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Schottky Barrier Dependent 2DEG Model for GaN/AlInGaN/AlN/GaN Heterostructure

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Abstract

In this paper we present analytical model for two-dimensional electron gas (2DEG) and surface barrier height (SBH) in GaN/AlInGaN/AlN/GaN heterostructure. An analytical expression for 2DEG charge density n_s has been derived which is dependent on thickness of AlInGaN and GaN cap layers of heterostructure and mole fraction of Al and In. We have also shown the effect of mole fraction variation on n_s and SBH. The model has excellent agreement with experiment data available in literature for given mole fraction and thickness of layers. This makes the model to be a useful tool in advance design and characterization of GaN/AlInGaN/AlN/GaN heterostructure.

Keywords

GaN/AlInGaN/AlN/GaN heterostructure, Nanomaterials, Nanotechnology, Surface barrier height, 2DEG

Introduction

III-V compound semiconductor devices are mainly based on alloys of the components GaN, InN and AlN. Most of the work in conventional nitride research and technology is based on binary and ternary compound semiconductor, now the use of quaternary material is recommended. It is a new type of material that opens additional possibilities for materials engineering. The performance of AlGaN/GaN HEMT is mainly due to high mobility 2DEG at the heterointerface. AlGaN/GaN has potential application in the field of high frequency and high-power electronic devices because of the strong piezoelectric and spontaneous polarization and high density 2DEG between AlGaN and GaN junction. With increase in Al mole fraction, there is increase in current carrying capability of devices, higher polarization charge and larger band offset at the heterointerface and higher current-carrying capability of the devices [1]. High Al content in AlGaN/GaN HFETs causes the change in system properties. For high content of Al, large lattice mismatch occurs between AlGaN and GaN. Due to this large lattice mismatch the critical thickness of a fully strained AlGaN barrier is decreased. As a result, the uncontrolled local strain relaxation occurs at the heterointerface, due to generation of misfit dislocations and causes cracks. High Al composition also increase electron scattering reducing the hall mobility. These degrade 2DEG transport and increase noise. In literature, it is mentioned that introduction of AlN layer at the AlGaN/GaN interface increases the carrier density and effectively reduces the alloy scattering of 2DEG and provides better carrier confinement. Some studies suggest using an alternative of AlGaN layer. One of them is use of AlInN layer instead of AlGaN as proposed by Kuzmik [2]. The AlInN growth suffers from miscibility gap in the AlN-InN phase diagram

which reduces the hall mobility due to alloy scattering and increased roughness [3]. Due these problems in ternary alloy more research is going on quaternary AlInGaN alloy [4-11].

To resolve the problem of lattice mismatch in heterostructure we can adjust lattice parameter by varying the composition of AlInGaN. It is found in literature that using lattice matched AlInN/GaN heterostructure with In composition 18%, provides higher 2DEG. Lattice parameter and energy band gap can be independently controlled by varying the In and Al compositions in quaternary $Al_xIn_yGa_{1-x-y}N$ alloys.

It is a challenge to realize the enhancement-mode GaN-transistor due to the presence of large polarization sheet charge density at AlGaN/GaN heterointerface. One of the solutions of this problem is use lattice matched quaternary AlInGaN layer in place of ternary layer because it has low spontaneous polarization mismatch to GaN. Low strain at heterostructure will also improve the long-term reliability of device with positive threshold voltage of about 2 V [5, 6].

Compound semiconductors and nanomaterials are interconnected in several ways due to their unique properties and applications at the nanoscale. Compound semiconductors can be engineered at the nanoscale to create nanostructures like quantum dots, nanowires, and nanorods. These nanostructures exhibit novel electronic, optical, and magnetic properties due to quantum confinement effects, surface states, and size quantization. This manipulation at the nanoscale often enhances the performance of semiconductor devices compared to their bulk counterparts. Nanomaterials derived from compound semiconductors offer tuneable properties due to their size and shape. By controlling the size and shape of nanoparticles or nanostructures, researchers can fine-tune characteristics such as bandgap, conductivity, photoluminescence, and catalytic activity [12]. AlGaN/GaN heterostructures are highly relevant to nanoscience and nanotechnology due to their unique properties and various applications at the nanoscale. AlGaN/GaN heterostructures can be engineered at the nanoscale to create advanced electronic and optoelectronic devices. Nanofabrication techniques enable the creation of nanosized transistors, HEMTs, and nanowire-based devices using these heterostructures. The nanoscale dimensions significantly impact the performance and functionality of these devices. AlGaN/GaN heterostructures can contribute to nanotechnology-driven advancements in energy-related devices. For instance, nanoscale engineering of these structures can enhance the performance of nanoscale photovoltaic devices, light-emitting diodes for energy-efficient lighting, and nanoscale sensors for energy harvesting or storage applications [13].

The quaternary compound semiconductor has number of advantages over ternary compound semiconductor. Use of quaternary AlInGaN barrier layer in nitride HEFTs started about fifteen years ago but recently some quaternary devices realized which have better performance [10, 11], especially for ultraviolet light emitting diodes [14] and radio-frequency high-power transistors [15-18]. When cap layer is placed on top of the AlGaN/GaN structure, the band diagram and properties change drastically. The value of 2DEG electron concentration ns reduces with increase in thickness of GaN cap layer. Various properties of AlInGaN/AlN/GaN heterostructure have been investigated such as sheet density, hall mobility, etc.

In the present work, we present analytical model for the heterostructure GaN/AlInGaN/AlN/GaN by combining the advantages of quaternary and AlN spacer layer. In our model we have replaced the ternary compound semiconductor with quaternary compound semiconductor, and we put an AlN spacer to reduce the scattering losses. The model shows the effect of GaN cap layer on AlInGaN/AlN/GaN structure (Table 1).

Experimentation

Band diagram

The schematic energy band diagram of the GaN/AlInGaN/AlN/GaN heterostructure is shown in figure 1. Band diagram of any structure is determined by several important factors such as doping effect in the unintentionally doped GaN/AlInGaN/AlN/GaN system, piezoelectric and spontaneous polarization and existence of surface states related to vacancy-impurity complex of the material. There is a reduction in polarization effect compared to AlGaN/GaN structure [10]. In AlGaN/GaN heterostructure, if the mole faction of Al increases, there is problem of lattice mismatch between AlGaN and GaN. If in the AlInGaN/GaN structure

Table 1: Parameter list.

Parameter	Symbol	Unit
Fundamental charge	Q	C
AlInGaN piezoelectric charge density	$q.\sigma$	C/cm^2
Dielectric permittivity	E	F/cm
2DEG electron concentration	n_s	cm^{-2}
SBH	$q.\varphi_B$	eV
Difference between the Fermi level and CB minimum at the GaN heterointerface	E_F	eV
CB offset	ΔE_c	eV
Surface donor level the top	Ed	eV
Constant surface donor density	n_0	$cm^{-2}eV^{-1}$

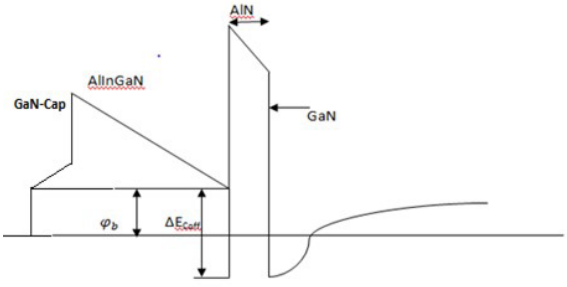

Figure 1: Conduction band diagram of the AlInGaN/AlN/GaN heterostructure.

we keep the Al mole faction constant and increase the In mole faction, the tensile strain in barrier-layer decreases and eventually turns into a compressive strain (decrease in piezoelectric polarization) while spontaneous polarization remain constant. As a result, total polarization is reduced.

Theoretical modeling

Polarization sheet carrier concentration

σ_{pz} is polarization induced charge density in tensile-strained GaN/AlInGaN/AlN/GaN heterostructure is dependent on the degree of polarization (piezoelectric and spontaneous) and tends to increase with the increase in the composition of Al [4]. The total polarization and the corresponding sheet carrier density increases with the increase in strain and decreases with increasing degree of relaxation in heterostructure [10]. To determine the amount of polarization-induced charge density σ_{pz} at the $Al_xIn_yGa_{1-x-y}N$/AlN/GaN interface, the following set of linear interpolation based on the physical properties of AlN, InN and GaN were used:

The lattice constant of the $Al_xIn_yGa_{1-x-y}N$ alloy:

$$a_{Al_xIn_yGa_{1-x-y}N} = 3.548y + 3.112x + 3.189(1-x-y)\,\text{Å} \quad (1)$$

Piezoelectric constants:

$$e_{31} = -0.36(1-x-y) - 0.57x - 0.58y\ \text{C/m}^2 \quad (2)$$

$$e_{33} = -0.36(1-x-y) - 1.55x - 0.97y\ \text{C/m}^2 \quad (3)$$

Elastic constants:

$$C_{13} = 99x + 94y + 158(1-x-y)\ \text{GPa} \quad (4)$$

$$C_{33} = 389x + 200y + 267(1-x-y)\ \text{GPa} \quad (5)$$

The piezoelectric polarization in the C-axis due to tensile strain in the $Al_xIn_yGa_{1-x-y}N$ epilayer is given by:

$$P_{pzAlInGaN} = 2\frac{a_{GaN} - a_{AlInGaN}}{a_{AlInGaN}}\left(e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right) \quad (6)$$

$$P_{pz}(AlN) = \left(-1.808\eta - 7.888\eta^2\right) \quad (7)$$

$$P_{sp}(AlN) = -0.0898 \quad (8)$$

$$P_{AlN} = P_{pz}(AlN) + P_{sp}(AlN) \quad (9)$$

Where η is:

$$\eta = \frac{x(a_{GaN} - a_{AlN}) + y(a_{GaN} - a_{InN})}{xa_{AlN} + ya_{InN} + a_{GaN}(1-x-y)} \quad (10)$$

The spontaneous polarization between AlInGaN and GaN can be written as:

$$P_{spAlInGaN} = P_{sp}\left(Al_xIn_yGa_{1-x-y}N\right) - P_{sp}(GaN) \quad (11)$$

$= -0.52x + 0.003y - 0.029\ \text{C/m}^2$

$$P_{AlInGaN} = P_{spAlInGaN} + P_{pzAlInGaN}$$

Using equation 7 and equation 8, the amount of polarization-induced sheet charge density at the $Al_xIn_yGa_{1-x-y}N$/GaN interface can be expressed as:

$$\left|\sigma_{pz}\right| = \left|P_{pe}\left(Al_xIn_yGa_{1-x-y}N\right) + P_{sp}\left(Al_xIn_yGa_{1-x-y}N\right) - P_{GaN} - P_{AlN}\right| \quad (12)$$

Sheet carrier concentration

Analyzing the electric field within the GaN cap layer, the influence of the Fermi level (E_F) can be disregarded as it is typically much smaller than other significant quantities such as the electric field itself. This simplification is justified based on the observation that E_F is on the order of a few thermal voltage values K_BT [7]. From the electrostatic analysis, one can write $E_2 = \frac{q\phi_B + E_1 d_{cap,GaN}}{d_{AlInGaN+AlN}}$, as shown in figure 1. To maintain the continuity of displacement at the GaN/AlInGaN interface E_1 and E_2 must be related as $\varepsilon E_2 = q\sigma - \varepsilon E_1$. At the AlInGaN/GaN interface, one can also write $E_2 = \frac{q(\sigma - n_s)}{\varepsilon}$. Combining these equations, one can arrive at the electron concentration (as function of $q\phi_B$):

$$n_s = \frac{\sigma_{pz} - \frac{q\phi_B\varepsilon}{qd_{AlInGaN+AlN}}}{1 + \frac{d_{cap,GaN}}{d_{AlInGaN+AlN}}} \quad (13)$$

There is a balance between the constant surface donor density (n_0) and the occupation of donor states above the Fermi level, indicating that the donor impurities near the surface have fully occupied. A constant surface donor density (n_0) below the donor level (E_d) at the GaN cap top equals to the number of empty donor surface state above the Fermi level. This must be equal to the 2DEG concentration, $n_s = n_0(q\phi_B - E_d)$ [19]. Therefore, one can arrive to below mentioned analytical expression for n_s:

$$n_s = \frac{n_0\left(\frac{\sigma d_{AlInGaN+AlN}}{\varepsilon} - \frac{E_d}{q}\right)}{\frac{1}{q} + \frac{n_0\left(d_{cap,GaN} + d_{AlInGaN+AlN}\right)}{\varepsilon}} \quad (14)$$

According to equation 14, the 2DEG density must monotonically decrease with increasing cap layer thickness d_{GaN}. It is given in literature for ternary alloy that value of n_s saturate for higher value of cap thickness. The expression for the SBH as analytically obtained is shown below. SBH decreases with increasing $d_{cap,GaN}$.

$$q\phi_B = \frac{n_0E_d\left(d_{cap,GaN} + d_{AlInGaN+AlN}\right) + \sigma d_{AlInGaN+AlN}}{n_0\left(d_{cap,GaN} + d_{AlInGaN+AlN}\right) + \frac{\varepsilon}{q}} \quad (15)$$

Results and Discussion

In this paper we studied the relationship between the sheet charge density (n_s) and SBH by varying different parameter such as thickness of AlInGaN, GaN cap thickness and mole fraction of Al and In. Value n_0 and E_d are linearly

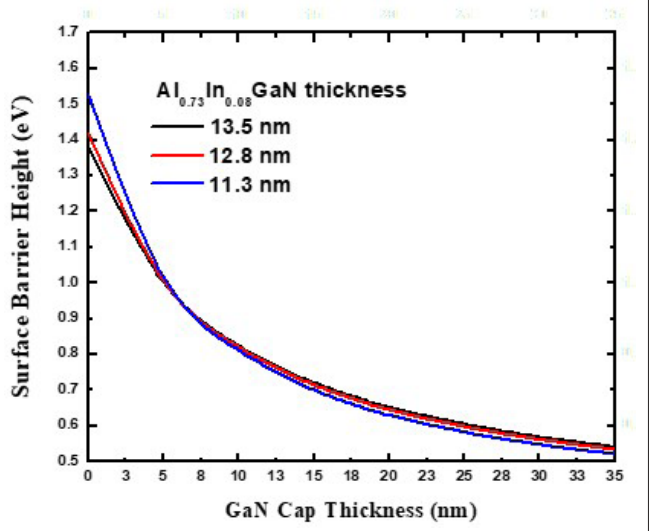

Figure 2: Variation of the SBH with the GaN cap thickness for different $Al_{0.73}In_{0.08}GaN$ thickness.

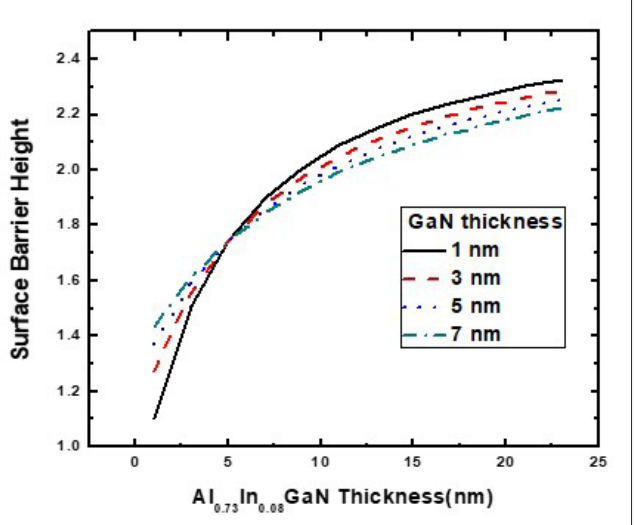

Figure 3: Variation of SBH with the $Al_{0.73}In_{0.08}GaN$ barrier thickness for different GaN cap layer thickness.

related to the mole fraction of Al given by Goyal et al. for ternary alloy [20]. By matching with the experimental data, we derived the relation of n_0 and E_d with mole fraction of Al and In. It is given by $n_0 = (2.9\ x - y - 0.893)10^{13}$ $cm^{-2}eV^{-1}$ and $E_d = 0.2x + 0.04y + 0.42$ in eV. As given in the literature, and our observation, the values of n_0 and E_d are not affected by thickness of layers. Figure 2 shows the variation of SBH with GaN cap thickness for different values of AlInGaN, it is noted that variation in SBH mostly depends on the GaN cap thickness and only slightly varies with AlInGaN thickness d1. The Al mole fraction is taken here as 0.66 and In mole fraction as 0.14. Figure 2 shows that SBH decreases with increase in GaN thickness. To the best of our knowledge, no experimental data is available for the SBH in GaN/AlInGaN/AlN/GaN heterostructure in the literature. Theoretically, we can conclude that the value of SBH approaches zero as the thickness of GaN increases. We note that for lower thickness of AlInGaN, sheet charge density n_s in higher. As shown in figure 3 our modeled SBH varies with AlInGaN thickness and with different values of GaN thickness. As AlInGaN thickness increases, the span of SBH decreases.

In figure 4, we compare our model for GaN/AlInGaN/AlN/GaN structure with experimental data on n_s obtained by hall measurement conducted with different thickness cap layer by Chen et al. [21]. Figure 5 shows the the modeled value of n_s with change in GaN thickness for different values of AlInGaN thickness for Al mole fraction x = 0.73, In mole fraction y = 0.08. It shows that as cap thickness increases, the value of n_s decreases. In this case, we used model parameters n_0 and E_d. The model can match experimental result quite well. Figure 6 shows the modelled value of n_s for variation in mole faction of In and Al respectively when thicknesses of GaN and AlInGaN are kept constant. The incorporation of In reduces the 2D electron density n_s in this structure. There is small change in n_s with In mole fraction when all other parameters kept constant. In figure 6, effect of Al mole fraction on n_s is shown, as value of Al mole fraction increases the value of n_s is also

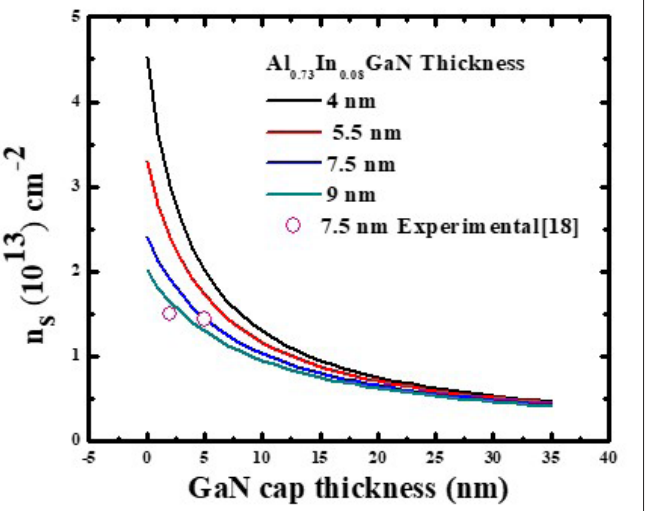

Figure 4: The modeled 2DEG value of the GaN/AlInGaN/AlN/GaN heterostructure is shown. The values of 2DEG experimental points reported in [19] (for Al mole fraction x = 0.73, In mole fraction y = 0.08 and GaN cap thickness = 2 nm and thickness = 5 nm).

increased. Effect of Al mole fraction is more as compared to the In mole fraction. If mole fraction of Al is higher, then the value of n_s increases with increase in mole fraction of In.

Conclusion

As per our knowledge this is first attempt to present theoretical model for GaN/AlInGaN/AlN/GaN structure. We have provided a model for AlInGaN/AlN/GaN structure with GaN cap layer. It is physics-based model and explains the effect of cap layer on 2DEG density and SBH. With cap layer there is a variation in n_s value with the thickness AlInGaN as shown in results. Our model explains the effect of mole fraction variation of Al and In and thickness of the AlInGaN and AlN layer on 2DEG. We have compared our data with experimental result. The proposed model agrees well with experiment data. Mole fraction on Al and In also

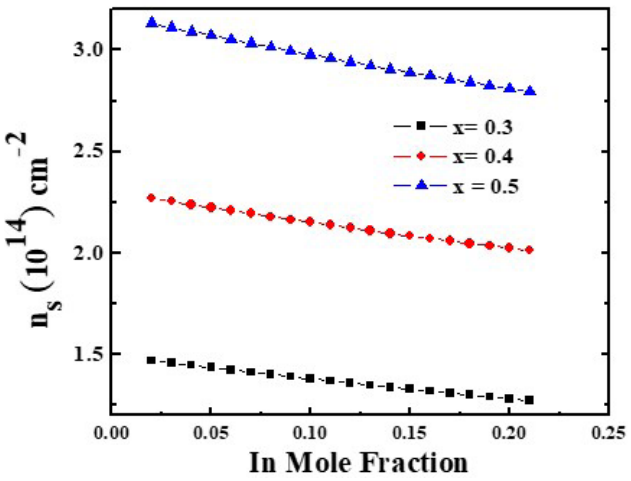

Figure 5: Variation in sheet charge density n_s with change in In mole fraction with different values of Al mole fraction and thickness of cap layer = 2 nm and AlInGaN layer = 7.5 nm.

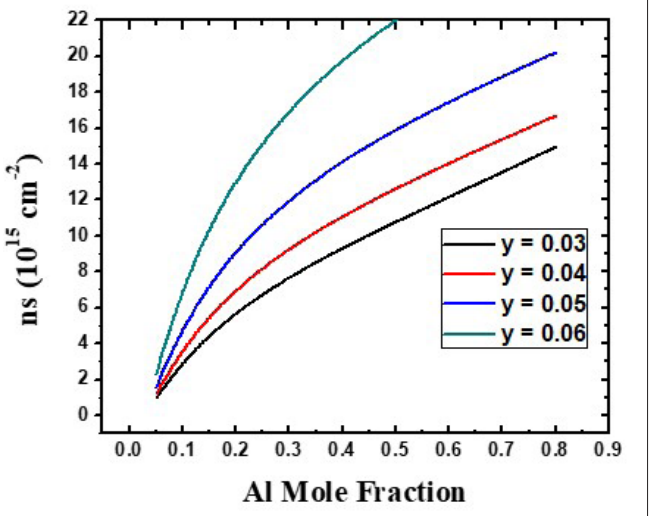

Figure 6: Variation of value of n_s with change in Al mole fraction for different value of In mole fraction and thickness of cap layer = 2 nm and AlInGaN layer = 7.5 nm.

effect on various electrical characteristic of GaN/AlInGaN/AlN/GaN heterostructure. According to our model, effect of variation in In mole fraction is higher than variation in mole fraction of Al. Nanotechnology has opened avenues for diverse applications across scientific domains. Expanding on studies that delve into the properties of nanomaterials, this research presents promising opportunities for deeper exploration in nanotechnology field.

Acknowledgments

None.

Conflict of Interest

None.

References

1. Khan MA, Yang JW, Simin G, Gaska R, Shur MS, et al. 2000. Lattice and energy band engineering in AlInGaN/GaN heterostructures. *Appl Phys Lett* 76(9): 1161-1163. https://doi.org/10.1063/1.125970
2. Kuzmík J. 2001. Power electronics on InAlN/(In) GaN: prospect for a record performance. *IEEE Electron Device Lett* 22(11): 510-512. https://doi.org/10.1109/55.962646
3. Wang J, Sun LL, Liu J, Zhou MZ. 2013. A surface-potential-based model for AlGaN/AlN/GaN HEMT[J]. *J Semicond* 34(9): 094002. https://doi.org/10.1088/1674-4926/34/9/094002
4. Ketteniss N, Khoshroo LR, Eickelkamp M, Heuken M, Kalisch H, et al. 2010. Study on quaternary AlInGaN/GaN HFETs grown on sapphire substrates. *Semicond Sci Technol* 25(7): 075013. https://doi.org/10.1088/0268-1242/25/7/075013
5. Ahl JP, Hertkorn J, Koch H, Galler B, Michel B, et al. 2014. Morphology, growth mode and indium incorporation of MOVPE grown InGaN and AlInGaN: a comparison. *J Cryst Growth* 398: 33-39. https://doi.org/10.1016/j.jcrysgro.2014.03.043
6. Liu Y, Egawa T, Jiang H. 2006. Enhancement-mode quaternary AlInGaN/GaN HEMT with non-recessed-gate on sapphire substrate. *Electron Lett* 42(15): 884-886. https://doi.org/10.1049/el:20061150
7. Goyal N, Iñiguez B, Fjeldly TA. 2012. Analytical modeling of bare surface barrier height and charge density in AlGaN/GaN heterostructures. *Appl Phys Lett* 101(10): 103505. https://doi.org/10.1063/1.4751859
8. Reuters B, Hahn H, Pooth A, Holländer B, Breuer U, et al. 2014. Fabrication of p-channel heterostructure field effect transistors with polarization-induced two-dimensional hole gases at metal-polar GaN/AlInGaN interfaces. *J Phys D Appl Phys* 47(17): 175103. https://doi.org/10.1088/0022-3727/47/17/175103
9. Reuters B, Wille A, Ketteniss N, Hahn H, Holländer B, et al. 2013. Polarization-engineered enhancement-mode high-electron-mobility transistors using quaternary AlInGaN barrier layers. *J Electron Mater* 42: 826-832. https://doi.org/10.1007/s11664-013-2473-7
10. Soh CB, Chua SJ, Tripathy S, Chow SY, Chi DZ, et al. 2005. Influence of composition pulling effect on the two-dimensional electron gas formed at $Al_yIn_xGa_{1-x-y}N$/GaN interface. *J Appl Phys* 98(10): 103704. https://doi.org/10.1063/1.2132090
11. Rahbardar Mojaver H, Manouchehri F, Valizadeh P. 2016. Theoretical evaluation of two-dimensional electron gas characteristics of quaternary $Al_xIn_yGa_{1-x-y}N$/GaN hetero-junctions. *J Appl Phys* 119(15): 154502. https://doi.org/10.1063/1.4946842
12. Xu X, Hou Y, Sun C, Wei Z, Wang, Y. 2013. Effect of surface area and surface area to volume ratio on the catalytic activity of CeO_2 nanoparticles. *J Nanosci Nanotechnol* 13(10): 6915-6920. https://doi.org/10.1166/jnn.2013.7859
13. Feng S, Li L, Liu H, Zhang X, Zhu D. 2010. Thermal conductivity of nanoparticle chain: a molecular dynamics study. *Nanosci Nanotechnol Lett* 2(2): 121-126.
14. Ghosh J, Ganguly S, Goyal N. 2016. Analytical modeling of 2DEG and surface barrier height in GaN/AlGaN/GaN heterostructures. In Proceedings of International Conference on Emerging Electronics, Mumbai, Maharashtra, India.
15. Muramoto Y, Kimura M, Nouda S.2014. Development and future of ultraviolet light-emitting diodes: UV-LED will replace the UV lamp. *Semicond Sci Technol* 29(8): 084004. https://doi.org/10.1088/0268-1242/29/8/084004
16. Lecourt F, Agboton A, Ketteniss N, Behmenburg H, Defrance N, et al. 2013. Power performance at 40 GHz on quaternary barrier InAlGaN/GaN HEMT. *IEEE Electron Device Lett* 34(8): 978-980. https://doi.org/10.1109/LED.2013.2266123

17. Kolbe T, Knauer A, Chua C, Yang Z, Kueller V, et al. 2011. Effect of temperature and strain on the optical polarization of (In)(Al) GaN ultraviolet light emitting diodes. *Appl Phys Lett* 99(26): 261105. https://doi.org/10.1063/1.3672209

18. Morales FM, Mánuel JM, García R, Reuters B, Kalisch H, et al. 2013. Evaluation of interpolations of InN, AlN and GaN lattice and elastic constants for their ternary and quaternary alloys. *J Phys D Appl Phys* 46(24): 245502. https://doi.org/10.1088/0022-3727/46/24/245502

19. Gordon L, Miao MS, Chowdhury S, Higashiwaki M, Mishra UK, et al. 2010. Distributed surface donor states and the two-dimensional electron gas at AlGaN/GaN heterojunctions. *J Phys D Appl Phys* 43(50): 505501. https://doi.org/10.1088/0022-3727/43/50/505501

20. Goyal N, Iñiguez B, Fjeldly TA. 2012. Analytical modeling of bare surface barrier height and charge density in AlGaN/GaN heterostructures. *Appl Phys Lett* 101: 103505. https://doi.org/10.1063/1.4751859

21. Chen HY, Tu PT, Yeh PC, Tzeng PJ, Sheu SS, et al. 2022. AlInGaN/GaN HEMTs with different GaN cap layer on low resistivity silicon substrate. In International Symposium on VLSI Technology, Systems and Applications. Hsinchu, Taiwan.