Design and Performance Analysis of Ultrathin Nanowire FET Ammonia Gas Sensor

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Abstract
In this work, an ultrathin 3 nm nanowire field-effect transistor (NWFET) based ammonia gas sensor is designed, and its sensitivity is analyzed at room temperature. The designed NWFET for gas sensing is observed to have a higher ratio of $I_{ON}$ to $I_{OFF}$ than $10^9$, lower DIBL and better gate controlling due to a higher surface to volume ratio. The gas-sensing performance analysis has been done for three different catalysts, iridium (Ir), ruthenium (Ru), and palladium (Pd), by gradually increasing the work function by a difference of 50 meV. The device showed higher OFF current sensitivity compared to ON current sensitivity. The power consumption and threshold voltage are observed to be least for palladium catalytic gate electrodes making palladium the most favorable catalytic for ammonia gas for the designed gas sensor.

Keywords Nanowire field-effect transistor · Gas sensor · Palladium catalytic gate electrodes · Sensing response · Ammonia gas

1 Introduction
Various types of the gas sensor have been designed, studied, and fabricated based on different sensing mechanisms and sensing material, and many new designs and materials are being studied presently [1, 2]. The demand for small-sized and integrated circuit compatible gas sensors has made the researcher keener towards organic and nanomaterial FET type gas sensors [3, 4]. These gas sensors play a vital role in the safety of chemical industries, factories by monitoring any leakages [5]. Among various gases, ammonia (NH₃) gas is the crucial base material for different chemical products and is used in food packaging industries, agriculture, medical diagnostics labs, and fertilizer industries [6]. However, ammonia is a colorless gas with a suffocating smell and, if accidentally leaked, could be hazardous to living beings [7].

The semiconductor nanowires FET are observed to have higher surface-area-to-volume ratio, lower resistance, and higher aspect ratio, making it ideal for designing gas sensors [8]. The sensing mechanism of the designed device is based on the deposition/absorption of gas molecules to the surface of the catalytic gate electrode [9, 10]. The deposition/absorption of gas molecules on metal electrodes disturb its composition and lead to the change in work function of the metal electrode, which affects the analog parameters of transistors. In the proposed gas sensor, the effect of change in metal function on threshold voltage has been studied on transfer characteristics. The relation of change in work function ($\Delta \phi_m$) to the partial pressure ($P$) of detectable gas is shown in Eq. (1) [11].

$$\Delta \phi_m = \phi_{m(const)} - \frac{RT}{4F} \ln(P)$$

In this paper, we have discussed the device design and simulation model and parameters of the proposed device in section (2), followed by results and performance analysis in section (3) and conclusion in section (4).

2 Device Design and Simulation Parameters
The three-dimensional schematic structure of the proposed nanowire FET is shown in Fig. 1a. The diameter of the cross-section is chosen as 3 nm, where the inner...
core has n-p-n configuration on silicon nanowire of diameter 2 nm, which is coated with silicon dioxide all-around of 1 nm thickness [12, 13]. A thin layer of the catalytic metal electrode (Ir/Ru/Pd) is coated on the oxide layer, all around the channel. The vertical length of the proposed NWFET is 50 nm with a channel length of 30 nm, and drain and source region length is 10 nm each. The source and drain are doped with an N-type uniform doping profile of $1 \times 10^{18}$/cm$^3$ and $1 \times 10^{20}$/cm$^3$; whereas the channel is doped with a P-type doping profile of $1 \times 10^{15}$/cm$^3$. The two-dimensional structure of the designed silicon NWFET has been used for current simulation, which is shown in Fig. 1b. The various design parameters of the device are mentioned in Table 1.

For simulation, the Silvaco TCAD Atlas tool has been used. The Shockley-Read-Hall model and band-to-band tunneling have been used for generation-recombination of electron-hole pairs, and self-consistent coupled Schrödinger Poisson model has been used to derive electron density. The non-equilibrium green function model (NEGF model) solves these coupled equations through a stable and oscillation-less iteration [14, 15]. The obtained solution of electron density is incorporated in the drift-diffusion model to get current and current density [16, 17].

### 3 Result and Discussion

#### 3.1 Device Performance and Characteristics Discussion

At room temperature, the transfer characteristic ($I_D-V_{GS}$) of the proposed device is shown in Fig. 2a for $V_{DS} = 1$ V has been obtained for the design parameter given in Table 1. The ON-current ($I_{ON}$) at $V_{GS} = 1.5$ V is noticed as $6.70 \times 10^{-7}$ (A/μm) and $8.67 \times 10^{-7}$ (A/μm), whereas the OFF-current ($I_{OFF}$) is observed as $5.67 \times 10^{-16}$ (A/μm). The device is observed to have a lower DIBL and high $I_{ON}$ to $I_{OFF}$ ratio in the order of $10^9$. The sub-threshold swing of 57.80 mV/dec and threshold voltage 0.589 V has been observed. The output characteristics ($I_D-V_{DS}$) for $V_{GS} = 0.6$ V and $V_{GS} = 0$ V (inset) has shown in Fig. 2b. From the inset graph in Fig. 2b, it can be observed that even though the $V_{DS}$ is increased to 1 v, the device remains in OFF state only, and OFF current is $1 \times 10^{-14}$ A/μm, which shows higher controllability of gate voltage on the device.

#### 3.2 Performance Analysis of Nanowire FET Gas Sensor for Three Different Metal Catalysts

The three different metals i.e. Iridium (Ir), Ruthenium (Ru) and Palladium (Pd) are selected as the catalyst metal electrodes due their higher sensitivity towards ammonia gas. In Table 2 the work function of the above-mentioned metal catalysts is listed. Considering the exposure of constant flow of ammonia gas at constant pressure on the proposed gas sensor, change in its drain current characteristics is studied by increasing the metal work function with a small value of 50 meV gradually. In the obtained transfer ($I_D-V_{GS}$) characteristics for each change in work function, change in $I_{OFF}$ to $I_{ON}$ ratio and threshold voltage can be observed. The sensing mechanism of the proposed gas sensor is based on the change in metal work function due to the absorption or deposition of ammonia on the surface of catalytic gate metal. As the ammonia gas settle

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**Table 1** Various design parameters of proposed cylindrical NWFET

| S. no. | Design parameters         | Values                  |
|--------|---------------------------|-------------------------|
| 1      | Channel length            | 30 nm                   |
| 2      | Gate work function        | 4.7 eV                  |
| 3      | SiO$_2$ thickness         | 1 nm                    |
| 4      | Si layer thickness        | 2 nm                    |
| 5      | Source doping concentration | n-type $1 \times 10^{15}$/cm$^3$ |
| 6      | Drain doping concentration | n-type $1 \times 10^{20}$/cm$^3$ |
| 7      | Channel doping concentration | p-type $1 \times 10^{15}$/cm$^3$ |
down on the surface of these catalyst, dissociate into nitrogen gas, hydrogen gas and hydrogen ion [18–20] as shown in Fig. 3. These hydrogen ions penetrate into the gate metal, which changes the structural composition of metal catalysts resulting in a change metal work function [21, 22]. Increasing the concentration of detectable gas will increase the work function more. The change in metal work function affects analog parameters, such as OFF-current (I_{OFF}), ON-current (I_{ON}), transconductance and threshold voltage, etc.

Figure 4a–c, transfer characteristics of the proposed device for palladium, ruthenium, and iridium shown respectively is obtained by step-wise linearly incrementing work function from 50 to 200 meV with step size of 50 meV. In the transfer characteristics of the three metal catalysts, it can be observed that the drain current curve shifts downwards with increasing work function. The palladium metal which has lowest work function among three has higher ON-Current and lower OFF-Current compared to that of iridium and ruthenium.

Since the threshold voltage depends directly on metal work function as shown in Eqs. (2) and (3) [11], hence increasing work function increases the threshold voltage which is shown in Fig. 5. So, increasing the concentration of detectable gas on metal surfaces will increase the device’s threshold voltage, which could be used as a sensing parameter for the proposed gas sensor. As the change in OFF and ON-state current in the device is very significant, hence drain current response have considered as sensing response parameter of the device and the current sensitivity and sensitivity response for mentioned three catalytic metals are studied. Table 3 shows the different threshold voltage observed by varying ΔΦ_M for all three metal catalysts.

\[ V_{fb} = \phi_m - \phi_s \pm \Delta \phi_m \] (2)

\[ V_{th} = V_{fb} + \varphi_{min,th} \frac{Q_d}{C_i} + 2\phi_F \] (3)

### 3.3 Sensitivity Analysis

Sensitivity of proposed nanowire FET gas sensor for ammonia is more in OFF state at V_{GS} = 0 V than ON state as in the off

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**Table 2** Work functions of incorporated metal catalysts

| Sl. no. | Metal catalyst | Gate work function |
|---------|----------------|--------------------|
| 1       | Iridium (Ir)   | 5.2 eV (single crystal) |
| 2       | Ruthenium (Ru) | 5.4 eV              |
| 3       | Palladium (Pd) | 4.8 eV              |

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**Fig. 2** a Transfer characteristics (ID-VGS) of the proposed cylindrical NWFET device for VDS = 1 V. bID-VDS Characteristics of proposed NWFET at VGS = 0.6 V and VGS = 0 V (in inset)

**Fig. 3** Two-dimensional Schematic view showing dissociation of ammonia on the surface of gate metal of proposed NWFET gas sensor

**Fig. 4** a ID-Vgs characteristics of proposed NWFET-based NH3 gas sensor for palladium gate catalyst. b ID-Vgs characteristics of proposed NWFET-based NH3 gas sensor for ruthenium gate catalyst. c ID-Vgs characteristics of proposed NWFET-based NH3 gas sensor for iridium gate catalyst
State higher work function induces more minority charges in the channel [11]. The increase in work function of device leads to formation of depletion layer at interface of an oxide layer and channel even in absence of gate bias which requires more positive gate voltage to switch-ON the device [23, 24]. The change in OFF current is referred as OFF-state current sensitivity, which can be obtained from the ratio of OFF current when no-gas/air exposed to device to OFF current when the detectable gas is exposed to device, which is mathematically expressed by following Eq. (4) [11].

\[
S_{\text{OFF}} = \frac{I_{\text{OFF(air)}}}{I_{\text{OFF(gas)}}}
\]  

(4)

Similarly, the change in ON current is referred as ON-state current sensitivity which can be obtained from the Eq. (5) expressed below [11].

\[
S_{\text{ON}} = \frac{I_{\text{ON(gas)}} - I_{\text{ON(air)}}}{I_{\text{ON(air)}}}
\]  

(5)

The sensitivity curve for both ON and OFF state with respect to change in work function for iridium, palladium and ruthenium catalytic metal is shown in the Fig. 6. Tables 4, 5 and 6 shows ON and OFF current, it’s ratio and sensitivity in OFF and ON state for iridium (Ir), ruthenium (Ru) and palladium (Pd) gate metal respectively. Here, we can observe that the palladium gate metal NWFET gas sensor has higher OFF current sensitivity compared to the iridium and ruthenium gate metal NWFET gas sensors.

The outcome forms the sensitivity calculation from the proposed NWFET-based NH3 gas sensor with Ir, Ru and Pd gate metal for different gas molecule concentration equivalent work function have been shown in Tables 4, 5 and 6 respectively. From these Tables 4, 5 and 6 we can conclude that maximum ON-state current sensitivity (\(S_{\text{ON}}\)) is reported to be -0.385, 0.061 and 0.182 form maximum gas concentration equivalent to 200 meV. Sensing Response of the proposed device as function of gate voltage for varying metal work function can obtained from the ratio of drain current in presence of ammonia to drain current in absence of ammonia [6] can be calculated from the expression by Eq. (6).

\[
\text{Sensing Response} = \frac{I_{\text{D(NH3)}}}{I_{\text{D(air)}}}
\]  

(6)

Since increase in concentration of detectable gas (ammonia) is considered as higher change in metal work function and the sensing response for higher change in work function i.e. 200 meV is maximum. It can be very clearly observed from the Fig. 7a that the NWFET gas sensor with Palladium gate metal electrode is highly sensitivity in OFF state and least sensitivity in ON state. In Fig. 7b and c, It can be observed that proposed device shows more sensitivity response when the gate voltage is equal to or higher than the threshold voltage i.e. VGS =1.08 V and VGS = 1.28 V for both iridium and ruthenium metal electrode respectively compared to OFF-state (VGS = 0 V).

### 4 Conclusion

The proposed nanowire FET gas sensor has higher OFF current sensitivity for palladium metal electrode as compared to other two metal electrodes as sensing response for palladium increases by 90.2% by increasing work function (\(\Delta \phi_m\)) from 50 to 200 meV where for iridium and ruthenium metal electrode sensing response increases by 78.5% and 31.81%
respectively. The threshold voltage for palladium metal electrode gas sensor is always below 0.9 V whereas for ruthenium and iridium metal electrode gas sensor, it is always more than 1 V; hence the palladium metal electrode gas sensor would be a wise choice for VLSI circuit operating at lower voltages. The designed gas sensor has higher gate controllability, even

![Diagram](image)

Fig. 7  a Sensing response as a function gate Voltage for Palladium metal gate. b Sensing response as a function gate Voltage for iridium metal gate. c Sensing response as a function gate Voltage for ruthenium metal gate

the drain voltage of 1 V won’t be able to switch ON the gas sensor which reduces the chances of getting false alert in case of voltage spikes in applied voltages. The designed device has higher ION/IOFF ratio in order of 10^9 which checks the leakage current in device and reduces the chances of false alert due to

![Diagram](image)

Fig. 8 Threshold voltage plot increment in work function of catalyst electrode of proposed NWFET GS

| ΔΦm   | I_{OFF}      | I_{ON}       | I_{ON}/I_{OFF} | S_{OFF} | S_{ON} |
|-------|--------------|--------------|----------------|---------|--------|
| 50 meV | 5.49×10^{-16} | 7.17×10^{-7} | 1.405×10^9     | –       | –      |
| 100 meV | 6.12×10^{-16} | 6.22×10^{-7} | 1.01×10^9      | 0.89    | –0.193 |
| 150 meV | 7.58×10^{-16} | 5.88×10^{-7} | 0.77×10^9      | 0.72    | –0.238 |
| 200 meV | 6.12×10^{-16} | 4.74×10^{-7} | 0.774×10^9     | 0.897   | –0.385 |

Table 4 Sensitivity calculation of proposed NWFET-based NH3 gas sensor with Ir gate metal

| ΔΦm   | I_{OFF}      | I_{ON}       | I_{ON}/I_{OFF} | S_{OFF} | S_{ON} |
|-------|--------------|--------------|----------------|---------|--------|
| 50 meV | 5.46×10^{-16} | 1.34×10^{-7} | 0.2×10^9       | –       | –      |
| 100 meV | 5.57×10^{-16} | 1.366×10^{-7}| 0.245×10^9     | 0.980   | 0.019  |
| 150 meV | 5.48×10^{-16} | 1.38×10^{-7} | 0.251×10^9     | 0.996   | 0.029  |
| 200 meV | 5.73×10^{-16} | 1.423×10^{-7}| 0.248×10^9     | 0.952   | 0.061  |

Table 5 Sensitivity calculation of proposed NWFET-based NH3 gas sensor with Ru gate metal

| ΔΦm   | I_{OFF}      | I_{ON}       | I_{ON}/I_{OFF} | S_{OFF} | S_{ON} |
|-------|--------------|--------------|----------------|---------|--------|
| 500 meV | 6.12×10^{-16} | 4.74×10^{-7} | 0.774×10^9     | 0.897   | –0.385 |
| 1000 meV | 6.12×10^{-16} | 4.74×10^{-7} | 0.774×10^9     | 0.897   | –0.385 |
| 1500 meV | 6.12×10^{-16} | 4.74×10^{-7} | 0.774×10^9     | 0.897   | –0.385 |
| 2000 meV | 6.12×10^{-16} | 4.74×10^{-7} | 0.774×10^9     | 0.897   | –0.385 |

Table 6 Sensitivity calculation of proposed NWFET-based NH3 gas sensor with Pd gate metal
leakage current. The current sensitivity increases with increase in concentration of ammonia gas on the surface of device, where the threshold voltage increases with increase in concentration of exposed ammonia gas, hence the threshold voltage of device can also be considered as one of sensing parameters. Compared to ruthenium and iridium metal, palladium metal seems to be favorable option for catalyst metal for detection of ammonia for the designed nanowire FET gas sensor.

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Data Availability Current submission does not contain the pool data of the manuscript but the data used in the manuscript will be provided on request.

Declarations

Consent to Participate Informed consent.

Consent for Publication Consent is granted.

Conflict of Interest The authors declare that they have no conflict of interest.

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