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# Radiation from shallow oxygen impurity in AlGaN/GaN HEMT structures in magnetic field

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## Abstract

The electrically excited impurity emission from AlGaN/GaN high electron mobility transistor (HEMT) structures in external magnetic field varying from 1.2 T to 1.5 T was investigated in this work at temperature of 4.2 K. We have observed the sharp emission line at  $(263 \pm 1) \text{ cm}^{-1}$  with FWHM of  $(5.8 \pm 0.8) \text{ cm}^{-1}$ , which we have attributed to radiative electronic transitions in residual oxygen impurity atoms. The blueshift of resonant transition frequency due to presence of external magnetic field was observed. The width of the peak was found to be defined mainly by the thermal broadening at 4.2 K.

## 1. Introduction

The unique properties of terahertz (THz) electromagnetic waves interaction with matter give a number of promising applications in medical diagnostics, security surveillance, explosives and drugs identification to name just a few. Thus it is desirable to have compact and conveniently tunable (electrically, for example) THz sources. The approaches of electrically pumped compact semiconductor THz emitters such as quantum cascade lasers [1, 2], 2DEG plasma oscillators [3, 4, 5], emitters utilizing electron transitions between Landau levels in external magnetic field [6, 7] or radiative electron transitions in shallow impurities [8, 9, 10] has been proposed so far.

On the other hand, one always has to be aware of parasitic radiative channels which may coexist in the solid state THz emitters. For example, it was shown recently that significant impurity electroluminescence can be excited in n-GaN epilayers and in AlGaN/GaN heterostructures [10, 11]. In Ref. [11] we have demonstrated that the intensity of impurity electroluminescence was proportional to residual shallow impurity concentration later confirmed by the secondary ion mass spectroscopy (SIMS). Moreover, the low frequency noise in AlGaN/GaN transistors developed of the same heterostructure was found to be two orders of magnitude higher than that measured in high electron mobility transistors (HEMTs) fabricated on different heterostructures grown on sapphire and SiC substrates [12]. The effective trap density extracted from noise measurements correlated with the results of SIMS and THz electroluminescence (TEL) measurements and the low-frequency noise was proven to be a very sensitive figure of merit parameter for the field effect transistors and material quality assessment [11, 12, 13]. Despite the fact the TEL spectroscopy is less sensitive to the total amount of trap density, it is suitable for direct evaluation of shallow im-

purity atom species in semiconductor heterostructures after the material growth and the device fabrication. Moreover, this technique has important advantages over conventional THz absorption spectroscopy: (i) any solid state component with two electric contacts can be used as the source for TEL spectroscopy; (ii) optical losses in the heterostructure and optional passivation layers can be neglected in most of the cases in the THz frequency range.

The oxygen atoms are present in AlGaN and GaN epilayers grown by metalorganic chemical vapour deposition (MOCVD) method, therefore monitoring of residual oxygen impurities is required. Theoretical and experimental research on shallow impurities such as oxygen, silicon, carbon traces in epitaxial GaN layers has been conducted [10, 14, 15]. However, to our knowledge no attempts to study impurity emission properties of AlGaN/GaN structures in external magnetic fields and at temperature of 4.2 K were reported so far. The aim of this work was to investigate the shallow impurities in unintentionally doped AlGaN/GaN HEMT structures at liquid helium temperature and subjected to external magnetic field by the means of TEL. The direction of the magnetic field was normal to the sample surface and the maximum applied strength reached up to 1.5 T. At pumping voltage of  $U_p = 20 \text{ V}$  we have observed the sharp emission peak which we have attributed to electron transition from the conduction band bottom to the ground energy state of residual oxygen impurity. The blueshift of resonant emission peak induced by the Landau quantization of conduction band electronic states was observed. The emission peak at lower energies was also observed, however, its origin was not determined and further investigation is required.

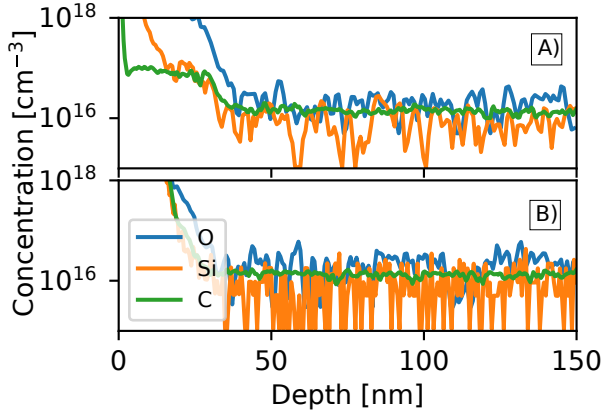
## 2. Samples and experiment

The investigated samples were formed on the structure of GaN/Al<sub>0.2</sub>Ga<sub>0.8</sub>N HEMT grown on Al<sub>2</sub>O<sub>3</sub> (wafer #TG2196) and SiC (wafer #Hx2688) substrates along *c*-axis by the MOCVD. The 20 nm-thick low temperature (LT) nucleation

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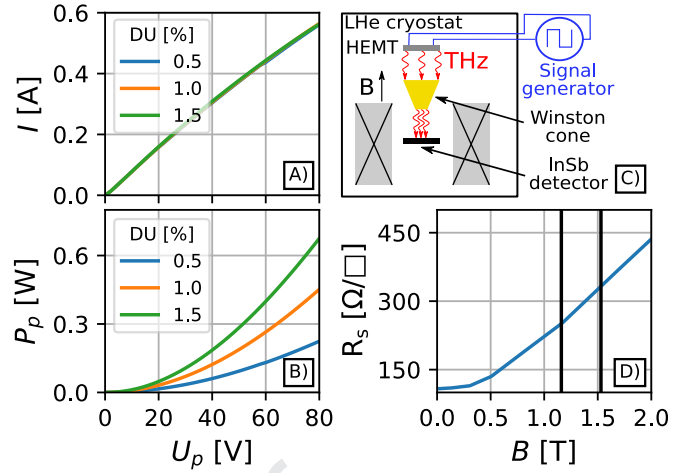
**Figure 1:** Concentration of residual impurity atoms in the investigated AlGaIn/GaN/Al<sub>2</sub>O<sub>3</sub> (A) and AlGaIn/GaN/SiC (B) HEMT structures as a function of depth measured from the top surface of the structure.

layer (GaN in #TG2196 and AlN in #Hx2688) was followed by 1000 nm-thick high resistivity GaN buffer, 500 nm-thick unintentionally doped GaN layer and 1 nm AlN spacer. On the top, 25 nm in thickness Al<sub>0.2</sub>Ga<sub>0.8</sub>N layer was grown. The two-dimensional electron gas (2DEG) formed at the AlGaIn/GaN interface with sheet concentration  $n_s = 1.15 \times 10^{13} \text{ cm}^{-2}$  and  $n_s = 8.0 \times 10^{12} \text{ cm}^{-2}$  while sheet resistance was equal to  $106 \text{ } \Omega/\square$  and  $58 \text{ } \Omega/\square$  at 4.2 K for samples grown on Al<sub>2</sub>O<sub>3</sub> and SiC, respectively. Residual doping level of the heterostructure layers was estimated using the secondary-ion mass spectrometry. Distribution of main residual impurities for sample #TG2196 are shown in Fig. 1 A. Concentrations of O, C and Si residual impurities were found to be  $\sim 2 \times 10^{16} \text{ cm}^{-3}$ ,  $\sim 1.4 \times 10^{16} \text{ cm}^{-3}$  and  $9 \times 10^{15} \text{ cm}^{-3}$  at the depth above 35 nm from the top surface of the sample, i.e. in GaN buffer. The heterostructure design and densities of residual dopants were very similar for sample #Hx2688 (Fig. 1 B). More details can be found in Ref. [12].

An active channel of the investigated device was  $2 \times 2 \text{ mm}^2$  in size. In order to have an electrical connection to the channel two  $0.1 \times 2 \text{ mm}^2$  Ti/Al/Ni/Au ohmic contacts were formed using a rapid thermal annealing (RTA) technique.

Pulsed current-voltage characteristics and pulsed electrical power dependencies on applied pulse voltage are shown in Fig. 2 A) and B) respectively for duty cycle values of 0.5 %, 1 % and 1.5 %. We can see, that the heating of the sample is the same in all cases despite higher electrical power was provided. This demonstrates that excessive heat is effectively removed from the sample at given pumping powers.

The sample was installed inside the oversized stainless steel light pipe and immersed in a liquid helium bath (see Fig. 2 B). It was situated outside the superconducting coil but was exposed to weak residual magnetic field which was estimated through geometrical magnetoresistance (Fig. 2 D). The sample was biased with the square voltage pulses of amplitude  $U_p$  which was changed from 10 V to 40 V, and modulation frequency was fixed at 33 Hz. The width



**Figure 2:** A) The pulsed current-voltage characteristics and B) the pulse power dependence on pulse voltage at DU values of 0.5 %, 1 % and 1.5 %. C) The experiment setup. D) Magnetoresistance of AlGaIn/GaN/Al<sub>2</sub>O<sub>3</sub> sample. Vertical bars enclose the region in which emission spectra were measured.

of the pulse was varied in the interval from 0.30 to 0.75 ns which corresponded to the duty cycle (DU) of 1–2.5%. The THz radiation coming from the sample was registered as cyclotron resonance phenomena induced photocurrent in the detector [16]. In our case, a magnetically tuneable meander-shaped *n*-type InSb detector was placed in a constant magnetic field created by a superconducting coil. By sweeping the magnetic induction from 0 to 5 T we were able to tune the electron cyclotron frequency of the detector in the interval from 0 to 8.67 THz ( $0\text{--}290 \text{ cm}^{-1}$  in wavenumber domain). However, the detection in frequency range from 5 to 6.6 THz ( $167\text{--}220 \text{ cm}^{-1}$ ) was suppressed due to the Reststrahlen band of InSb. A Winston cone was used to concentrate the radiation on the detector. The output of the cone could be blocked with an externally actuated copper shutter in order to study side effects. The photocurrent change in the detector was registered with a lock-in amplifier.

### 3. Results and discussion

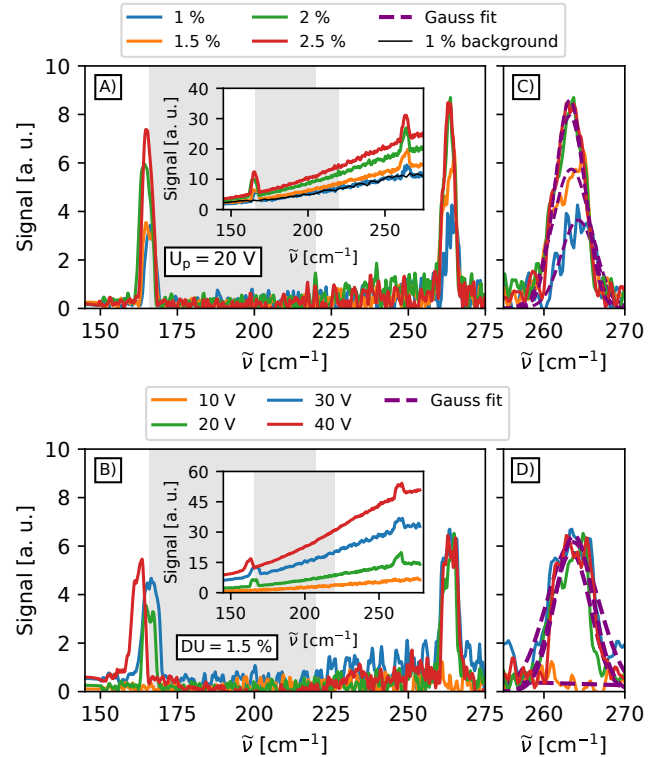
The emission spectra for the HEMT on the Al<sub>2</sub>O<sub>3</sub> (#TG2196) measured at various DU values at fixed  $U_p = 20 \text{ V}$  are shown in the inset of Fig. 3 A. The energy of the peak at  $263 \text{ cm}^{-1}$  is close to the ionization energy of shallow oxygen impurity ( $O_{c-1s}$ ) in wurzite GaN lattice, which was predicted theoretically [14] and reported experimentally in electroluminescence experiments without external magnetic field at the temperature of 20 K [13]. Also we observed emission at lower energies,  $163 \text{ cm}^{-1}$  for HEMT on Al<sub>2</sub>O<sub>3</sub> and at  $147 \text{ cm}^{-1}$  for HEMT on SiC. These peaks are too close to the Reststrahlen band of our detector and require additional research using other methods. In this paper we will concentrate on the emission at  $263 \text{ cm}^{-1}$ . The emission nature at lower energies will not be discussed here.

Spectrum when the optical path between emitter and detector was closed is shown for  $DU = 1\%$  (see background

line in the inset of Fig. 3 A). It demonstrates the background signal measured with the detector at a given DU value. Note, that the background signal was also registered in the Reststrahlen region of InSb where the detection of THz radiation is suppressed. This indicates that our detector picks up the signals that are not related to the THz emission from the sample. The amplitude of the pick-up signal is rising with the magnetic field, as well as with the electric pulse amplitude and duration. For further analysis, this background line was numerically subtracted from the measurement results (Fig. 3 A) and the obtained curves were fitted using Gauss functions (Fig. 3 B). The sharp peak at position of  $(263 \pm 1) \text{ cm}^{-1}$  which FWHM value is  $(5.8 \pm 0.8) \text{ cm}^{-1}$  was attributed to the emission from shallow oxygen impurity atoms.

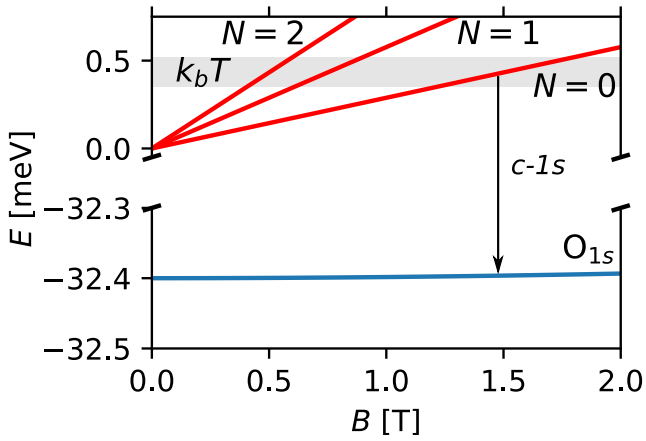
The electroluminescence spectra were also measured for a constant duty cycle  $DU = 1.5\%$  when pulse voltage was changed every 10 V in the interval from 10 V to 40 V and results are presented in Fig. 3 C. It was found, that the emission peaks appear in the spectrum when applied voltage amplitude is higher than 10 V which corresponds to electric field strength above 50 V/cm. It is worth noting that the value of threshold electrical field of impurity electroluminescence reported in bulk GaN is about 500 V/cm [10], however in our previous works we have observed that the threshold electrical field could be smaller in AlGaIn/GaN heterostructures most likely due to the optimized performance of ohmic contacts [11, 13]. Also, it is interesting to note that after subtraction of the background line we have found that the amplitude and FWHM of ( $O_{c-1s}$ ) emission peak were independent of applied bias voltage up to 40 V (Fig. 3 D). Such a behaviour is not common to impurity-assisted THz electroluminescence in bulk samples, where it increases together with pump voltage. Calculations show, that only about 0.33 % of total injected electric current flows through buffer layer in our samples. This gives a relatively low number of drifting electrons in the buffer which can cause impact impurity ionisation. Since an increased voltage heats free electrons in the channel, the density of acoustic phonons increases and the scattering of electrons by acoustic phonons in the buffer becomes more efficient. The more efficient scattering could compensate the increased injected electron number and momentum. This phenomenon could result to TEL signal independent on applied voltage.

The experimentally determined frequency  $(263 \pm 1) \text{ cm}^{-1}$  of the oxygen impurities related emission peak is at a higher frequency than the theoretically calculated value of  $261.3 \text{ cm}^{-1}$  [14]. In order to address this frequency shift it is important to remember that the external magnetic field normal to the sample surface was present. Therefore, Landau quantization of electron energy states in conduction band and/or diamagnetic shift of the impurity energy levels could be responsible for the change in electron transition energy. Magnetoresistance measurements revealed that the magnetic field felt by the sample was in the range from 1.16 to 1.53 T (Fig. 1 D) when resonant frequency of the detector was tuned between 150 and  $280 \text{ cm}^{-1}$ . Landau quantization led to the electronic levels with energies  $E_N = (N + 1/2)\hbar\omega_c$



**Figure 3:** A) Emission spectra of AlGaIn/GaN HEMT at 4.2 K for pumping pulse duty cycle DU values which are increased by the step of 0.5% in the interval from 1 to 2.5% when  $U_p = 20 \text{ V}$  after subtraction of electrical pick-up background. The inset shows the original spectra when the radiation is reaching the detector (solid curve) and is blocked (black solid curve) at  $DU=1\%$ . B) The Gauss fit of the spectral feature observed at  $263 \text{ cm}^{-1}$  for different DU values at  $U_p = 20 \text{ V}$ . C) Emission spectra at  $DU = 1.5\%$  for  $U_p = 10\text{-}40 \text{ V}$  increased in steps of 10 V without the background. Inset: emission spectra as measured. D) The Gauss fit of the spectral feature observed at  $263 \text{ cm}^{-1}$  for different pulse voltages at  $DU = 1.5\%$ . The shaded regions in A), B) and their insets represent the Reststrahlen band of InSb.

with  $N = 0, 1, 2, \dots$ . Here  $\omega_c = eB/m^*$  is the angular cyclotron frequency,  $e$  – the elementary charge and  $m^*$  – electron effective mass. The lowest energy level ( $N = 0$ ) for electrons in the conduction band of GaN calculated including the spin split is shown in Fig. 4. At  $B = 1.53 \text{ T}$  the estimated energy shift from conduction band bottom at  $B = 0 \text{ T}$  is  $\sim 3 \text{ cm}^{-1}$ , which is higher than the experimentally observed shift. On the other hand, the calculated Rydberg energy and cyclotron energy ratio  $\gamma = 0.018$  at  $B = 1.53 \text{ T}$ . The condition  $\gamma \ll 1$  holds, therefore, impurity potential can be treated as hydrogen atom-like and the applied external magnetic field is considered as a small perturbation only. For  $1s$  state the diamagnetic shift is less than 1 % of ionization energy, and it should affect the energy of  $O_{c-1s}$  transition insignificantly. Thus, the Landau quantization effect gives the main contribution to energy shift of resonant emission line



**Figure 4:** Energy of the lowest three Landau levels in GaN in magnetic field is depicted by solid lines. Shaded region shows  $k_bT$  broadening at 4.2 K. Dashed line represents the  $1s$  energy level of oxygen impurity in GaN. Vertical arrow represents the radiative electron transition from conduction band to  $O_{1s}$  level.

related to oxygen impurities in GaN at magnetic fields below 1.5 T. The difference between experimentally and theoretically determined emission peak energy shift could result from the fact that Landau level energy was calculated neglecting the non-parabolicity of the conduction band. In addition, the  $k_bT$  energy at 4.2 K is  $\sim 2.8 \text{ cm}^{-1}$ , and it is comparable to the observed energy shift.

As it was pointed out before, the estimated FWHM value of the emission peak is  $(5.8 \pm 0.8) \text{ cm}^{-1}$ . On the other hand, the  $k_bT$  thermal broadening of impurity energy levels is  $\sim 2.8 \text{ cm}^{-1}$  at  $T = 4.2 \text{ K}$ . What we actually measure in our experiment is the convolution between thermally broadened  $c - 1s$  emission line of the oxygen impurities and the detector spectral response function. It is known that the width of InSb cyclotron resonance line is  $\sim 5.7 \text{ cm}^{-1}$  at  $T = 4.2 \text{ K}$  and  $B = 5 \text{ T}$  [17]. If we assume that thermal broadening of impurity levels and detector spectral response function are described by Gauss functions of widths  $c_1$  and  $c_2$  respectively, their convolution is a Gaussian function with FWHM  $= \sqrt{c_1^2 + c_2^2}$  [18]. Such evaluation gives FWHM of around  $6.3 \text{ cm}^{-1}$  which is in a good agreement with the experimentally observed value. Since, the actual width of  $O_{c-1s}$  emission line was not measured directly we could suppose that its width should be of about  $2.8 \text{ cm}^{-1}$ , i.e. the value defined by the thermal broadening. On the other hand, continuum to bound electron transitions in bulk semiconductors usually give much broader emission spectral features of  $40 \text{ cm}^{-1}$  to  $60 \text{ cm}^{-1}$  in width [8, 9, 10]. In our case it is possible that Joule heating of epilayers is weak due to optimized resistance of ohmic contacts (see Fig. 2 A and Fig. 2 B) and as the result a narrow  $c - 1s$  emission peak is observed in the experiment.

## 4. Conclusions

The THz electroluminescence from AlGaIn/GaN high electron mobility transistor structures grown on  $\text{Al}_2\text{O}_3$  and SiC substrates was investigated experimentally at the temperature of 4.2 K and magnetic field up to 1.5 T. The peak resulting from electron transition from conduction band bottom to ground state of residual oxygen impurities was observed at  $(263 \pm 1) \text{ cm}^{-1}$  for the sample grown on  $\text{Al}_2\text{O}_3$ . It was found that the external magnetic field of 1.5 T blueshifts transition energy by about  $2 \text{ cm}^{-1}$ . Also, an indirect estimation of the width of  $c - 1s$  electroluminescence peak shows that its value should be around  $3 \text{ cm}^{-1}$ . Relatively strong electroluminescence at position around  $147 \text{ cm}^{-1}$  (#Hx2688) and  $163 \text{ cm}^{-1}$  (#TG2196) were observed. The origin of these peaks was not identified and therefore, further investigation is required.

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