Optica Applicata, Vol. XXXV, No. 3, 2005

Piezoelectric effect and spontaneous polarization in computer modelling of A^{III}–N heterostructures

TOMASZ PIASECKI*, WOJCIECH KOŚNIKOWSKI, BOGDAN PASZKIEWICZ

Faculty of Microsystem Electronics and Photonics, Wrocław University of Technology, Janiszewskiego 11/17, 50-372 Wrocław, Poland

*Corresponding author: T. Pasecki, tomasz.piasecki@pwr.wroc.pl

The Ga, Al and In nitrides (A^{III}–N) are complete material system suitable in high power and high temperature electronic devices such as $Al_xGa_{1-x}N$/GaN heterostructure field effect transistor (HFET). The examples of computer modelling of A^{III}–N heterostructures were shown. A^{III}–N materials exhibit strong piezoelectric and spontaneous polarization. The computer modelling results showing the influence of layer polarity on carrier distribution in $Al_xGa_{1-x}N$/GaN heterostructure were shown. Only in Ga-faced heterostructures 2-dimensional electron gas (2DEG) is formed. The effect of $Al_xGa_{1-x}N$ layer relaxation on 2DEG concentration in $Al_xGa_{1-x}N$/GaN heterostructure was examined. The difference in spontaneous polarization in $Al_xGa_{1-x}N$ and GaN caused high 2DEG concentration even in $Al_xGa_{1-x}N$/GaN heterostructures with relaxed $Al_xGa_{1-x}N$ layer. Polarization field in $Al_xGa_{1-x}N$ layer in $Al_xGa_{1-x}N$/GaN heterostructure was enough for achieving high 2DEG concentrations in undoped heterostructure. Strained $Al_xGa_{1-x}N$ layer was introduced into typical HFET heterostructure. GaN layer above an interlayer was depleted and the negative influence of using non semi-insulating GaN layer in HFET transistor was reduced.

Keywords: A^{III}–N, computer modelling, heterostructure, 2-dimensional electron gas (2DEG), strain, piezoelectric effect, spontaneous polarization, heterostructure field effect transistor (HFET).

1. Introduction

The nitrides of 3rd group elements (gallium, aluminium, indium) are complete wide-bandgap semiconductors material system A^{III}–N. They may be used in blue or UV optoelectronic devices or high temperature electronic devices. It is possible to compose the ternary or quaternary A^{III}–N alloys, which allows to manufacture heterostructures necessary in modern semiconductor devices. Reported high 2-dimensional electron gas (2DEG) sheet concentration in AlGaN/GaN heterostructures and high electron mobility in 2DEG suggest using the AlGaN/GaN heterostructure in 2DEG-based devices such as heterostructure field effect transistor (HFET) [1, 2]. A^{III}–N materials, unlike the traditional semiconductors such as A^{III}–B^{V} or Si, exhibit strong piezoelectric effect and spontaneous polarization [3, 4]. These phenomena have

to be taken into account in device design process. One of the tools used in device design process is computer modelling. The peculiarities of A^{III}–N heterostructures computer modelling are discussed in this paper.

2. Piezoelectric effect and spontaneous polarization in A^{III}–N

The fabricated heterostructures usually consist of epitaxial layers made of materials which have different bulk crystalline cell sizes. In this case the crystalline cell of epitaxial layer is deformed. If the thickness of grown layer is lower than the critical thickness, then the layer is strained. In other case the strain is relaxed.

The strain in piezoelectric material causes the piezoelectric effect that is inducing a static charge at the layer boundaries which sheet density equals to the piezoelectric polarization P_{PI}:

$$P_{PI} = 2\frac{a - a_0}{a_0}\left(e_{31} - e_{33}\frac{c_{13}}{c_{33}}\right)$$

where: a – strained layer lateral cell size, a_0 – bulk lateral cell size, e_{ij} – piezoelectric constants, c_{ij} – elasticity factors.

The A^{III}–N materials are ionic crystals with hexagonal wurzite crystalline structure (Fig. 1).

Epitaxial layers are grown in $\langle 0001 \rangle$ or $\langle 000{-}1 \rangle$ orientation. However, the proportions of crystalline cell size differ from the ideal wurzite. It causes that the centres of positive and negative charges in crystalline cell are located in different places and the cell itself is an electric dipole and the crystal exhibits strong spontaneous polarization. This phenomenon has been predicted by simulations [3] and proved experimentally [5]. The calculated values of piezoelectric and spontaneous polarizations in fully strained AlGaN layer are shown in Fig. 2**a**.

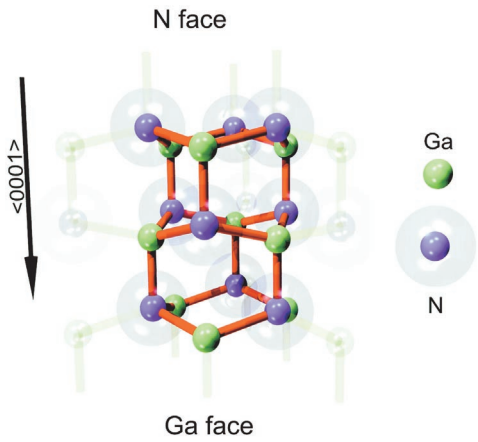

Fig. 1. GaN crystalline cell structure.

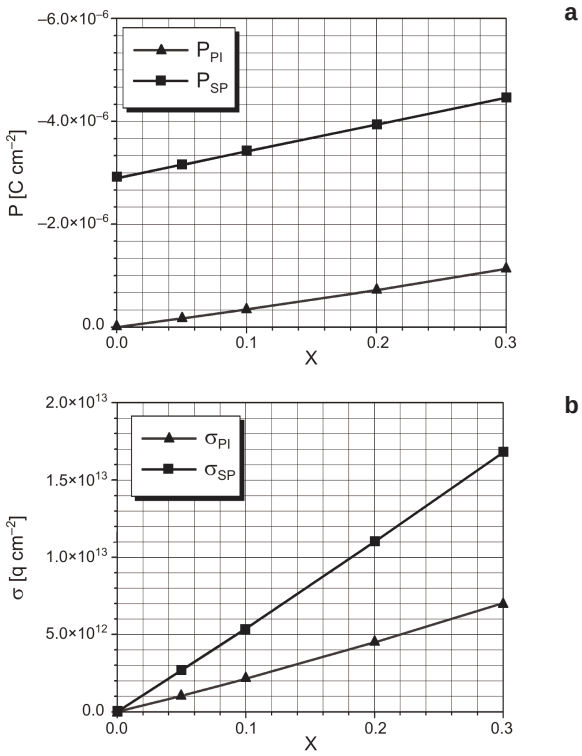

Fig. 2. Calculated values of polarization in strained $Al_xGa_{1-x}N$ layer (**a**); sheet charge density at $Al_xGa_{1-x}N$/GaN interface for different aluminium content x (**b**).

Spontaneous polarization in A^{III}–N materials results in the induction of static charges at the device structure boundaries and at the heterojunctions [6]. The sheet charge density caused by spontaneous polarization at the heterjuncjtions is equal to the difference between spontaneous polarization of neighbouring materials. Calculated values of sheet charge concentrations caused by both effects at strained $Al_xGa_{1-x}N$/GaN heterointerface are shown in Fig. 2**b**. Sheet charge concentrations are of the same order of magnitude as expected 2DEG sheet concentration and these charges have to be taken into account in A^{III}–N heterostructures modelling.

3. Influence of layer polarity on heterostructure properties

The crystalline cell of A^{III}–N materials, GaN for instance (Fig. 1), is asymmetric along $\langle 0001 \rangle$ direction. The 3rd and 5th group atoms are located at different planes. If the growth direction of heterostructure layers is the same as $\langle 000\text{–}1 \rangle$ direction the heterostructure is called N-faced, otherwise it is called Ga-faced. The polarization vector is oriented in the $\langle 0001 \rangle$ direction. As shown in Fig. 2**a** in AlGaN layer both piezoelectric and spontaneous polarization have negative value.

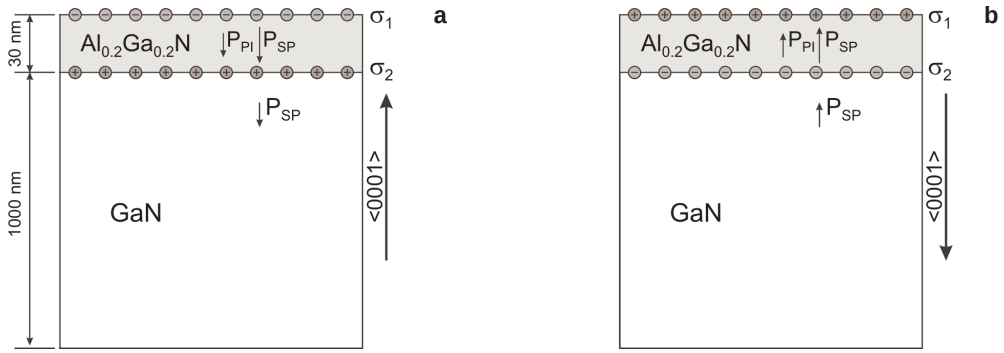

Fig. 3. Modelled N-faced (**a**) and Ga-faced (**b**) $Al_xGa_{1-x}N/GaN$ heterostructures.

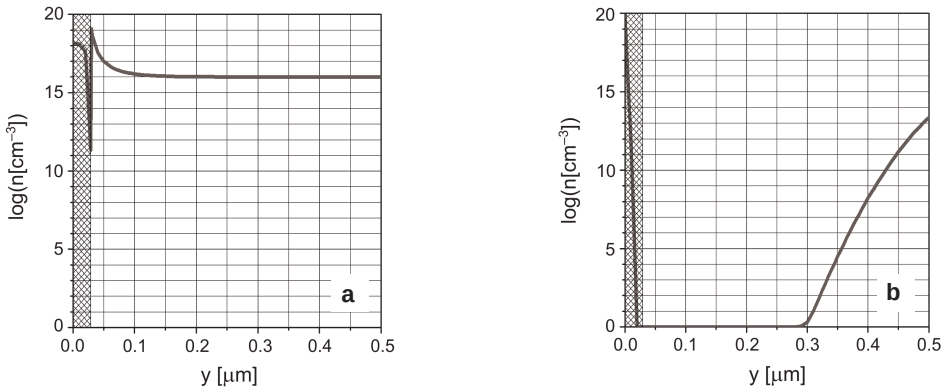

Fig. 4. Electron concentration in modelled heterostructures: Ga-faced (**a**), N-faced (**b**) [8].

The Ga- and N-faced $Al_xGa_{1-x}N/GaN$ heterostructures were simulated using elaborated software [7] (see Fig. 3).

$Al_xGa_{1-x}N$ layer was assumed to be fully strained. The directions of polarization vectors and static charge at the $Al_xGa_{1-x}N$ layer boundaries are shown. The carrier distribution across heterostructures is shown in Fig. 4. At the Ga-faced AlGaN/GaN heterojunction there is 2DEG with high sheet concentration (Fig. 4**a**). In N-faced heterostructure there is no 2DEG and the undoped GaN layer is depleted (Fig. 4**b**).

4. Polarization effect on 2DEG sheet concentration in AlGaN/GaN heterostructure

The simple model of strained $Al_xGa_{1-x}N$ layer relaxation in $Al_xGa_{1-x}N/GaN$ heterostructure was introduced in simulation software. Layers thicker than the critical thickness were simulated as fully relaxed with no piezoelectric polarization, otherwise

the layer was treated as fully strained. The series of simulations were performed for $Al_xGa_{1-x}N$/GaN heterostructures differing in aluminium content in $Al_xGa_{1-x}N$ layer and $Al_xGa_{1-x}N$ layer thickness. The sheet carrier concentration in 2DEG formed below the heterojunction was calculated. Results are shown in Fig. 5.

Higher aluminium content in $Al_xGa_{1-x}N$ layer increased 2DEG sheet electron concentration. As the aluminium content in $Al_xGa_{1-x}N$ of certain thickness layer increases, the strain relaxation may occur causing rapid decrease of 2DEG sheet electron concentration. However, due to spontaneous polarization, the 2DEG sheet electron concentration in relaxed layer was still high – about 30% lower than in strained layer of similar aluminium content. The $Al_xGa_{1-x}N$ layer does not have to be intentionally doped to reach high 2DEG sheet concentration. In wide range of

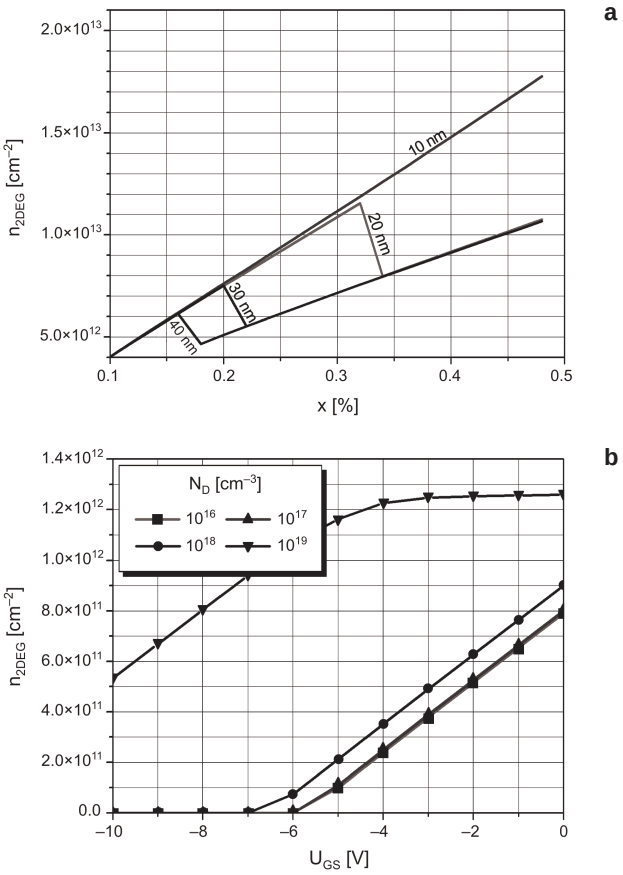

Fig. 5. 2DEG sheet concentration in $Al_xGa_{1-x}N$/GaN heterostructure dependence on: $Al_xGa_{1-x}N$ layer thickness and aluminium content (**a**), $Al_xGa_{1-x}N$ electron concentration and Schottky gate bias voltage (**b**).

concentrations its dependence on gate bias voltage does not change. Even undoped $Al_xGa_{1-x}N$ layers may be used due to "piezoelectric doping" phenomenon [9].

5. Influence of strained AlGaN interlayer on carrier concentration in GaN buffer

One of major obstacles in using A^{III}–N materials in microelectronic devices is the impossibility of depositing semi-insulating GaN epitaxial layers. In HFET transistor a semi-insulating GaN buffer layer should be used to minimize parasitic leakage currents flow through buffer layer.

A method of lowering carrier concentration in GaN buffer layer by introducing a strained 20 nm $Al_{0.1}Ga_{0.9}N$ interlayer into GaN buffer (Fig. 6**a**) was investigated. The static charge at the boundaries of interlayer causes depleting of the GaN layer

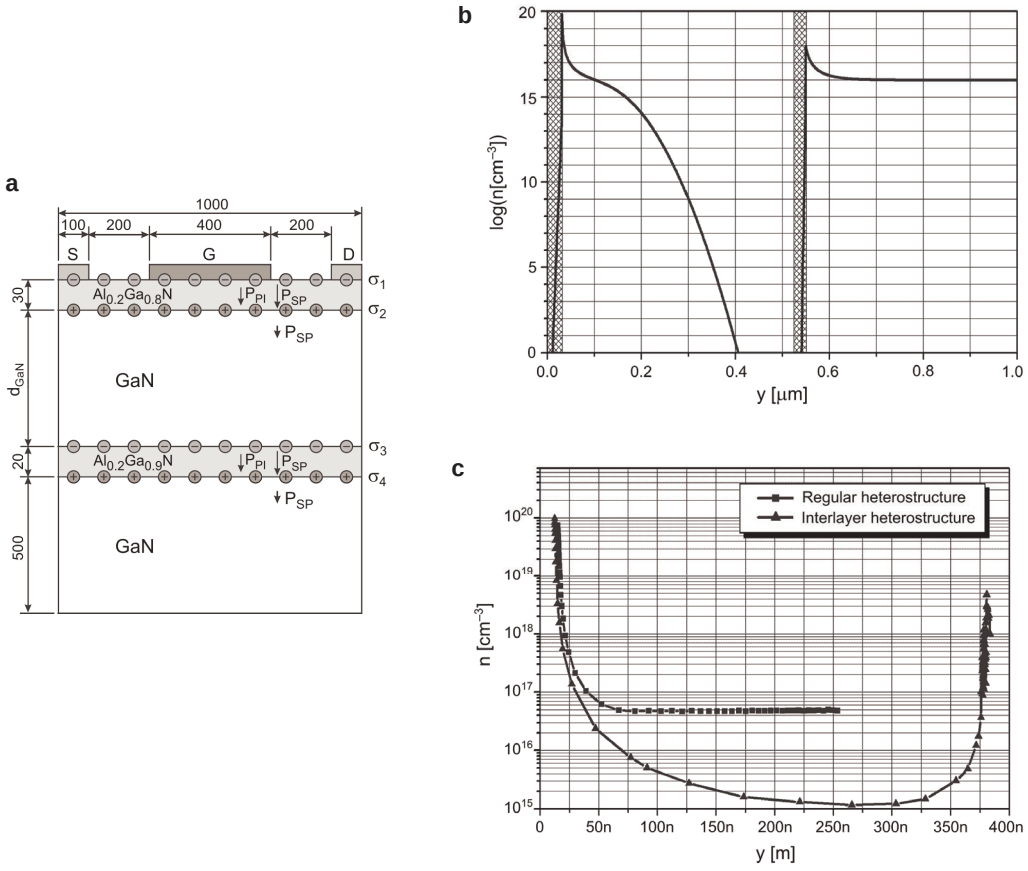

Fig. 6. HFET heterostructure with strained $Al_{0.1}Ga_{0.9}N$ interlayer: schematic overview (**a**), simulated electron concentration across heterostructure (**b**), *C-V* measurements of regular and interlayer HFET heterostructure (**c**).

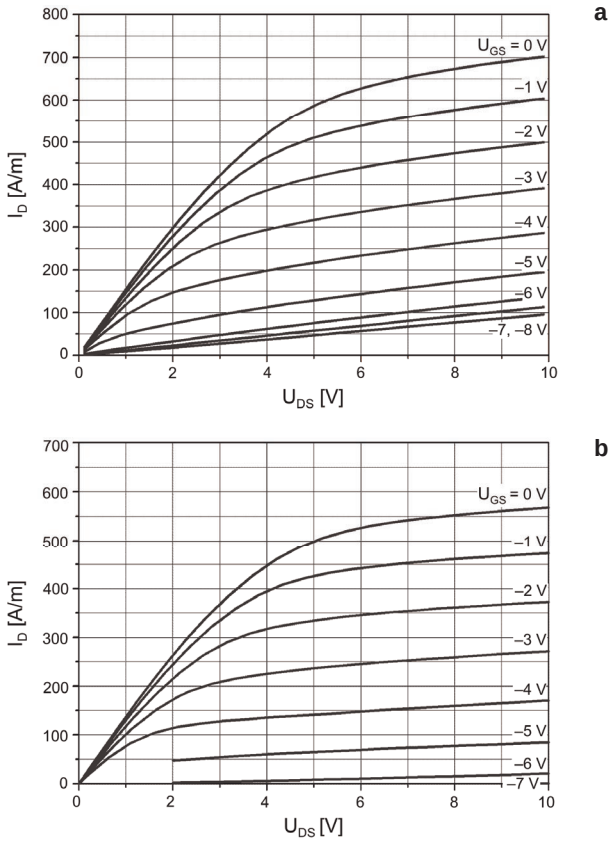

Fig. 7. Simulated output *I-U* characteristic of HFET: regular (**a**), with $Al_{0.1}Ga_{0.9}N$ interlayer (**b**).

above in similar way as in N-faced AlGaN/GaN heterostructure presented earlier in Fig. 4**b**. Heterostructure was simulated. The electron distribution across simulated heterostructure is shown in Fig. 6**b**. Interlayer heterostructure was fabricated and compared with regular HFET heterostructure grown at the similar conditions by *C-V* measurements (Fig. 6**c**).

Simulation showed that the depletion of GaN layer above the interlayer reached the 2DEG area causing the GaN layer below the 2DEG to be less conductive. This should limit the parasitic current. Below the interlayer the second 2DEG area was formed. It may be used in two-channel HFET to increase source–drain current in high power applications [10]. *C-V* measurements of interlayer heterostructure confirmed that electron concentration above the interlayer is lowered in comparison with the traditional heterostructure.

A 2D simulation of HFET based on heterostructure with AlGaN interlayer was performed using APSYS software. In a simulated device the source and drain contact were not connected to the second 2DEG area below the $Al_{0.1}Ga_{0.9}N$ interlayer. The output *I-U* characteristic of regular and interlayer HFETs are presented in Fig. 7.

Introducing of strained AlGaN interlayer caused great improvement in DC *I-U* characteristic. The parasitic source–drain current noticeable at high gate bias in regular HFET heterostructure was reduced. The modified HFET transistor allows the complete source–drain current cut-off at –7 V gate bias.

6. Conclusions

The spontaneous polarization and piezoelectric effect in A^{III}–N heterostructures have significant influence on A^{III}–N microelectronic devices performance and should not be ignored in device designing and modelling. The layer polarity is important as it has great influence on carrier distribution within heterostructure. These phenomena may be utilized to reduce the significance of A^{III}–N materials drawbacks such as lack of semi-insulating layers.

Acknowledgements – This work was supported partially by Polish State Committee for Scientific Research in Grant 4T11B 012 23 and Wrocław University of Technology (Poland) statutory grant.

References

[1] SHUR M., GELMONT B., KHAN M.A., *Electron mobility in two-dimensional electron gas in AlGaN/GaN heterostructures and in bulk GaN*, Journal of Electronic Materials **25**(5), 1996, pp. 777–85.

[2] SHUR M.S., KHAN A., GELMONT B., TREW R.J., SHIN M.W., *GaN/AlGaN field effect transistors for high temperature applications*, [In] *Compound Semiconductors 1994. Proceedings of the Twenty First International Symposium*, 1995, pp. 419–24.

[3] BERNARDINI F., FIORENTINI V., VANDERBILT D., *Spontaneous polarization and piezoelectric constants of III-V nitrides*, Physical Review B: Condensed Matter **56**(16), 1997, pp. R10024–7.

[4] BERNARDINI F., FIORENTINI V., *Polarization fields in nitride nanostructures: 10 points to think about*, Applied Surface Science **166**, 2000, pp. 23–9.

[5] DRABIŃSKA A., KORONA K.P., BOŻEK R., BARANOWSKI J.M., PAKUŁA K., TOMASZEWICZ T., GRONKOWSKI J., *Investigation of 2D electron gas on AlGaN/GaN interface by electroreflectance*, Physica Status Solidi C: Conferences and Critical Reviews **0**(1), 2002, pp. 329–33.

[6] AMBACHER O., SMART J., SHEALY J.R., WEIMANN N.G., CHU K., MURPHY M., SCHAFF W.J., EASTMAN L.F., DIMITROV R., WITTMER L., STUTZMANN M., RIEGER W., HILSENBECK J., *Two-dimensional electron gases induced by spontaneous and piezoelectric polarization charges in N- and Ga-face AlGaN/GaN heterostructures*, Journal od Applied Physics **85**(6), 1999, pp. 3222–33.

[7] PIASECKI T., PASZKIEWICZ B., PASZKIEWICZ R., TŁACZAŁA M., *FDM Modelling of Wurzite AIII–N Heterostructures for HFET Fabrication*, [In] *Proceedings Thermal Problems in Electronics Microtherm 2005*, Łódź, Poland, June 19–22, 2005, pp. 113–8.

[8] PIASECKI T., KOŚNIKOWSKI W., *Komputerowe modelowanie przyrządów opartych na heterostrukturze AlGaN/GaN/Al_2O_3*, Elektronika 2-3, 2005, p. 50 (in Polish).

[9] SHUR M.S., BYKHOVSKI A.D., GASKA R., *Two-dimensional hole gas induced by piezoelectric and pyroelectric charges*, Solid-State Electronics **44**(2), 2000, pp. 205–10.

[10] GASKA R., SHUR M.S., FJELDLY T.A., BYKHOVSKI A., *Two-channel AlGaN/GaN heterostructure field effect transistor for high power applications*, Journal of Applied Physics **85**(5), 1999, pp. 3009–11.

Received June 6, 2005