтены технологические ограничения, такие как непреднамеренное встраивание атомов Ga, зависимость

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подвижности и насыщенной скорости 2ДЭГ от его концентрации, а также критическая толщина AlGaN, напряженного относительно GaN. Найдена оптимальная толщина барьерного слоя, обеспечивающая минимальное слоевое сопротивление R_S ~ 250 Ω/□, в то время как насыщенный ток стока увеличивается с ростом толщины барьера и содержания алюминия, но ограничен растрескиванием слоя из-за механических напряжений. Полученные результаты представляют практические рекомендации по проектированию барьерного слоя в транзисторах на основе GaN.

Ключевые слова: GaN, AlGaN, транзистор, двумерный электронный газ, уравнения Пуассона–Шрёдингера, слоевое сопротивление, критическая толщина

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Introduction

High-electron-mobility transistors (HEMTs) based on III-nitride heterostructures are finding increasing use in modern electronics. Gallium nitride, with its unique combination of properties such as a wide bandgap, high electron saturation velocity, high breakdown electric field strength, and relatively high electron mobility [1], offers superior performance compared with silicon and conventional III-V semiconductors. These advantages, particularly in terms of breakdown voltage and thermal stability, make GaN especially suitable for high-power applications.

In GaN-channel heterostructures, the AlGaN barrier layer is a critical element. Conventional designs typically employ a barrier layer with a thickness of 20–30 nm and an aluminum mole fraction of 20–30%, which provides a good balance of performance and reproducibility in metalorganic vapor phase epitaxy (MOVPE) production. However, increasing performance demands on electronic components are driving the development of novel heterostructure architectures. For example, operation at higher frequencies requires heterostructures with thinner barrier layers. For some applications, low sheet resistance is crucial, while for others, high operating current is desired, necessitating optimization of the barrier layer's thickness and composition while accounting for practical technological constraints.

In this paper, we analyze the effect of AlGaN barrier thickness and Al mole fraction in AlGaN/AlN/GaN heterostructures, taking into account technologically relevant constraints.

Materials and Methods

A typical HEMT heterostructure, consisting of a thick GaN channel, a thin (~1 nm) AlN interlayer, and an $Al_xGa_{1-x}N$ barrier of variable Al mole fraction x and thickness d was selected as the model system. The GaN layer was assumed to be fully relaxed, while both the interlayer and the barrier were treated as elastically strained to the GaN lattice. The two-dimensional electron gas (2DEG) concentration N in the channel of the heterostructures was obtained through a numerical self-consistent solution of the coupled 1D Poisson and Schrödinger equations [2] using a predictor-corrector approach for faster convergence [3]. Spontaneous and piezoelectric polarization, as well as a position-dependent electron effective mass were taken into account. All calculations were performed for room temperature, and background doping was assumed to be negligible in comparison with polarization-induced charge. Any underlying buffer layers that might be present were also disregarded due to their minimal direct effect on the 2DEG characteristics.

Unintentional incorporation of Ga atoms into subsequently grown Al-containing layers is a well-known effect in epitaxial growth of HEMT heterostructures, particularly in MOVPE, where Al mole fraction in nominally binary AlN interlayer can be as low as ~0.45 instead of ~1 [4, 5].

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However, it is still unclear whether the measured mole fraction reflects "true" atomic distribution or it is simply a measurement artifact due to poor spatial resolution or surface roughness [6]. For our heterostructures, the nominally 1-nm-thick AlN interlayer was estimated to be ~1.5 nm $Al_{0.65}Ga_{0.35}N$, so we used these values in calculations. The Al mole fraction in the AlGaN barrier layer was also limited to a maximum value $x = 0.65$.

The calculation of 2DEG mobility that accounts for multiple occupied subbands and all relevant carrier-scattering mechanisms can be computationally demanding. Moreover, such calculations often fail to reproduce the experimentally observed mobility-density dependences a priori [7]. For this reason, the dependence of the 2DEG mobility μ on the 2DEG concentration *N* was approximated using empirical fits based on the highest experimentally measured mobilities obtained for our heterostructures. This semi-empirical approach implicitly accounts for dominant (intrinsic, unavoidable, as we believe) density-dependent scattering mechanisms and has previously demonstrated good predictive capability in our earlier studies [8, 9], where the predictions were experimentally verified. The dependence of the 2DEG saturation velocity $v_{sat}(N)$ on the 2DEG density *N* was taken from [10].

In addition, the mechanical stability of the AlGaN barrier layer was considered. Due to the smaller in-plane lattice constant of AlN compared to GaN, an AlGaN film grown on GaN experiences tensile strain. As the layer thickness increases, the elastic strain energy accumulates, and once this energy exceeds a critical threshold, the layer may relax through the formation of surface cracks. The corresponding critical thickness d_{cr} for crack initiation was estimated using the Griffith fracture criterion [11].

Results and Discussion

The calculated values of the 2DEG concentration *N* for various Al mole fraction *x* and barrier thickness *d*, combined with the mobility dependence $\mu(N)$, were used to obtain the sheet resistance $R_S = (e \cdot N \cdot \mu)^{-1}$, shown in Fig. 1, *a*. These results reveal well-defined optimal thickness values over a wide compositional range $x > 0.30$ in terms of minimal sheet resistance $R_S \approx 250$ Ω/□ (the red dashed line in Fig. 1, *a*). These optima result from a trade-off between increasing 2DEG concentration and the accompanying reduction in mobility at high carrier densities. The optimal thickness values remain below the critical thickness (solid black lines in Fig. 1) for all Al mole fractions. It should be noted that for the barrier layers with the Al mole fractions $x > 0.54$, the optimal thickness falls below 2 nm, and when the 2DEG is located very close to the surface, additional scattering mechanisms, such as remote surface roughness scattering [12] or scattering by charged surface states [13] may become significant. These effects are not considered in the present study; however, they do not appear to be inevitable and can be mitigated through proper optimization of the growth process.

The saturation drain current was estimated as $I_D = e \cdot N \cdot v_{sat}$. This expression is appropriate for the high-field (velocity-saturation) regime, where the electron drift velocity approaches the saturation limit, such as at sufficiently high drain voltage. The resulting values of I_D as a function of Al mole fraction *x* and barrier thickness *d* are shown in Fig. 1, *b*. As one can see, in contrast to R_S, the saturation drain current does not exhibit an optimum with respect to *x* and *d*. Instead, it increases monotonically with increasing barrier thickness and Al mole fraction, indicating a 'more is better' behavior, despite the reduced saturation velocity for the high 2DEG density. In practice, however, this trend is constrained by the strain accumulated in the AlGaN layer, which limits the maximum achievable thickness and Al content before cracking. At the same time, when considering barrier layers with thicknesses equal to the critical value, a thinner barrier with a higher Al mole fraction provides a higher drain current than a thicker barrier with a lower Al mole fraction. Under these conditions, the maximum saturation drain current achievable for AlGaN/GaN-based transistors grown by MOVPE technology is ~2.6 A/mm for $_x$ = 0.65. This value should be regarded as a rough upper-limit estimate, since the model used does not account for several phenomena that may limit the drain current, such as self-heating, source and drain contact resistance, short-channel transport effects, etc.

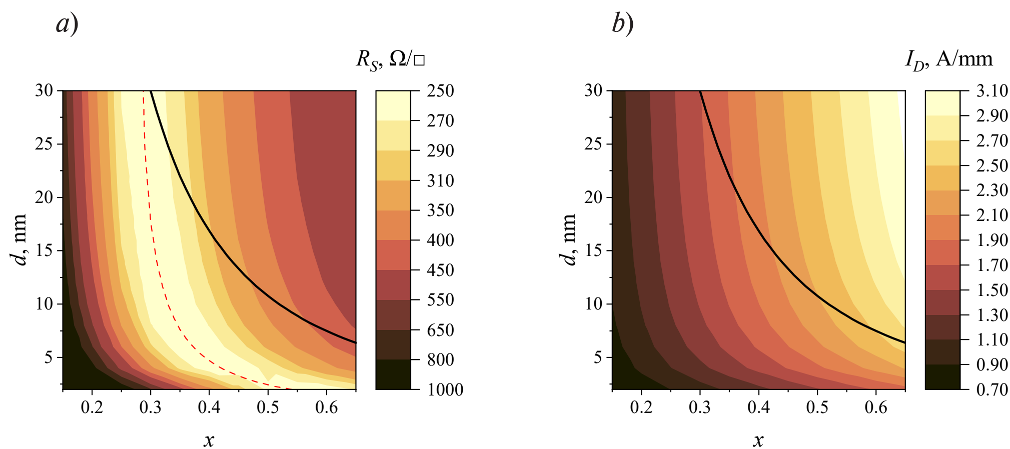

Fig. 1. Dependence of sheet resistance R_S (*a*) and saturation drain current I_D (*b*) on the Al mole fraction *x* and thickness d of $Al_xGa_{1-x}N$ barrier layer.

The black solid line represents the critical thickness of the AlGaN layer coherently strained to GaN. The red dashed line indicates the minimal sheet resistance of ~250 Ω/□

Conclusion

In this work, we analyzed the influence of AlGaN barrier thickness and aluminum mole fraction on the transport properties of AlGaN/AlN/GaN heterostructures under technologically relevant constraints. Self-consistent Poisson–Schrödinger simulations combined with semi-empirical transport modeling revealed well-defined optimal barrier thicknesses that minimize the sheet resistance to ~250 Ω/□ over a range of Al compositions, while the saturation drain current increases monotonically with increasing Al mole fraction and barrier thickness. It was also shown that higher Al content is favorable for achieving a high saturation drain current, and the achievable values are ultimately constrained by strain-induced critical thickness limitations. The presented results provide practical guidelines for optimizing AlGaN barrier design in GaN-based high-electron-mobility transistors.

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