ATLANTIS PRESS

Advances in Computer Science Research, volume 58

Modeling, Simulation and Optimization Technologies and Applications (MSOTA 2016)

A Restrain Method of Polarization Effect in GaN/AlGaN RTD

Haipeng Zhang[1,2*], Xiliang Hao[1,2], Mi Lin[1], Xiang Ning[1], Bin Wang[1,2], Jian He[1,2] and Biao Han[1,2]

[1]Electronics and Information College, Hangzhou Dianzi University, Hangzhou, China, 310018

[2]Smart-City Research Center of Zhejiang Province, Hangzhou, China, 310018

[*]Corresponding author

Abstract—**Polarization effects and polarization charges on the interfaces between GaN and AlGaN in GaN/AlGaN RTD on c-plane GaN substrate destroy its RT conditions. To pave the way for electron transportation through GaN/AlGaN RTD in the mode of resonant tunneling, the influence from polarization effects was analyzed and a way to restrain it on the NDR characteristic was found. Since the polarization field is along the negative C crystal orientation, while the external applied field is orthogonal to the original crystal plane, the effective polarization field was modeled and device simulations of the polarization effects in GaN/AlGaN RTDs with different initial crystal planes of GaN substrates were carried out. The results indicate that to select an initial crystal plane of GaN substrate by increasing the c-plane drift angle from 0 to $\pi/2$ is very helpful to recover and enhance the RT conditions since it is capable of reducing effective polarization field, forming RT quantum state energy levels on both sides of potential barriers and improving electron transmission. Therefore, the crystal planes between $\{2\ \bar{2}\ 0\ 1\}$ and a-plane are optional as the initial crystal plane of GaN substrate for related power levels of related practical applications.**

Keywords-GaN/AlGaN; RTD; polarization effects; c-plane drift angle; NDR; low voltage

I. INTRODUCTION

Wide-band III-V compounds are one cluster of the most attractive semiconductors for the microelectronics, optoelectronics and power electronics industries. They are the optional materials for high frequency devices, high power devices, optoelectronic devices [1-11]. The main reason for this originates from their direct band gap tunable along a wide range of energies and that they appear higher electron mobility, thermal conductivity and wider band gap than silicon counterparts. With the development of III-Nitrides materials and devices, more and more attention are paid to the studies on GaN/AlGaN-based RTD (resonate tunneling diode) [7-10,12]. Resonant tunneling diodes (RTDs) which display a Negative Differential Resistance (NDR) are exploited in digital applications (Multi-Value Logic) as well as in analog applications (ADC, frequency divider or multiplier, oscillator), leading to simpler circuits, with a large gain in low power consumption and high frequency performance [7,8,10,12,13]. Generally, single crystal GaN exists in the form of wurtzite structure due to its relative higher thermal stability. However, in the wurtzite GaN based quantum well hetero-structures, resonate tunneling is not yet controlled due to strong polarization effects across the hetero-interfaces, which may block or cut off the vertical electronic transport in between conduction bands in RTDs devices. Ga cation center and N anion center do not overlap each other in GaN crystal of wurtzite structure, which leads to polarization effects and polarization charges on the interfaces between GaN and AlGaN in GaN/AlGaN RTD device. When the lattice constant and thermal expansion coefficient mismatch between GaN epitaxial layer and the substrate layer or buffer layer, deformation will be incurred in GaN epitaxial layers due to withstand stress (pressure, tensile stress), which breaks the covalent bonds and symmetry of atoms and changes the arrangement of the Ga cations and N anions, thus result in a piezoelectric polarization field. The polarization fields and charges are up to the orders of MV/cm and 1e13cm^{-2} respectively, which may generally destroys the RT conditions of GaN/AlGaN RTD [1-6, 9]. Only limited theoretical studies have been reported on AlGaN/GaN RTDs [7-10, 12, 13].

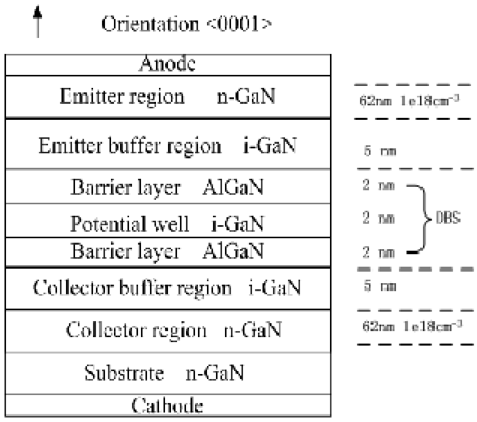

FIGURE I. CROSS SECTION VIEW OF GAN/ALGAN RTD

II. CONVENTIONAL GAN-BASED RTD STRUCTURE

Conventional GaN-based RTD consists of cathode, emitter region, DBS (Double Barriers) region, collector region and anode on a homogenous epitaxial GaN substrate along <0001> or $\langle 000\bar{1} \rangle$ direction. Its cross section view is illustrated as Figure Ⅰ. In the conventional GaN-based RTD structure, piezoelectric polarization only occurs across barrier layers while only spontaneous polarization occurs across other GaN layers. Assume the positive polarization orientation along

Copyright © 2016, the Authors. Published by Atlantis Press.
This is an open access article under the CC BY-NC license (http://creativecommons.org/licenses/by-nc/4.0/).

<0001> direction, which is reverse to the orientation of spontaneous polarization. However, the orientation of piezoelectric polarization depends on the property of stress the concerned material layer is beard [1].

III. POLARIZATION EFFECTS IN GAN/ALGAN RTD

The spontaneous polarization density of AlxGa1-xN (x is the composite of Al.) can be expressed as in [14]:

$$P_{SP}(Al_xGa_{1-x}N) = -0.09x - 0.034(1-x) + 0.019x(1-x). \tag{1}$$

Since its crystal lattice constant is less than that of GaN, it bears the tensile stress from the interface between AlGaN and GaN. Therefore the piezoelectric polarization orientation across AlGaN barrier layer is along $<000\bar{1}>$ direction, as can be seen in Figure II. Thus, the nonlinear piezoelectric polarization density of AlxGa1-xN can be expressed as in reference [14]:

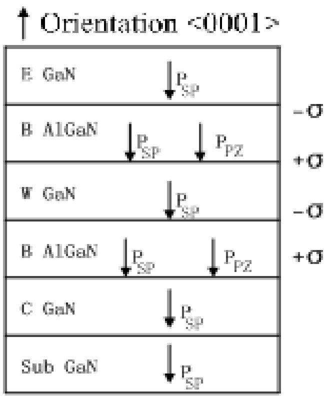

FIGURE II. DISTRIBUTION OF POLARIZATION DIRECTIONS AND CHARGES

$$P_{PZ}(Al_xGa_{1-x}N) = x\cdot P_{PZ}(AlN) + (1-x)\cdot P_{PZ}(GaN), \tag{2}$$

Where,

$$\begin{aligned} P_{PZ}(AlN) &= -1.808\cdot\varepsilon + 5.624\cdot\varepsilon^2, \varepsilon<0 \\ P_{PZ}(AlN) &= -1.808\cdot\varepsilon - 7.888\cdot\varepsilon^2, \varepsilon>0 \\ P_{PZ}(GaN) &= -0.918\cdot\varepsilon + 9.541\cdot\varepsilon^2 \end{aligned}, \tag{3}$$

Where the stress density of epitaxial layer 'ε' is a function of x with 'a' as corresponding crystal lattice constants in the term of subscribes and the crystal lattice constant of AlxGa1-xN is calculated according to the Vegard law.

$$\varepsilon(x) = \left[a_{sub} - a_{epi}(x)\right] / a_{epi}(x). \tag{4}$$

The total polarization effect can be characterized as the polarization charge sheet on the heterogeneous interface between AlGaN and GaN epitaxial layers in the term of bound polarization charge density on the interface [1] :

$$\sigma = \frac{1}{q}\left(P_{tot}^{+} - P_{tot}^{-}\right) = \frac{1}{q}\left[P_{SP}^{+} + P_{PZ}^{+} - \left(P_{SP}^{-} + P_{PZ}^{-}\right)\right]. \tag{5}$$

The bound polarization charge densities on GaN/AlGaN and AlGaN/GaN interfaces are calculated irrespectively at -1.38e13cm^{-2} and 1.38e13cm^{-2} with equations (1)-(5). Therefore, the polarization fields across the barrier layers are reverse to the external applied electric field, which destroys one of the resonate tunneling conditions and conceals the NDR characteristic of the RTD similar to that illustrated in Figure I. Its current-voltage characteristic curve is obtained by TCAD simulation and can be seen in Figure III indicated by "c-plane".

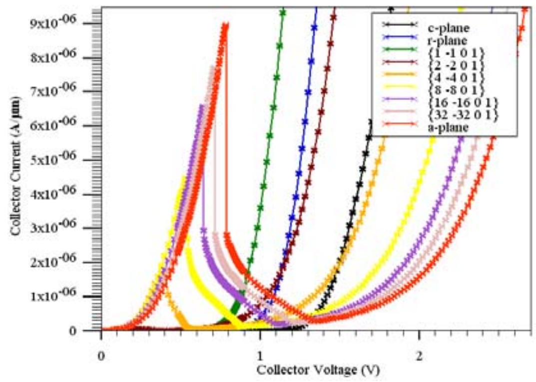

FIGURE III. CURRENT-VOLTAGE CHARACTERISTICS OF GAN/ ALGAN RTD

Assume that the orientation of the initial GaN substrate is an arbitrary crystal direction between c-direction and a-direction, and the angle between the arbitrary crystal direction and c-direction is 'α' and defined as c-plane drift angle, that is to say, 'α' lies in the plane that is defined by the crossing vectors of c-direction and a-direction. The polarization field is along c-direction while the external applied electric field is along the negative arbitrary crystal direction. That is to say the angle 'α' is the same as the angle between c-direction and the direction of the external applied electric field. Thus, the effective interface polarization charge density can be expressed as:

$$\sigma_{eff} = \sigma\cos\alpha = \sigma\left|\frac{(a_1,a_2,c_1)\cdot(b_1,b_2,c_2)}{\left|(a_1,a_2,c_1)\right|\cdot\left|(b_1,b_2,c_2)\right|}\right| = \sigma\left|\frac{c_2}{\left|(b_1,b_2,c_2)\right|}\right| \tag{6}$$

with

$$0 \le \alpha \le \frac{\pi}{2}, (a_1,a_2,c_1) = (0,0,1)$$

where, a_1, a_2, b_1 and b_2 are plane Cartesian coordinates, which can be obtained by the linear exchanges from the plane hexagon coordinates $a_1^{'}, a_2^{'}, b_1^{'}$ and $b_2^{'}$ as following:

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 & -1/2 \\ 0 & \sqrt{3}/2 \end{bmatrix} \begin{bmatrix} a_1^{'} \\ a_2^{'} \end{bmatrix} \quad with\ a_3^{'}\ ommited,$$
$$\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 1 & -1/2 \\ 0 & \sqrt{3}/2 \end{bmatrix} \begin{bmatrix} b_1^{'} \\ b_2^{'} \end{bmatrix} \quad with\ b_3^{'}\ ommited. \tag{7}$$

Equations (6)-(7) mean that the larger α is the weaker the influence from polarization field on the NDR characteristic of the RTD is. It is obviously that the maximum of α is π/2. Moreover, the effective interface polarization charges begin to transfer to the lateral surfaces of epitaxial layers and the effective interface polarization charge density is also reduced since both Gallium and Nitrogen ions emerge on the interfaces between AlGaN and GaN as α increases from 0 to π/2. Generally, the width and length of RTD device are much larger than the thickness of any epitaxial layer, which means the polarization field is much more significantly reduced at last and its direction becomes orthogonal to the direction of external applied electric field.

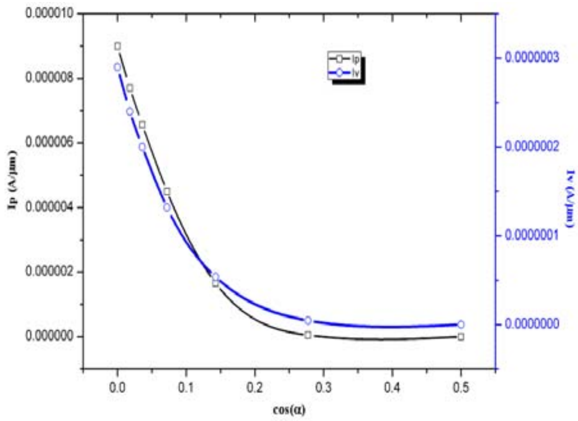

FIGURE IV. PEAK AND VALLEY CURRENTS VS. COS(α) ALGAN RTD

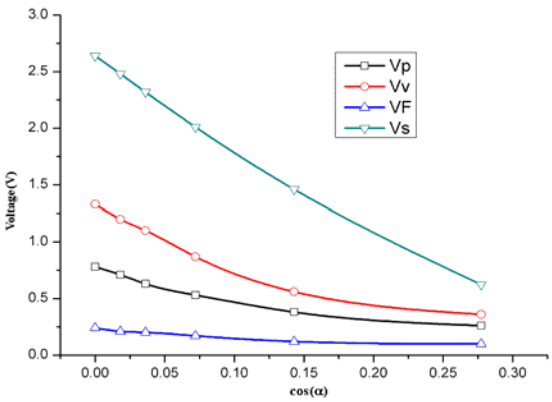

FIGURE V. VP, VV, VF AND VS VS. COS(α)

IV. VERIFICATIONS AND DISCUSSIONS

To characterize the influence from polarization field on the NDR characteristic of the RTD, c-plan, r-plan, a-plane and some planes between r-plan and a-plane were chosen as the planes of the initial GaN substrates respectively for verification through TCAD simulations with the similar structure design to that illustrated in figure I in Green Function Method. The simulation results are illustrated in Figure III-Figure VIII.

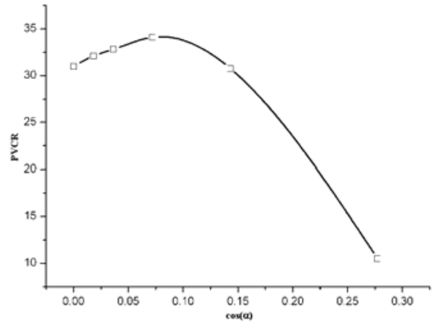

FIGURE VI. FIGURE 6. PVCR VS. COS(α)

As can be seen in Figure III that the NDR characteristics of the proposed GaN/AlGaN RTDs appear more and more significant with the increase of α. No obvious NDR characteristic was observed for the cases of c-plane, r-plane and $\{1\ \bar{1}\ 0\ 1\}$, which might suggest that a angle threshold of α exists for a certain crystal plane between $\{1\ \bar{1}\ 0\ 1\}$ and $\{2\ \bar{2}\ 0\ 1\}$. The proposed GaN/AlGaN RTDs are featured of the same order current as the result in [10], [12] and [15] at much lower peak and valley voltages. Moreover, the peak and valley currents and all feature voltages increase nonlinearly with α as illustrated in Figure IV and Figure V respectively. Figure VI indicates that the PVCR of the proposed GaN/AlGaN RTD increases with α to a maximum value at about 34.09 for $\{8\ \bar{8}\ 0\ 1\}$ and then decreases slowly to about 31 for a-plane. The observed minimum value of PVCR is at about 10.49 for $\{2\ \bar{2}\ 0\ 1\}$, which is enough to satisfy the PVCR requirement for low voltage and low power loss MVL and supercomputer design applications.

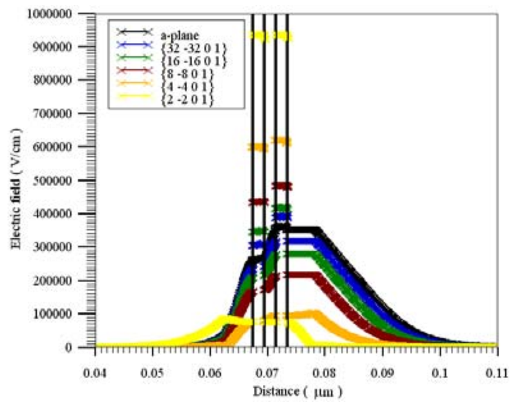

FIGURE VII. ELECTRIC FIELD DISTRIBUTIONS OVER DBS REGIONS

Figure VII illustrates the simulation results of electric field distributions over DBS regions of the proposed GaN/AlGaN RTDs with different initial crystal planes of GaN substrates. As can be seen in Figure VII that the effective tunneling field increases and the reverse polarization field decreases while the initial crystal plane varies from r-plane to a-plane. At the same time, the electron transmission of the main well states also increase with the initial crystal plane as illustrated in Figure VIII since the main well states commence to correspond to those quantum states in emitter region as can be seen in Figure IX (c) and (e)-(i). The reason is that the polarization charge densities between the potential barriers decrease with the c-plane drift angle — α, which leads to reduced effective polarization fields, closed quantum states on both sides of potential barriers and improved electron transmission through potential barriers. Thus, the RT conditions are recovered and enhanced as α increases.

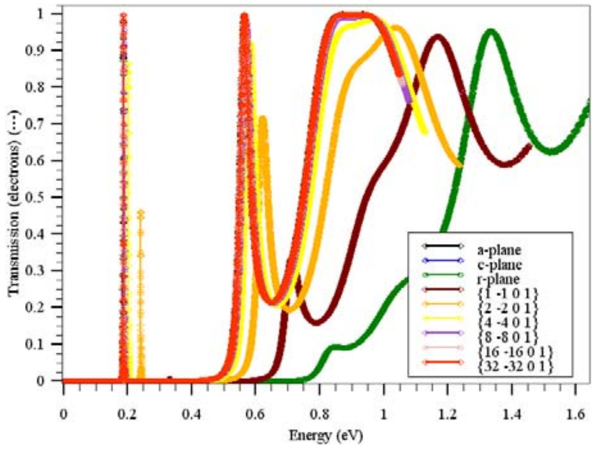

FIGURE VIII. ENERGY OF QUANTUM STATES IN WELL AND EMITTER REGIONS AT APPLIED VOLTAGE

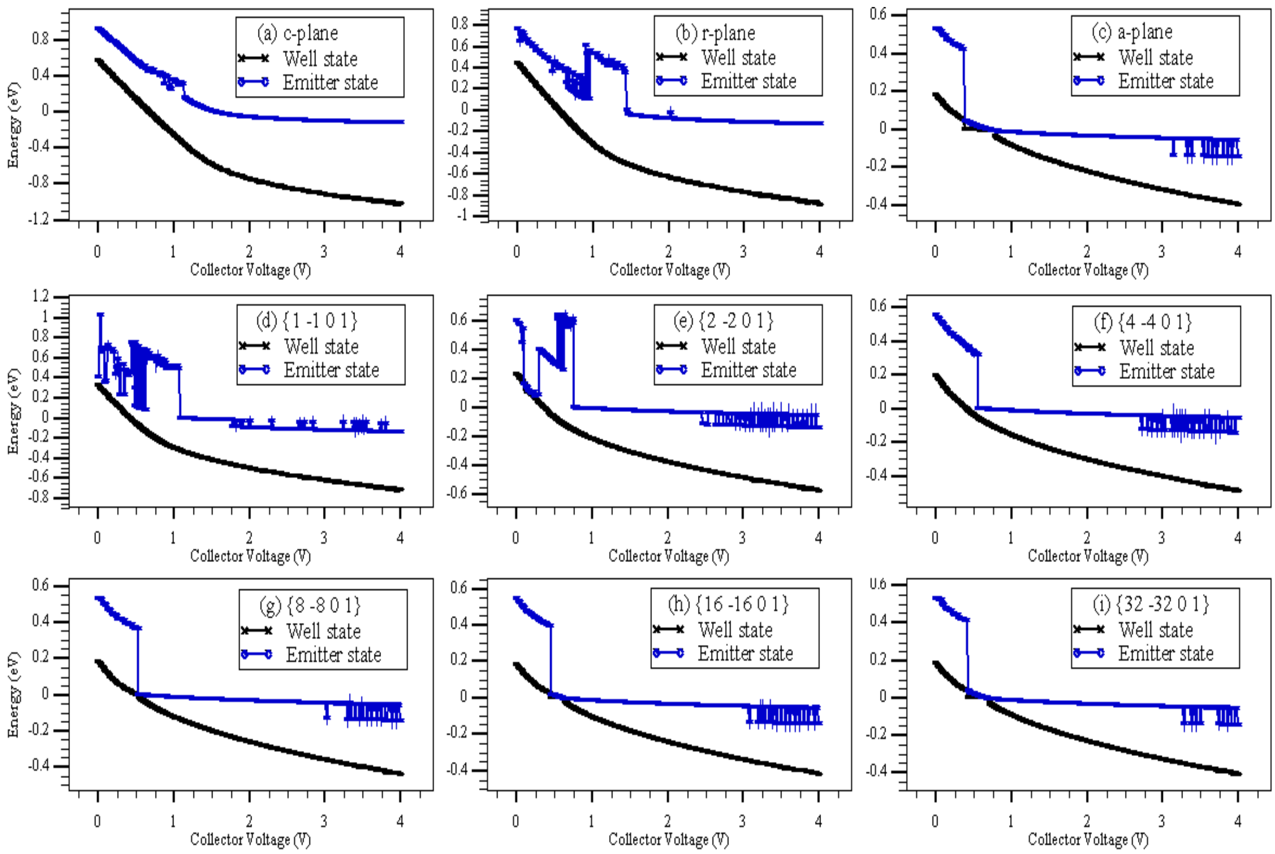

FIGURE IX. ENERGY OF QUANTUM STATES IN WELL AND EMITTER REGIONS AT APPLIED VOLTAGE

V. CONCLUSIONS

Based on the studies and experiments it might be concluded that to select an initial crystal plane by increasing the c-plane drift angle from 0 to π/2 is very helpful to recover and enhance the RT conditions of GaN/AlGaN RTD since it is capable of reducing effective polarization field across the barriers, forming RT quantum state energy levels on both sides of potential barriers and improving electron transmission through potential barriers. As a result, the GaN/AlGaN RTD with the crystal plane $\{2\ \bar{2}\ 0\ 1\}$ as the initial crystal plane of substrate commence to appear practical NDR characteristic for low voltage and low power loss MVL application, which might be approximately defined as critical RT crystal plane. Even the NDR characteristic of a-plane RTD is observed at less than half peak and valley voltages of the result in [10], [12] and [15]. Besides, the GaN/AlGaN RTD with the crystal plane $\{8\ \bar{8}\ 0\ 1\}$ as the initial crystal plane of substrate appears the maximum PVCR at about 34.09.

ACKNOWLEDGEMENTS

This work was supported by National Natural Science Foundation of China (Granted No.61302009)and Zhejiang Smart-City Regional Collaborative Innovation Centre (No Granted No.).

REFERENCES

[1] O. Ambacher, J. Smart, J. R. Shealy, N. G. Weimann, K,Chu, et al., "Two-dimensional electron gases induced by spontaneous and piezoelectric polarization charges in N- and Ga-face AlGaN/GaN heterostructures," J. Appl. Phys., Vol.85, pp.3222-3233, March 1999.

[2] F. D. Sala, A. D. Carlo and P. Lugli, "Free-carrier screening of polarization fields in wurtzite GaN/InGaN laser structures," Appl. Phys. Lett., Vol.74, pp.2001-2004 , April 1999.

[3] S. H. Park and S.L. Chuang, "Spontaneous polarization effects in wurtzite GaN/AlGaN quantum wells and comparison with experiment," Appl. Phys. Lett. , Vol.76, pp.1981-1983, April 2000.

[4] F. Sacconi, A. D. Carlo and P. Lugli, "Modeling of GaN-based resonant tunneling dildes:influence of polarization fields," phys. Stat. sol. (a) Vol.190, pp.295-299, 2002.

[5] S. Heikman, S. Keller, Y. Wu, S. S. James, P. D. Steven, et al., "Polarization effects in AlGaN/GaN and GaN/AlGaN/GaN heterostructures," J. Appl. Phys., Vol. 93, pp.10114-11018, June 2003.

[6] A. E. Romanov, T. J. Baker, S. Nakamura and J. S. Speck, "Strain-induced polarization in wurtzite III-nitride semipolar layers," J. Appl. Phys., Vol.100, pp.023522-1-023522-10, July 2006.

[7] S. H. Park and J. I. Shim, "Effects of Polarization Field on Vertical Transport in GaN/AlGaN Resonant Tunneling Diodes," Journal of the Korean Physical Society, Vol.60, pp.1957-1960, June 2012.

[8] S. Chowdhury and D. Biswas, "Performances comparison of Si, GaAs and GaN based resonant tunneling diode in presence and absence of electric field," IJ-Nano, vol.1, pp.39-45, November 2012.

[9] N. Y. Tang, "Simulation of Polarization effect in GaN/AlN Resonant Tunneling Diode," Advanced Materials Research, Vol.774-776, pp.691-694, September 2013.

[10] S. Sankaranarayanan, S. Ganguly and D. Saha, "Polarization modulation in GaN-based double-barrier resonant tunneling diodes," Appl. Phys. Express, Vol.7, pp.095201-1-095201-4, August 2014.

[11] H. P. Zhang, X. Ning, M. Lin, Y. X. Yu, X. Meng, et al., "A GaAs/AlGaAs Based Asymmetrical DBS (ADBS) RTD," In Proceedings of ICCT2015, Hangzhou China, pp.380-385, October 2015.

[12] A. Rached, A. Bhouri, S. Sakr, J.L. Lazzari and H. Belmabrouk, "Self-consistent vertical transport calculations in $Al_xGa_{1-x}N$/GaN based resonant tunneling diode," Superlattices and Microstructures, Vol.91, pp.37-50, Janury 2016.

[13] E. J. Miller and E. T. Yu, "Direct measurement of the polarization charge in AlGaN/GaN heterostructures using capacitance-voltage carrier profiling," Appl. Phys. Lett., Vol.80, **pp.**3551-3553, May 2002.

[14] V. Fiorentini, F. Bernardini and O. Ambacher, "Evidence for nonlinear macroscopic polarization in III-V nitride alloy heterostructures," Appl. Phys. Lett., Vol.80, pp.1204-1206, Febrary 2002.

[15] S. Chowdhury, A. Santara, P. Mukhopadhyay and D. Biswas, "Advanced AlGaN/GaN resonant tunneling diode on silicon substrate for negligible scattering and polarization effects," Physics of Semiconductor Devices, Environmental Science and Engineering, Switzerland: Springer International Publishing, 2013, pp.285-288.