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Comprehensive Analytical Modeling of AlGaN/GaN based Heterostructure Gas Sensor

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Currently we are facing major problem regarding the environmental pollution due to industry-emitting gases and industrial waste, which can induce environmental hazards and causes serious health problems for human beings. So, volatile organic compounds (VOCs) sensors have generated a lot of attention from researchers over the last decade. As acetone is among the VOCs that extensively used for all research laboratories, industries and human consumables, thus, acetone concentration level monitoring is beneficial for biomedical and environmental research. The Schottky diode AlGaN/GaN heterostructure has therefore been analytically modeled to effectively detect acetone. As a consequence of spontaneous and piezoelectric polarization, the inbuilt high density 2DEG produced over at the interface of AlGaN/GaN is highly sensitive to surface state alterations. Owing to the polarity of acetone, the electrostatic potential of the AlGaN surface is amended when the sensing device is introduced to acetone (dipole moment = 2.9 Dy). This potential alteration leads the 2D electron gas to be modified and hence the current to change. The TCAD tool is used to simulate the Schottky diode sensor and I-V curves generated at various temperatures for different gas concentration levels.From the *I-V* curves the sensitivity is determined with a biasing voltage of 0.5 V at an elevated temperature of 450 K, around 72 % response in the presence of 100 ppm gas is being recorded as this model estimates the sensing properties. It is also observed that the sensitivity saturates after 450 K hence the optimum operating temperature of 450 K is determined and the device also demonstrates good linearity and response at different temperatures. The sensitivity changes as per the change in surface coverage which is ultimately increases due to the increase in gas concentration up to certain limit. Hence the reliance of the area surface coverage on the various gas concentrations has been taken into account.

Keywords: Volatile organic compounds, Heterostructure, 2D electron gas, Polarisation,Gas sensing.

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1. INTRODUCTION

By virtue of superb material characteristics such as large and direct bandgap, high temperature, actinic stability, saturation velocity, break-down voltage and high drift velocity etc., the group III-N elements have drawn attraction among the scientists worldwide during last deade [1-5], facilitating them to be extensively significant in electronics, optoelectronics and sensor application [6-9]. The AlGaN/ GaN material platform is widely involved in sensor implementation amongst the other III-N element owing to inadequacy of Fermi-level pinning [10]. Recent times, AlGaN/GaN heterostructure sensor devices have been analyzed for various types of measured quantity species, including ions [11], polar liquids [12], noxious [13] and combustible gas [14] and fluids [15].The elegance of this structure is clearly depends in its aboriginal hetero-interfacial characteristics imputes the creation of 2DEG because of piezoelectric as well as spontaneous polarization [16]. Now at hetero-interface, the said 2DEG of high density is intently spaced to the facet, thereby being extremely sensitive with any modification with the surface states, i.e. any alteration of the atmosphere [17]. Therefore, AlGaN/GaN heterostructure devices will be the promising contender for the applications of gas sensing, even within corrosive environments.

Till date, heterostructure based on AlGaN/GaN sensors are most often used for hydrogen [18], NOX [19], CO [20], and NH_3 [21] sensing applications. However, very less research has been done on volatile organic compounds (VOCs), particularly acetone sensors based upon AlGaN/ GaN heterostructure [22]. The physics of acetone adsorption are yet to be understood in the structured devices of AlGaN/GaN. Acetone may produce some serious consequences mentioned earlier on human health, despite its low toxic effects [4]. Inbreathetion above the level of 500 ppm, on the other hand, may lead to slackness and sleepiness [23]. So the environmental level of acetone in industrial belt therefore required to be watched and regulated. In addition, acetone diagnosis can become a good biomarker to track food and vegetable standard [25].

We demonstrated the acetone sensing performance of the acetone in this current attempt. The acetone sensing ability of the AlGaN/GaN Schottky diode at lower temperatures with varying concentration of acetone vapor is being exhibited in this current conversation. Some research and analysis on the sensing technique of the heterostructure built upon AlGaN/GaN and the thermodynamics of acetone adsorption and sensing attributes of the device have recently been

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The results were presented at the International Conference on Innovative Research in Renewable Energy Technologies (IRRET-2021) investigated [2]. Also the Schottky parameters and the sensitivity have been reported [1]. In order to effectively detect different gases such as acetone, a MSM Schottky diode type structural system has been used [26]. In some studies, a separate sort of metal-semiconductor-metal (MSM) with successive Schottky diode system is been implemented [2, 3]. In most of the recent work deal with only experimental approach rather than analytical approach. But in this paper a analytical model has been shown which can predict the different sensing characteristics.

2. DEVICE STRUCTURE

Fig. 1 illustrates the design of the modeled device. One wide GaN buffer surface (1.5 μm) is smeared on Si (111) with 50 nm AlN nucleation film. The tensile strain with least fault exhibits a 20 nm thick AlGaN barrier layer on GaN. Because of the presence of piezoelectric polarization at the tip of AlGaN/GaN, 2DEG having density with 1.23×10^{12} cm^{-2} is instigated.

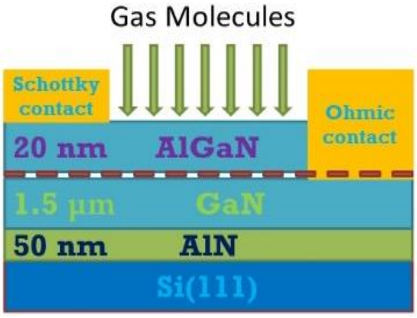

Fig. 1 – Proposed device structure schematic

3. THEORETICAL FRAMEWORK

As completely strained pseudomorphic coating of AlGaN is built upon GaN, the interface induces piezoelectric polarisation [27] and can be represented by

$$P_{PZ,AlGaN} = 2\frac{a_{GaN} - a_{AlGaN}}{a_{AlGaN}}\left(e_{31,AlGaN} - e_{33,AlGaN}\frac{c_{31,AlGaN}}{c_{31,AlGaN}}\right), (1)$$

where the lattice parameters of GaN and AlGaN expressed by 'a_{GaN}' and 'a_{AlGaN}' respectively, the piezoelectric constants and elastic-stiffness constants of AlGaN shown as e_i and c_{ij}, respectively. The equation (2) demonstrate, the spontaneous polarizations for diverse Aluminium (Al) molar fractions and the total polarization propelled charge is computed which is provided in equation (3) [16, 28]

$$P_{SP,Al_xGa_{1-x}N} = -0.09x - 0.034(1-x) + 0.021x(1-x), (2)$$

where the mole fraction of Aluminium (Al) expressed by 'x' and the spontaneous polarization charge is represented by 'P_{SP}'.

$$\sigma_{total} = P_{SP,tot} - P_{SP,GaN} + P_{PZ,tot}, \quad (3)$$

where the polarization sheet charge density is shown by σ_{total}.

4. ANALYTICAL SENSOR MODEL

While reducing gases make contact with the semiconductor layer then adsorption happens at the top surface and contributes negatively charged electrons significantly to the whole surface [29, 30].Those contributed negatively charged electrons provide the modification of electronic state of the plane. As a result, the work-function is amended and thus the density of 2DEG modifications which essentially affect the current transmission.The concentration of 2DEG is altered as follows:

$$n_s + \Delta n_s = \frac{\sigma}{q} - \frac{\left(\phi_B - \Delta\phi_B + E_F - \Delta E_C\right)}{q\,\frac{d_{AlGaN} + \Delta d}{\varepsilon_{AlGaN}}}, \quad (4)$$

where the polarization impact sheet charge density denoted by 'σ' , Schottky barrier elevation among metal/AlGaN and their change are demonstrated as 'ϕ_B' and '$\Delta\varphi_B$' respectively, Fermi energy level at the border with regard to the GaN conduction band (CB) edge is designated by E_F, conduction band (CB) offset at the AlGaN/GaN edge is indicated by 'E_C', width of the AlGaN streak is denoted by 'd_{AlGaN}', 2DEG offset from the hetero-interfaces and permittivity of the AlGaN are signified by Δd and 'ε_{AlGaN}', respectively [31]. The electron concentration of AlGaN at the conduction band (CB) is conveyed as:

$$n = n_i\left[\exp\left(\frac{E_F - E_i}{kT}\right)\right], \quad (5)$$

where the concentration of the intrinsic carrier is 'n_i', intrinsic Fermi level in AlGaN are 'E_F and 'E_i' separately, 'k' shows the Boltzmann constant and 'T' specifies the absolute temperature in Kelvin (K). By moving the Fermi energy (E_F) level, the adsorption of reducing gas reassembles the electrons and modulates the Schottky barrier altitude. So, model formulation is hence as follows: $\phi_B = kT\ln\left(\frac{n+\Delta n}{n}\right)$, where due to gas adsorption, the revision of electron concentration in the conduction band (CB) is denoted by 'Δn'. The impact of this tiny alteration in the forward current of diode is followed by

$$I_0 = qAT^2A^*e^{\left(-\frac{\Delta\phi_B}{V_T}\right)}, \quad (6)$$

where the saturation current is 'I_0', the Richardson's constant is 'A^*', 'T' represents the temperature and 'A' is the contact area and at room temperature the thermal voltage is 'V_T'. The overall current flowing through the Schottky diode is mentioned as below

$$I_{total} = I_0\left(e^{\left(\frac{V}{\mu V_T}\right)} - 1\right), \quad (7)$$

where the ideality factor is denoted by 'η'.

5. RESULTS AND DISCUSSION

The sensor attributes are simulated at different operating bias conditions and varying temperatures, with a fixed gas concentration. The alteration of the current in the sensor at 100 ppm gas with bias voltage at different temperatures 300 K and 450 K is shown in Fig. 2 and Fig. 3, respectively. It is obvious that the current shift is more due to the rise in bias voltage. For the prospective modeling, the gas concentration is maintained at 100 ppm and the biasing voltage up to 1 V is also used, as a surge current is developed at a higher voltage level. It is assessed that the device demonstrates good linearity and response at different temperatures.

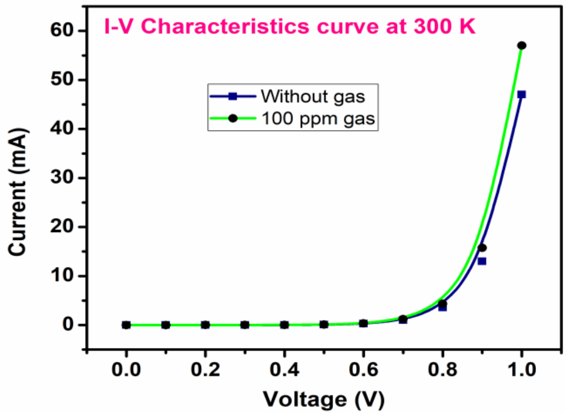

Fig. 2 – Imitated *I-V* response of AlGaN/GaN schottky diode in presence of air and 100 ppm of concentration of gas at room temperature

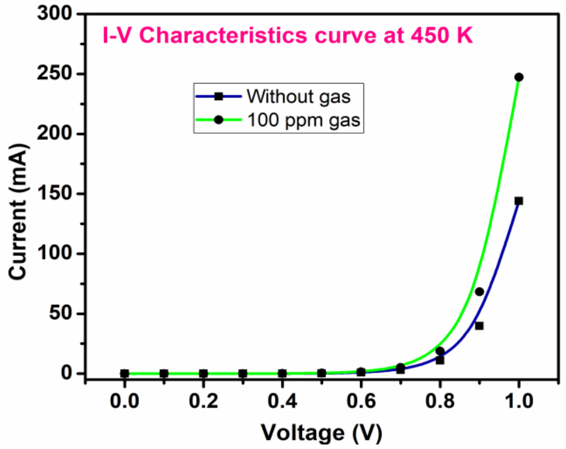

Fig. 3 – Imitated *I-V* response of AlGaN/GaN Schottky diode in presence of air and 100 ppm of concentration of gas at elevated temperature

Sensitivity profile of AlGaN/GaN Schottky diode as a function of temperature for 0.5 V with 100 ppm gas concentration is shown in Fig. 4. The sensor sensitivity is estimated according to the given relationship $S=\left[\dfrac{\left(I_g-I_a\right)}{I_a}\right]\times 100$, where current with the gas and without the gas is denoted by I_g and I_a respectively [32]. It can also be noted that with the rise in temperature, the amount of sensitivity in the response increases progressively. Beyond a certain temperature, the response is saturated, i.e., the sensor response does not really increase substantially beyond that temperature. The adsorption capacity of the AlGaN plane largely limits the response quantity. It can also be observed that the sensitivity basically saturates after 450 K. Hence, the optimal operating temperature for sensing is 450 K.

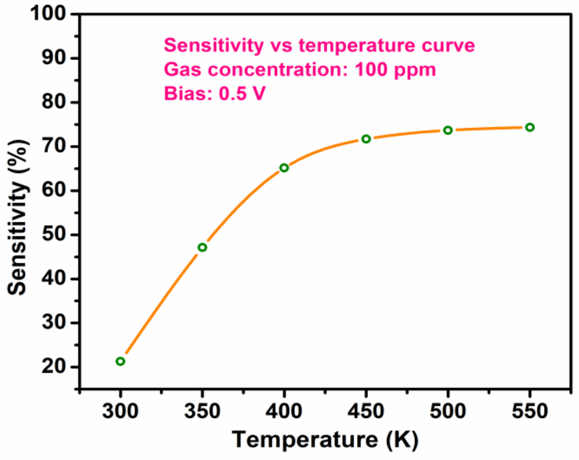

Fig. 4 – Sensitivity versus temperature profile of AlGaN/GaN Schottky diode for 0.5 V with 100 ppm gas concentration

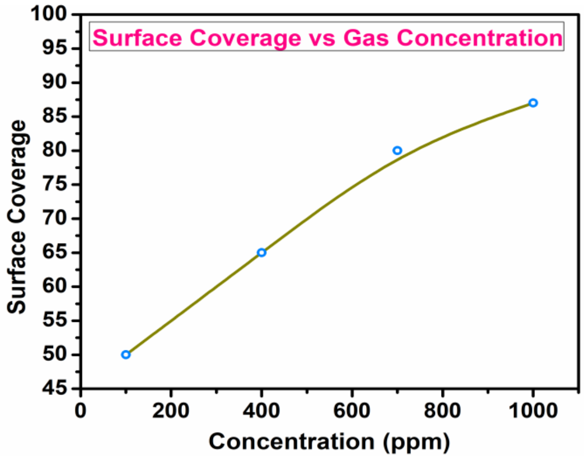

Fig. 5 – Surface coverage of the heterostructure at various gas concentrations

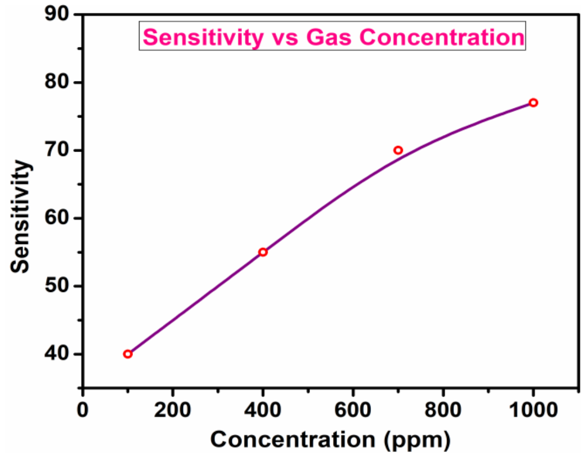

Fig. 6 – Sensitivity of the heterostructure at various gas concentrations

Fig. 5 shows the surface coverage of the heterostructure at various gas concentrations. The expression of the surface coverage at the AlGaN surface (θ_i) shown as [32] $\theta = \frac{K\sqrt{P_g}}{1+K\sqrt{P_g}}$, where the fractional surface coverage denoted by θ_i ($0 \le \theta_i \le 1$), effective equilibrium rate constant denoted as K and the partial pressure of gas is P_g. Now, $\Delta\phi_B$ is proportional to θ_i and is given by [32] $\Delta\phi_B = \Delta\phi_{B_{\max}}\theta_i$, where $\Delta\phi_{B_{\max}}$ can be expressed as the maximum Schottky barrier height change due to the saturation of gas coverage sites. With the increment in the gas concentration the surface coverage also increases and ultimately it increases the adsorption but after certain time surface coverage saturates in spite of further increase in gas concentration. As the surface coverage will change in the above manner, one can predict that the sensitivity will also be changing in the same fashion which is shown in Fig. 6 for clear understanding. Moreover, this sensitivity changes accordingly to the change in Δn.

6. CONCLUSIONS

With the increment of the gas concentration the surface coverage also increases due to adsorption but after a certain limit it will be get saturated so as the sensitivity. In strategic applications, this particular work characterizes a physics-based modeling approach to extremely responsive gas sensors. For extremely tough environmental application areas the substance qualities of GaN emphatically provide sturdiness to the proposed structure of the device. Due to the powerful adsorption of gas particles at the edge and the 2DEG reliance on the condition of surface charge, it is anticipated that sensor will react at a very low gas concentration level. This model is capable of showing *I-V* curves at various concentrations of gas, thus evaluates the device sensitivity.

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Комплексне аналітичне моделювання газового датчика з гетероструктурою на основі AlGaN/GaN

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Сьогодні людство стикається з серйозною проблемою, пов'язаною із забрудненням навколишнього середовища через викиди промислових газів і промислових відходів, які можуть становити небезпеку для навколишнього середовища і викликати серйозні проблеми зі здоров'ям людей. Так датчики летких органічних сполук (ЛОС) привернули велику увагу дослідників протягом останнього десятиліття. Оскільки ацетон належить до ЛОС, які широко використовуються у всіх дослідницьких лабораторіях, в промисловості та споживчих матеріалах, то моніторинг рівня концентрації ацетону є корисним для біомедичних та екологічних досліджень. Тому гетероструктура AlGaN/GaN діода Шотткі була аналітично змодельована для ефективного виявлення ацетону. Як наслідок спонтанної та п'єзоелектричної поляризації, двовимірний електронний газ високої щільності, що утворюється на межі розділу AlGaN/GaN, є дуже чутливим до змін стану поверхні. Завдяки полярності ацетону електростатичний потенціал поверхні AlGaN змінюється при введенні чутливого датчика в ацетон (дипольний момент = 2,9 Dy). Ця зміна потенціалу призводить до модифікації двовимірного електронного газу і, отже, зміни струму. Інструмент TCAD використовується для моделювання діодного датчика Шотткі та кривих *I-V*, отриманих при різних температурах для різних рівнів концентрації газу. За кривими *I-V* визначається чутливість за напруги зміщення 0,5 В при підвищеній температурі 450 K, реєструється близько 72 % відгуку в присутності газу з 100 ppm, оскільки ця модель оцінює чутливі властивості. Також спостерігається, що чутливість насичується після 450 K, отже, визначається оптимальна робоча температура 450 K; пристрій також демонструє гарну лінійність та відгук при різних температурах. Чутливість змінюється відповідно до зміни покриття поверхні, яка в кінцевому рахунку зростає через збільшення концентрації газу до певної межі. Отже, враховано залежність покриття поверхні від різних концентрацій газу.

Ключові слова: Леткі органічні сполуки, Гетероструктура, Двовимірний електронний газ, Поляризація, Датчик газу.