PNIN-GAA-Tunnel FET with Palladium Catalytic Metal Gate as a Highly Sensitive Hydrogen Gas Sensor

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Abstract—**This work reports an n$^+$ source pocket doped PIN gate all around tunnel FET (PNIN-GAA-TFET) with Palladium as a catalytic metal gate for hydrogen detection. The basis of sensing of H_2 molecules is the dissociation of H_2 into Hydrogen atoms followed by their diffusion into the Palladium (Pd) gate leading to formation of a dipole layer due to the polarization of H atoms at the Pd-SiO_2 interface. It is analyzed that the sensitivity of GAA-TFET based H_2 gas sensor is appreciably enhanced by many orders with the integration of n$^+$ source pocket at the tunneling junction. Moreover, for evaluating the stability of the sensor, the performance of the sensor is analyzed at ambient temperatures other than the room temperature. Results reveal that the PNIN-GAA-TFET based H_2 gas sensor is practically stable for the range of ±100K w.r.t. 300K. It is examined that for the entire pressure range the sensitivity of PNIN-GAA-TFET based H_2 gas sensor is maximum at the room temperature.**

keywords—Hydrogen gas; Hydrogen sensor; sensitivity; stability; temperature; tunnel FET.

I. INTRODUCTION

With the ever increasing demand to reduce greenhouse emissions comes the inevitable need to make a transition to cleaner fuels. H_2 presents itself as one of the frontrunners in this quest for zero emission fuels owing to its unique properties like its ability to burn with oxygen leading to the production of water as the only byproduct. Additionally, the commercial importance H_2 is clear from its use in a wide gamut of industries. H_2 is used as crucial component of rocket fuel in the aerospace industry, as a coolant and to provide an inert environment in steam turbine generators, in various processes in semiconductor device fabrication and for processes like gas cutting, welding and to produce smooth surface finish in industries like the automotive industry. With the advent of burgeoning fields like Hydrogen medicine, the importance of H_2 in the biomedical, pharmaceutical and healthcare industries cannot be undermined. However, H_2 is colorless and odorless. It burns in the presence of oxygen in the ultraviolet region of the EM spectrum making the flames invisible to human eyes. Among the many hypotheses put forth by experts who studied the Hindenburg disaster of 1937, the hydrogen hypothesis is most widely accepted, serving as a testimony to hydrogen's destructive nature, if handled carelessly [1]. Given the potential dangers associated with the use of H_2, it becomes imperative to develop accurate and reliable H_2 sensors before the gas becomes an integral part of our fuel economy.

Due to the aforementioned reasons, a H_2 gas sensor based on n$^+$ source pocket PIN Gate All Around Tunnel FET (PNIN-GAA-TFET) is proposed in this work. A conventional TFET is a reverse biased PIN transistor that is operated in reverse bias. TFETs were proposed as possible alternatives to the ubiquitous MOSFET that became a crucial component of modern circuit architecture over the latter half of the 20th century. MOSFETs suffer from short channel and hot carrier effects, which act as the primary impediments to their scale down. Furthermore, the primary carrier injection mechanism in TFETs is quantum mechanical Band-to-Band Tunneling (BTBT) as opposed to thermal carrier injection in MOSFETs. Therefore, Fermi-Dirac statistics limits the Subthreshold Swing (SS) of MOSFETs to kT/q (= 60 mV/decade at 300K), where k is Boltzmann's constant, T is the absolute temperature and q is the electronic charge. However, TFETs fall in the category of super-steep threshold devices with SS less than 60mV/decade [2, 3]. The introduction of an n$^+$ pocket further improves the characteristics of the TFET while the use of the Gate All Around (GAA) scheme enhances the gate controllability of the device. The ability of catalytic metals like Palladium (Pd) to adsorb H_2 gas on their surface is well known. Therefore, in the proposed device, the Pd is used as the gate metal on which H_2 gas is adsorbed. Once adsorbed on the surface of Pd, these H_2 molecules dissociate into H atoms and diffuse into the bulk of the metal. This leads to a formation of a dipole region at the Pd-SiO_2 interface in the device resulting in a modulation of the metal gate work function. There is, therefore, a concomitant change in the device characteristics which depends on the polarization of H atoms at the interface and, indirectly, on the pressure of H_2 gas over the Pd gate. These alterations in the device characteristics are the key transduction parameter for calibration of sensitivity of the sensor. Being active devices, Field Effect Transistors (FETs) can be effectively used to fabricate sensors as they intrinsically amplify signals producing a large change in drive current for a comparatively small change in the gate work function [4]. Therefore FET based H_2 sensors are more sensitive to the parameter being sensed as compared to other H_2 sensors. In this work, TFETs have been used due to the aforementioned advantages they have over other FETs. In addition, the temperature stability of the device, which is a crucial parameter of any practical sensor under consideration,

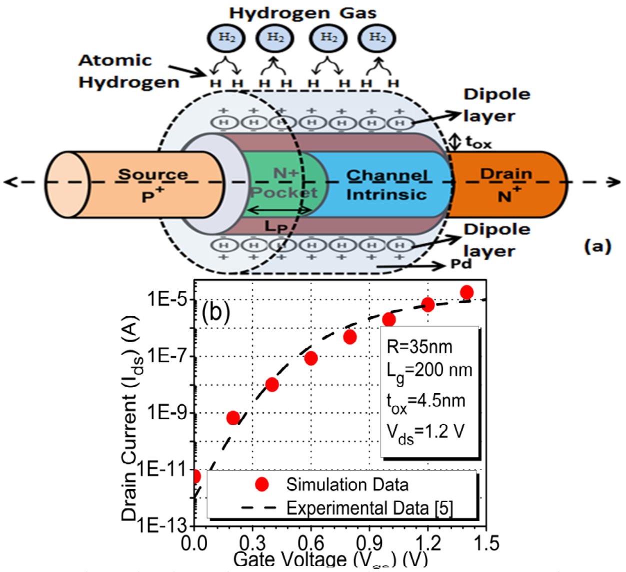

Fig. 1(a) Schematic view of n+ source pocket PIN GAA Tunnel FET. (b) Calibration of the GAA-TFET for transfer characteristics [5].

has also been studied. Numerical device simulation has shown promising results for use of PNIN-GAA-TFET as a viable H_2 sensor in future.

II. DEVICE ARCHITECTURE AND SIMULATION MODELS

Fig. 1(a) shows the schematic view of the PNIN-GAA-TFET H_2 gas sensor. The device consists of a p^+ source, an intrinsic (i) channel and an n^+ drain with an n^+ pocket at the source channel interface. The parameters of the PNIN-GAA-TFET have been optimized in our previous work [6]. The source (p^+) and drain (n^+) doping are 1×10^{20} cm^{-3} and 5×10^{18} cm^{-3} respectively. The structural parameters of the device such as channel length, channel radius, and gate oxide thickness are optimized to 50 nm, 10 nm and 3 nm respectively. The source pocket width and doping are 4 nm and 4×10^{19} cm^{-3} respectively. The sensing element is the Pd gate with a work function (Φ_M) of 5.1 eV. The use of the GAA scheme demands that the device have cylindrical symmetry. The GAA scheme allows for better electrostatic control of the device through the gate as compared to single and double gate devices. In addition, having a gate over the entire device increases the surface area over which adsorption of H atoms can take place. Since the Pd gate is the primary sensing element of the device, the GAA scheme also increases the sensitivity of the H_2 gas sensor. The modulation of Φ_M of the Pd gate on diffusion of H atoms, followed by the creation of dipole layer, has been incorporated to account for the influence of H_2 gas pressure as reported by D. Sarkar *et al.* in [7]. The proposed device has been calibrated with experimental data as obtained by Z. Chen *et al.* in [5].

The numerical simulation of the device has been performed on Silvaco Technology Computer Aided Design (TCAD). In the process of device simulation, it is essential to accurately simulate quantum mechanical BTBT of electrons from the source to the channel through the n^+ pocket. In general, one of two simulation models can be used for this purpose. The first is the Kane model which approximates the tunnelling barrier to be triangular in nature, while the second is the Non- Local BTBT model that accounts for the dynamic variation in the electric field at the tunnelling junction. Therefore, for the purpose of this work, the latter becomes a natural choice as it provides more accurate simulation results owing to its ability to perform numerical calculation over the true potential barrier that electrons moving from the source to the channel tunnel through in a physical device. The Concentration and Field Dependent Mobility model accounts for the drift and diffusion of charge carriers through the device by solving Poisson and carrier continuity equations, while the recombination of majority and minority charge carriers in the device is accounted for by the Shockley-Read-Hall (SRH) Recombination model. Being fermions, the majority carriers occupy energy states in accordance with Fermi-Dirac statistic. Hence, their distribution in the device is simulated using the Fermi-Dirac Statistical model. Finally, the Band Gap Narrowing (BGN) model is used for mathematically modelling doping induced shrinkage of the bandgap leading to changes in carrier transport across the junctions in the device, an effect commonly called band gap narrowing.

III. RESULTS AND DISCUSSIONS

The sensitivity (S) of a sensor measures the magnitude of variation of the sensor's output for a standardized change in the parameter being sensed. Hence in the present case, it is natural to define S as the ratio of change in drive current (I_{ds}) through the device to the OFF-state current (I_{OFF}) of the device, before and after the gas exposure respectively. In Fig. 2, S of GAA-TFET and PNIN-GAA-TFET are plotted w.r.t the H_2 gas pressure at T = 300 K. It is observed that the sensitivity of GAA-TFET is increased by many orders with the integration of n+ source pocket. This increased sensitivity offered by the PNIN-GAA-TFET is attributed to the steeper band bending at the tunneling junction due to the introduction of the n^+ pocket that lowers the width of tunneling barrier (L_{BW}), thus enhancing the drain current. This increased drain current leads to the enhanced S of the PNIN-GAA-TFET as compared to the GAA-TFET. It is observed that at a gas pressure of 10^{-11} Torr, the sensitivity increases from 86 (for GAA-TFET) to an order of 10^5 (for PNIN-GAA-TFET) due to the introduction of the n^+ pocket at the source-channel interface. As is clear from Fig. 2, the proposed H_2 gas sensor has an incredibly large sensitivity range. This large sensitivity range of the device is a consequence of the physical processes involved in the functioning of the device as a sensor.

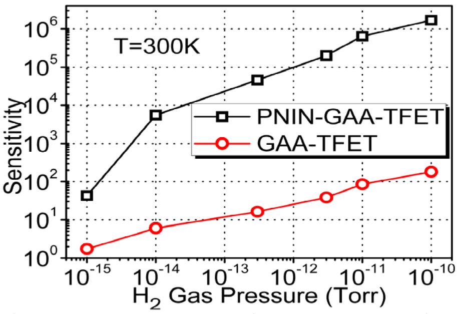

Fig. 2 Sensitivity w.r.t H_2 gas pressure for GAA-TFET and PNIN-GAA-TFET.

The device consists of a catalytic metal gate (Pd) forming an interface with a layer of dielectric insulator (SiO_2), which in turn forms an interface with a layer of semiconductor (Si). This forms a Pd-dielectric-semiconductor structure, which forms the primary sensing element of the device. Earlier experimental studies on such Pd-dielectric-semiconductor structures have revealed changes in the electrical properties, primarily the work function, of Pd due to changes in the partial pressures of gases, particularly H_2, on the surface of Pd, which indirectly leads to a change in the conductance of the semiconducting channel. The physical reasoning behind such changes can be explained as follows [8]. The H_2 gas on the surface of Pd has a tendency to dissociate into H atoms and get adsorbed on one of the interfaces of the Pd-dielectric-semiconductor structure. Following this, the adsorbed H atoms form a dipole layer along the adsorption interface and thus modulate the electrical properties of the structure. Dipole moment calculations indicate that the adsorption layer is formed at the Pd-SiO_2 interface, which means that the H atoms diffuse through the Pd layer to form the dipole layer at this interface. Therefore, this dipole layer modulates the work function of the Pd gate in turn, thus leading to the observed variations in device sensitivity. One important observation is the dependence of sensitivity on the large polarization of H atoms rather than the large number of H atoms adsorbed. Finally, experiments by Ekedahl L. *et al.* [9] have shown that the introduction of a small amount of O_2 over the Pd substrate leads to the formation, followed by desorption of water from the Pd surface. This leads to a decrease in partial pressure of H_2 on Pd and hence increases the dynamic range of the sensor to 10^{-14} Torr at 473 K. In this work, the simulator operates up to a lower bound of 10^{-15} Torr at 300 K, which is concurrent with the aforementioned experimental observation as the partial pressure of H_2 gas will decrease further with decrease in temperature. Also, no saturation limit on the adsorption of H atoms at the interface has been successfully found experimentally, which indicates the efficacy of this structure as a sensing element. All simulations in this work have been performed in an inert atmosphere of H_2 only.

The temperature affectability of TFET, semiconductor properties, H_2 gas and Pd interaction are the key motivations to analyze the stability of the sensor at ambient temperatures (other than the room temperatures). Thus, to account for the stability of PNIN-GAA-TFET H_2 gas sensor against temperature alterations, the sensitivity of the device is analyzed at various temperatures, at constant gas pressures as shown in Fig. 3. It is observed that, the sensitivity of PNIN-GAA-TFET H_2 gas sensor is maximum at T = 300 K for the entire pressure range. The reduction of sensitivity at elevated temperature owes to the reduction in the adsorption of H atoms at the adsorption interface with increase in temperatures. This can be attributed to the fact that the H atoms become more energetic as the temperature increase and the bonds between the adsorbent and adsorbate weaken. Therefore, desorption of H atoms takes place as temperature increases resulting in decreased sensitivity. The sensitivity also decreases at lower temperatures (T < 300 K), but the reduction is comparatively small w.r.t. higher temperatures (T > 300 K) as compared to 300 K. The decrease in sensitivity for T < 300 K can be attributed to the decrease in drive current at lower temperature. The sensitivity as a function of pressure at various ambient temperatures is shown in Fig. 4. It is clearly observed that with an increase in H_2 gas pressure, the sensitivity of PNIN-GAA-TFET gas sensor increases appreciably for each temperature. Experimentally, it is observed that the H response, and hence sensitivity, is proportional to the logarithm of pressure, thus explaining the observed simulation trends [9]. The sensitivity variation with temperature is due to the aforementioned reasons, with maximum sensitivity being observed for T = 300 K. Quantitatively, it is seen that for T = 200 K, with an increase in pressure from 10^{-14} Torr to 10^{-11} Torr, the sensitivity is enhanced from an order of magnitude of 10^2 to 10^4.

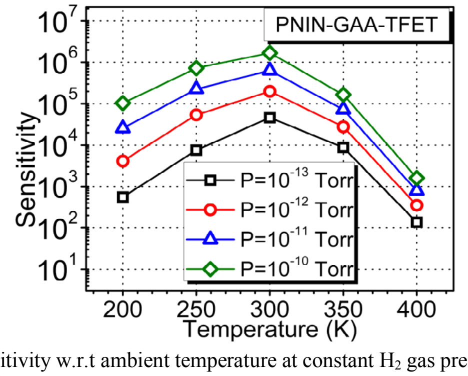

Fig. 3 Sensitivity w.r.t ambient temperature at constant H_2 gas pressure for PNIN-GAA-TFET.

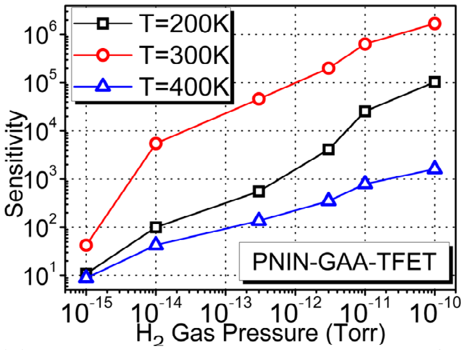

Fig. 4 Sensitivity w.r.t H_2 gas pressure at constant temperature for PNIN-GAA-TFET.

In addition to the sensitivity, the electrical parameters of the PNIN-GAA-TFET such as the surface potential and the nonlocal BTBT rate of electrons are also investigated for various gas pressures and ambient temperatures as shown in Figs. 5-7. With an increase in gas pressure, a remarkable increase in surface potential is observed as shown in Fig. 5. This enhanced potential leads to the steeper band bending at higher gas pressures and thereby an increase in the drain current at higher pressure. The nonlocal BTBT tunneling rate of electrons at the tunneling junction w.r.t. gas pressure for a temperature range of 200-400K is shown in Fig. 6. The steeper band bending at higher gas pressures lowers L_{BW} and thereby enhances the electron tunneling rate. Moreover, at elevated temperatures, the exponential temperature dependence of SRH and band gap narrowing increases the BTBT rate of electrons tremendously from an order of 10^{25} /cm^{3}s to 10^{27} /cm^{3}s. The influence of ambient temperature and gas pressure on the

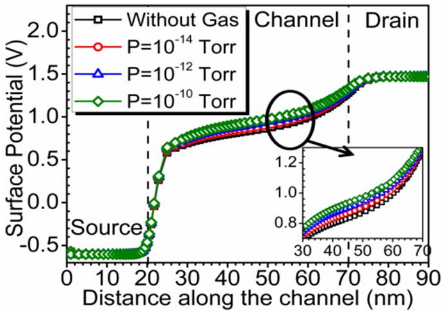

Fig. 5 Surface potential along channel length at constant H_2 gas pressures and at T=300K for PNIN-GAA-TFET.

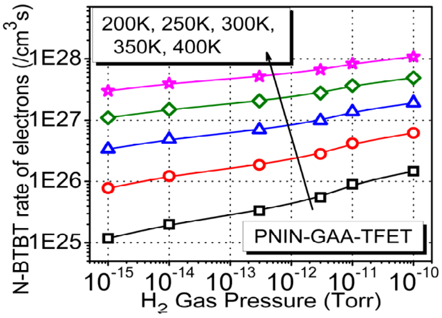

Fig. 6 Non local BTBT rate of electrons w.r.t H_2 gas pressure at constant temperatures for PNIN-GAA-TFET

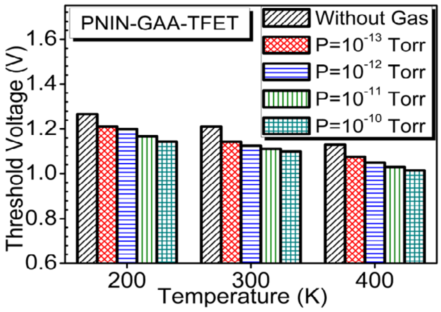

Fig. 7 V_{th} of PNIN-GAA-TFET as a function of temperatures at constant H_2 gas pressures.

threshold voltage (V_{th}) of the PNIN-GAA-TFET is shown in Fig. 7. It is observed that the enhanced BTBT rate of electrons at higher gas pressures switches ON the sensor earlier for the entire temperature range. Moreover, at elevated ambient temperature, the lowered bandgap and SRH exponential temperature dependence enhances the drive current of the sensor that, in turn, switches the sensor ON early [10].

IV. CONCLUSION

In this work, a highly sensitive PNIN-GAA-TFET based H_2 gas sensor has been proposed. The sensitivity of the device is compared with that of a conventional GAA-TFET and it is revealed that with the incorporation of n^+ source pocket, there is an extensive increase in device sensitivity up to an order of 10^6 at a gas pressure of 10^{-10} Torr. In addition, it is observed that with an increase in gas pressure, the sensitivity of the sensor increases considerably. Furthermore, the stability of the device is also examined for the wide temperature range. Results reveal that the PNIN-GAA-TFET based H_2 gas sensor is reasonably stable at 200-400K. The significantly high sensitivity of PNIN-GAA-TFET H_2 gas sensor may be beneficial to meet the escalating demand for H_2 gas sensors in a wide range of uses.

ACKNOWLEDGEMENTS

The authors would like to express their sincere gratitude to the Microelectronics Research Lab, Department of Engineering Physics, Delhi Technological University (formerly DCE). In addition, one of the authors (Jaya Madan) thanks the University Grant Commission (UGC) for providing the financial assistance required to carry out this research.

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