The Kondo effect in 2D electron gas of magnetically undoped AlGaN/GaN high-electron-mobility transistor heterostructures

N K Chumakov¹, I A Chernykh¹, A B Davydov², I S Ezubchenko¹, Yu V Grishchenko¹, I L Lev³,4, I O Maiboroda¹, V N Strocov², V G Valeev¹ and M L Zanaveskin¹

¹National Research Center “Kurchatov Institute”, 1, Akademika Kurchatova pl., Moscow, 123182, Russia
²P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Leninskii pr. 53, Moscow, 119991 Russia
³Moscow Institute of Physics and Technology, 9 Institutskiy per., Dolgoprudny, Moscow Region, 141701, Russia
⁴Swiss Light Source, Paul Scherrer Institute, 5232, Villigen-PSI, Switzerland

E-mail: valeyevvg@gmail.com

Abstract. Unusual observation of the Kondo effect in two-dimensional electron gas (2DEG) of magnetically undoped AlGaN/GaN high-electron-mobility transistor heterostructures is reported. The temperature-dependent zero-field resistivity data exhibited an upturn below 120 K, while the standard low-temperature weak-localization behaviour was revealed at T → 0. Magnetotransport characterization was carried out in the magnetic fields up to 80 kOe, applied perpendicular to the 2DEG plane, in the temperature range 1.8 ÷ 300 K. Negative low-temperature magnetoresistance with a magnitude of order of 1 % was detected. The data set is analysed in the frame of the multichannel Kondo model for d⁰-magnetic materials.

1. Introduction

Wurtzite AlGaN/GaN high electron mobility transistor (HEMT) heterostructures have been scrupulously studied for a couple of the last decades as potential candidates for the next generation high-power, high-temperature and microwave electronics. This interest is motivated by their capacity to achieve current density, operating temperatures, breakdown voltage and cut-off frequencies, significantly higher compared to all of the existing GaAs, Si and Ge systems [1]. The latter unique properties are caused by the ability to realize two-dimensional electron gas with sheet carrier concentrations of order of 10¹³ cm⁻², localized in the vicinity of the heterostructure interface, without intentional doping. This value is at least an order of magnitude larger than the electron densities achievable in other III–V material structures [2]. Accumulation of the high density 2DEG is attributed to the formation of a deep spike-shaped quantum well at the heterojunction, where a large conduction band offset coexists with large piezoelectric and spontaneous polarization [3].

Despite recent remarkable progress in the development of III-nitride functional systems, this family of semiconductor materials, however, continues to bring surprises. In the work presented, we report unusual observations of Kondo effect in AlGaN/GaN based HEMTs that were synthesized without incorporating any magnetic impurities.
2. Experimental details
The nitride heterostructures with 2DEG were grown on c-oriented sapphire substrate in SemiTeq STE3N MBE-system equipped with ammonia nitrogen (NH₃) source. Prior to deposition substrate was annealed during 1 h and then nitrided for 40 min at 850°C. Buffer layers were grown using Al and Ga fluxes corresponding to 200 nm/h and 270 nm/h AlN and GaN growth rates, respectively. Deposition started with 10 nm AlN layer, grown at 1020°C under high ammonia flux of 200 sccm. Combination of long substrate nitridation with thin AlN nucleation layer grown under relatively high ammonia flux allows to suppress the formation of inverted AlN domains on sapphire substrate [4]. Then Al shutter was closed, and substrate temperature was increased to 1120°C. To improve crystalline quality and smoothen the film surface, the following 200 nm high-temperature AlN layer was deposited with Ga additive as a surfactant [5]. Then gradient junction to Al₀.43Ga₀.57N with thickness of approximately 250 nm was achieved by gradual decrease of substrate temperature to 830°C followed by 140 nm of growth at constant temperature. Then second gradient junction to Al₀.1Ga₀.9N with thickness of approximately 140 nm was formed by reducing temperature of the Al effusion cell. Then 500 nm GaN layer was grown. The growth was finished by deposition of a barrier layer consisting of 2 nm AlN and 1 nm Al₀.5Ga₀.5N, and no magnetic doping was allowed throughout the whole procedure.

3. Results & Discussion
An NT-MDT Ntegra atomic force microscopy (AFM) system was used to characterize surface morphology of the samples. Film surface was examined at several points and found to be homogeneous with root-mean-square roughness less than 1.9 nm at several 10×10 μm² areas.

Figure 1. Band dispersions of the buried 2DEG. Experimental band structure measured at hν = 1066 eV for the (a) ΓK and (b) ΓM directions of the bulk Brillouin zone (BZ) (superimposed with calculated E(k) of bulk GaN, black dashed lines). The QWSs appear above the valence band continuum. (c–d) Zoom-in image of the QWSs around the Γ10-point (purple lines schematize their dispersions fitting the experimental k_F). (e–f) Normalized momentum-distribution curves around the Γ10-point for a series of E_B through the QWS bandwidth. The difference between the ΓM and ΓK dispersions manifests planar anisotropy of the 2DEG, and the absence of k_z dispersion confirms its 2D character. (g) Bulk BZ of GaN and 2D one of the GaN/AlGaN heterostructure.

Bulk Brillouin zone (BZ) of GaN and 2D one of the GaN/AlGaN heterostructure and ARPES experimental band dispersions in GaN-HEMTs [6] are shown in figure 1. The data were measured along ΓM (a) and ΓK (b) at the photon energy hν = 1066 eV bringing k_z to the Γ-point of the bulk Brillouin zone (BZ). Non-dispersive ARPES intensity coming from the AlN and AlGaN layers was
suppressed in the plots by subtracting the angle-integrated spectral component. The conduction band minimum - derived quantum well states (QWSs) appear as tiny electron pockets above the valence band (VB) dispersions of GaN. Their energy separation from the VB minimum is consistent with the GaN fundamental band gap of ~ 3.3 eV. Whereas the VB dispersions are broadened in binding energy $E_B$ primarily because of band bending in the QW region, the QWS dispersions stay sharp. This confirms their 2D nature insensitive to band bending as well as their localization in the deep defect-free region in GaN, spatially separated from the defect-rich GaN/AlN interface region, the latter being the fundamental operational principle of the HEMTs delivering high 2DEG mobility. Clear dispersion of the VB states manifests their 3D character, while the QWS are flat in $k_z$. A zoom-in of the QWS dispersions along the $\Gamma M$ and $\Gamma K$ azimuths is shown in figure 1 (d, e) with the corresponding momentum-distribution curves in figure 4 (e, f). Whereas the outer contour of these dispersions corresponds to the QWS1, the significant spectral weight in the middle is due to the QWS2. The occupation of QWS2 is of order of $5\% - 10\%$.

ARPES study revealed a noticeable anisotropy in 2DEG Fermi surface and indicated the directional coincidence of the high 2DEG conductivity and low 2DEG effective mass, signifying, that the system symmetry ($C_{3v}$) is lower than that of the bulk GaN hexagonal lattice ($C_{6v}$) due to influence of the interface plane, orthogonal to the c-axis. A parabolic fit of the QWS1 dispersions yields $m^*$ values of $(0.16 \pm 0.03) m_0$ along the $\Gamma M$ azimuths and $(0.13 \pm 0.02) m_0$ along $\Gamma K$, where $m_0$ is the free-electron mass, which thus differ from each other by ~ 22%, see [6] for more details.

The direct experimental evidence, that the two 2DEG QWSs are occupied partially in the system under study, is of special importance for what follows.

Magnetotransport characterization was carried out in the magnetic fields up to 80 kOe, applied perpendicular to the 2DEG plane, in the temperature range 1.8 ÷ 300 K. The temperature and magnetic field dependencies were measured in both the usual Hall and van der Pauw geometries. Temperature-dependent resistance $R_{xx}(T)$ data, given in figure 2 for a number of the field values, exhibits a pronounced upturn approximately below 120 K, indicating the classical Kondo behaviour, while the significant low-temperature resistance growth clearly demonstrates the existence of the weak localization and interaction corrections to the conductivity of the 2DEG at $T \to 0$.

The results above are characteristic of the Kondo effect and indicate the presence of localized magnetic degrees of freedom, similar to those of the undoped semiconductors ZnO, CaO, and MgO oxides, which demonstrate the so-called $d_0$-magnetism – the magnetism in these materials is not induced by magnetic impurities, but is due to the vacancies in the cation sublattice [7].

![Figure 2. The temperature dependence of resistance for different magnetic field: B = 0, 5 and 80 kOe. Zero-magnetic field data are fitted using the numerical renormalization group n-channel Kondo model [17] (see Eq. (2) below).](image-url)
There are several types of the appropriate defects in GaN, including various charge states of Ga vacancies ($V_{Ga}$), whose presence was confirmed by the measurements of the photoluminescence spectrum (yellow emission), Raman spectrum, and X-ray photoelectron spectroscopy [8], and vacancy complex of two positively charged N vacancies ($V_N$) and one doubly negative Ga vacancy ($V_{Ga}^{2-}$ - $2V_N^{-}$ - complexes) [9]. In particular, the composite spin $3/2$ with a local magnetic moment of about $3\mu_B$, associated with neutral $V_{Ga}$ center, is produced by ferromagnetically coupled spins of unpaired $2p$-electrons of the three nitrogen atoms surrounding each of the Ga vacancy, while the latter defect complex induces a net moment of $1\mu_B$, localized around the negative Ga center.

The set of data above confirms, that the 2DEG at hand is in fact a two-channel Kondo system – indeed, the two partially occupied QWSs of the itinerant electrons there form two channels, interacting with the localized magnetic degrees of freedom.

According to the n-channel Kondo model [10], naturally invoked for the further analysis, three scenarios are then possible, mainly depending on the relative values of the two parameters: the total spin $S$ of the defect, responsible for spin-flip scattering of the itinerant electrons, and the number $n$ of screening channels: undercompensated ($n<2S$), compensated ($n=2S$), and overcompensated ($n>2S$) cases. The compensated model is characterized by the absence of the residual moment below the Kondo temperature ($T_K$) – if $n=2S$, the localized spin is completely quenched by the Kondo effect. The number of channels in an undercompensated model (which is definitely not the case for the two defect types, mentioned above) is insufficient to screen the localized spin completely, and an effective local moment with spin $S-n/2$ remains which asymptotically decouples from the conduction band. An overcompensated scenario results in a composite local moment with spin $n-S$, which remains coupled to the rest of the conduction electrons by an effective matrix element of the order of the band width. [11].

The key further observation is the behaviour, demonstrated by the weak localization magnetoresistance and magnetoconductivity, see figures. 3 and 4 below: the picture like this would be impossible in a system with a random distribution of residual magnetic moments, coupled to the conduction band.

![Figure 3. Magnetoresistance measurement results of the 2DEG in AlGaN/GaN HEMT.](image)

![Figure 4. Magnetoconductivity $\Delta\sigma = \sigma(B,T) - \sigma(0,T)$, measured at 1.8, 3.4, 10 and 40 K (normalized to $G_0 = e^2/\pi h$).](image)

Indeed, as it was shown in [12], the interaction of electron spins with the magnetic moments frozen in random directions leads to the suppression of the interference corrections to the conductivity, while the Zeeman splitting of the localized spin states reduces the electron dephasing rate, thus enhancing
the effect of electron interference on conduction. In other words, if these interference contributions can be restored by an application of a spin-polarizing field, then a transport measurement may serve as a test for the presence of the localized magnetic degrees of freedom in a sample, [13]. But this is definitely not the case. (The weak antilocalization corrections due to the spin-orbit interaction, peaking out in the system in the fields up to ~ 0.2 kOe and sufficiently low temperatures [14], are beyond the parametric region of the current study).

Negative magnetoresistance of the AlGaN/GaN heterostructure with a temperature-dependent magnitude of order of 1% was observed for the temperatures up to 110 K, as shown in figure 3.

Figure 4 presents the experimental data for the magnetoconductivity, \[ \frac{\Delta \sigma(B, T)}{G_0} = 0.2 + \frac{1}{b \tau_{\phi}} \ln \left( \frac{\tau}{\tau_{\phi}} \right), \]

where \( b = B/B_\phi, B_\phi = h/4eD \tau, \tau \) is the electron transport relaxation time, \( D = v_F^2 \tau/2 \) - the 2D diffusion coefficient, \( v_F \) - the Fermi velocity and \( \tau_{\phi} \) - the electron dephasing time. Eq. (1) is formally valid, if \( B < B_\phi \) and \( \tau \ll \tau_{\phi} \). The best fit for the temperatures range 1.8 K \( \leq T \leq 40 \) K, where the interaction contribution to the conductivity is a relatively slow function of the temperature, and the fields \( B \geq 0.2kOe, \) was obtained for \( \alpha = 0.14, \tau_{\phi} = 1.3 \cdot 10^{-13} \text{s}, v_F = 0.6 \cdot 10^6 \text{m/s}; \tau_{\phi}(\text{ps}) = 6.17, 4.66, 1.35 \) and \( 0.27 \) at \( T = 1.8, 3.4, 10 \) and \( 40 \) K, correspondingly.

The temperature dependence of the electron phase relaxation time \( \tau_{\phi} \) found from the fit is given at figure 5. The \( \tau_{\phi} \propto T^{-1} \) behavior of the dephasing time there is known to be mainly determined by the inelasticity of electron-electron interaction [15].

We conclude, that the 2DEG in AlGaN/GaN based HEMT is a compensated two-channel Kondo system, and the appropriate possibility with the defect types mentioned above is to have a 2DEG with (dominated density of) the neutral \( \text{V}_{\text{Ga}}^{2-} \cdot 2\text{V}_{\text{N}}^+ \cdot \) complexes and/or singly charged Ga vacancies (\( \text{V}_{\text{Ga}}^{-} \)) [16] - indeed, only then the bare local spin \( S=1, \) necessary for the complete Kondo screening in the \( n=2 \) channel case.
Finally, we perform the comparison of zero-magnetic field temperature-dependent resistance measurement results with the corresponding prediction of the numerical renormalization group for an $n$-channel Kondo system [17] with the electron-electron and electron-phonon resistance contributions taken into account:

$$R(T) = R_0 + \alpha R \left[1 + \left(2^{1/8} - 1\right)\left(\frac{T}{T_K}\right)^2\right]^8 + \beta \frac{T}{T_m} + \gamma \left(\frac{T}{T_m}\right)^4. \quad (2)$$

The best fit in the temperature range $[50K, 300K]$, given by the solid line in figure 2, was obtained for $R_0 = 1.2416 \text{k}\Omega$, $S = 1$, $T_K = 136.7 \text{K}$, $T_m = 300 \text{K}$, $\alpha R = 330.2 \text{\Omega}$, $\beta = 312.3 \text{\Omega}$, $\gamma = 332.0 \text{\Omega}$. The material constants, characterizing the electron-electron and the electron-phonon scattering contributions to the system resistance (the third and the fourth summands in Eq. (2), correspondingly) were calculated by the method, described in [18]. A relatively high value of the Kondo temperature, obtained in the fitting procedure, explains the failure of our initial attempts to fit this data to perturbative Kondo’s approximation.

It is worth mentioning, that Eq. (2) a-priori fails to describe the resistance growth with $T$ lowering due to the weak localization and interaction corrections to the conductivity of 2DEG, the latter being the reason to use the dashed line for the low-temperature wing of the fitting curve.

4. Summary

The Kondo effect we observed recently in 2D electron gas (2DEG) of magnetically undoped AlGaN/GaN high-electron-mobility transistor heterostructures and the corresponding magneto-conductivity data are interpreted in terms of the two-channel Kondo model for $d_0$-magnetic materials. The magnetic degree of freedom in the system is attributed with $V_{Ga}^{2v} \sim 2V_{S}^{\mu}$ - vacancy complexes, each inducing a net moment of 1$\mu_B$, located around its negative Ga center in the 2DEG localization region, and/or singly charged Ga vacancies ($V_{Ga}^{\mu}$).

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References

[1] Medjdoub A F and Iniewski K (eds.) 2016 Gallium nitride (GaN): physics, devices, and technology (New York: CRC Press)
[2] Gurusisinghe M N, Davidsson S K and Andersson T G 2005 Phys. Rev. B 72 045316
[3] Ambacher O et al. 2000 J. Appl. Phys. 87 334-44
[4] Mayboroda I O, Ezubchenco I S, Grishchenko Yu V, Presniakov M Yu and Zanaveskin M L 2017 J. Surf. Invest. 11(6) 1135-44
[5] Mayboroda I O, Knizhnik A A, Grishchenko Yu V, Ezubchenko I S, Zanaveskin M L, Kondratev O A, Presniakov M Yu, Potapkin B V and Ilyin V A 2017 J. Appl. Phys. 122 105305
[6] Lev L et al. 2018 Nature Communications 9, Article number: 2653, 1–9
[7] Kapilashrami M, Xu J, Rao K V, Belova L, Carlegrim E and Fahlan M 2010 J. Phys.: Cond. Matter 22 345004
[8] Jin H, Dai Y, BaiBiao Huang and Whangbo M –H 2009 Appl. Phys. Lett. 94 162505
[9] Zhang Zh, Schwingenschoegl U and Roqan I S 2014 J. Appl. Phys. 116 183905
[10] Nozieres P and Blandin A 1980 J. Physique 41 193-211
[11] Cox D L and Zawadowski A 1998 Adv. Phys. 47(5) 599-942
[12] Hikami S, Larkin A I and Nagaoka Y 1980 *Prog. Theor. Phys.* 63 707-10; Wittmann H –P and Schmid A 1987 *J. Low Temp. Phys.* 69 131-49

[13] Vavilov M G, Kaminski A and Glazman L I 2003 *Physica* E 18 64-8; Vavilov M G and Glazman L I 2003 *Phys. Rev.* B 67 115310

[14] Spirito D, Di Gaspare L, Evangelisti F, Di Gaspare A, Giovine E and Notargiacomo A 2012 *Phys. Rev.* B 85 235314

[15] Altshuler B L, Aronov A G and Khmelnitsky D E 1982 *J. Phys.* C 15 7367-86

[16] Wang X, Zhao M, He T, Wang Zh and Liu X 2013 *Appl. Phys. Lett.* 102, 062411; Tang Zh-k, Zhang D -Y, Tang L -M, Wang L –L and Chen K -Q, 2013 *Eur. Phys. J.* B 86 284

[17] Hanl M, Weichselbaum A, Costi T A, Mallet F, Saminadayar L, Bauerle C and Von Delft J 2013 *Phys. Rev.* B 88 075146; Costi T A et al 2009 *Phys. Rev. Lett.* 102 056802

[18] Rizwana Begum K and Sankeshwar N S 2014 *Diam. Relat. Mater.* 49 87-95