Silicon Nanowire FET Hydrogen gas Sensor: Design Aspects

Monika Dubey
CSIR-Central Electronics Engineering Research Institute Pilani Rajasthan, India

Abstract -- Palladium (Pd) is considered as ideal hydrogen sensing material due to its properties as high sensitivity and selectivity to hydrogen gas, fast response and reversible room temperature operation.Silicon nanowire (SiNW) functionalized with Pd based hydrogen gas nanowire sensor having quantum confinement effect and high sensitivity because of high surface to volume ratio of SiNW. This paper highlights the design aspects with physical dimensions and response of palladium film functionalized silicon nanowire based hydrogen gas sensor.

Index Terms--Hydrogen sensor, Palladium (Pd) film,Silicon nanowire (SiNW), sensitivity.

1. INTRODUCTION

Silicon nanowire based gas sensors work at room temperature with lowest power consumption [1]. Hydrogen is used in many commercial processes such as hydrogenation, petroleum transformation, cryogenic cooling and many other chemical productions. Hydrogen gas is odorless, colorless and flammable (almost invisible) at concentration over 4%, it poses safety concerns and creates a need for effective hydrogen leakage sensor [2-3].

The hydrogen gas adsorption process allows reactions on a sensing surface if it is activated or if it possesses free electrons or holes. In this case the charge carriers can communicate with the gas and form a built-in potential difference with a sufficient amount of resistance, which is recognised as the gas sensor signal [5]. The effect of hydrogen on conductivity of the palladium is reversible with the formation of PdH_k[2][4].

2. SILICON NANOWIRE BASED HYDROGEN GAS SENSOR: DESIGN ASPECTS

For the simulation ofSiNW functionalized with Pd Films SILVACO Atlas 3D software has been used. At temperature above 50 K hydrogen atoms nomadize from hole to hole throughout the Pd. The calculated size of Pd atom is 0.24nm. Palladium functionalized Silicon nanowire has reversibility and selectivity (non-stoichiometry) for hydrogen gas sensing with the rapid formation of PdH_k ,where k=0 - 0.7. Because there are four Pd atoms and four octahedral holes per unit cell, maximum stoichiometry, $PdH_{0.7}$ represents 70%of the octahedral holes filled and absorbed 935 times hydrogen gas of its volume at STP[6]. Palladium hydride readily releases H_2 by the reverse process of hydrogen absorption.

$$Pd(s) + k/2\, H_2(g) \rightleftarrows PdH_k(s)$$

For lower H:Pd ratios, $PdH_{0-0.02}$, the nature of palladium remains very much like that of pure Pd and is referred to as the α-phase. The most notable difference between pure Pd and the α-phase is that the latter has a slightly lower conductivity and its unit cell dimensions are slightly larger. A β-phase occurs along with the α-phase for $PdH_{0.02-0.58}$ and the β-phase exists exclusively for $PdH_{0.58-0.7}$. The β-phase differs from the α-phase in that the material becomes increasingly brittle as the H:Pd ratio increases and for $PdH_{>0.5}$ the material is a semi-conductor.The conductance of palladium functionalized Silicon nanowire is smaller than that of pure SiNW due to electron depletion at the Pd and Si surface. For design purpose, the thickness of SiO_2 layer is between 10 nm.

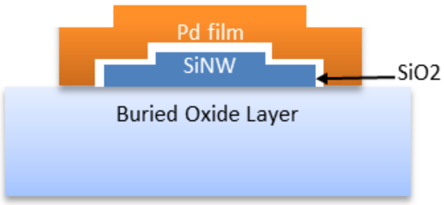

Fig:1 Cross sectional view of Pd functionalized Si nanowire FET sensor

The length of silicon nanowire varies as 1μm, 3 μm, 5 μm, 10μm and width and height of Si nanowire varies as 50nm, 70nm, 100nm, 200nm. The size of palladium film is according to the Si nanowire length varies from 0.8μm to 3μm, width and height varies as 50 nm, 70nm, 100nm, 200 nm. The calculated atom size of Pd atom is 0.24nm. When the Fin (L=800nm W=50nm H=50nm), number of moles of Pd is about $6.67\text{x}10^7$. The based on the amount of palladium, the maximum limit of absorption of Hydrogen is determined (the calculated total amount that will be consumed at t=∞). Initially, this value will be used in the kinetics calculation as the number of moles of hydrogen reagent present at t=0, k_{H2} (t=0).

$$k_{H2}\ (t=0)=mmolPd\text{x}\ (k\ mmol\ H/\ 1mmol\ Pd)\ \text{x}\ (1mmol\ H_2/\ 2mmol\ H)$$

The rate of hydrogen absorption is determined as

$$rate_{H2uptake} = -dk_{H2}/dt$$

The doping of source and drain is higher than of channel. The doping concentration is typically order of 10^{15} to 10^{16} per cm^3 for Si nanowire because SiNW doping concentration, with lower doping densities resulting in higher device sensitivity and 10^{18} to 10^{19} per cm^3 for source and drain.

3. SIMULATION RESULTS AND DISCUSSIONS

The changes of electrical characteristics are consistent regarding n-type SiNW surface functionalized with Pd because hydrogen is a reducing gas.

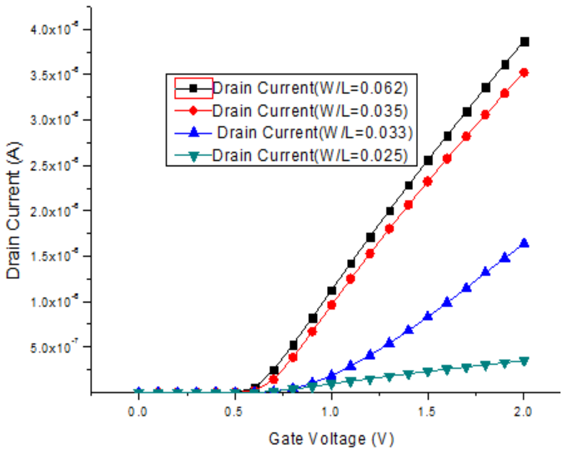

Fig:2 Id-Vg characteristics of n-type SiNW with different widths functionalized with palladium

Table:1Sensor performance with dimensions of SiNWs functionalised with Pd Film

SiNW (Dimensions)	Pd Fin (Dimensions)	Threshold Voltage (V)	Sensitivity for 0.03e charge of H_2 for conc. H/Pd=0.037 [5]
L=1µm W=50nm H=50nm	L=800nm W=50nm H=50nm	0.6V	85%
L=3µm W=70nm H=70nm	L=2000nm W=70nm H=70nm	0.6V	83.33%
L=5µm W=100nm H=100nm	L=3000nm W=100nm H=100nm	0.6V	70.2%
L=10µm W=200nm H=200nm	L=8000nm W=200nm H=200nm	0.6V	40.4%

When positive charged molecules bind on n-type SiNW surface it results in accumulation of the positive carriers thus increasing the conductance reading. The current-voltage characteristics of n-type Si- nanowire with different widths functionalized with palladium has shown in figure 2. The physical dimensions of the silicon nano wire have no influence up on the threshold voltage 0. 6 V but sensitivity of SiNWfunctionalized with palladium is decreasing with increasing the dimensions of SiNW, has shown in table 1.

4. CONCLUSION

Silicon nanowire (SiNW) having main transport channel of n-type modified by palladium (Pd) Film was designed with different physical dimensions for hydrogen detection. The change in physical dimensions effects on sensitivity of SiNW functionalized with Pd Film (fig 3).

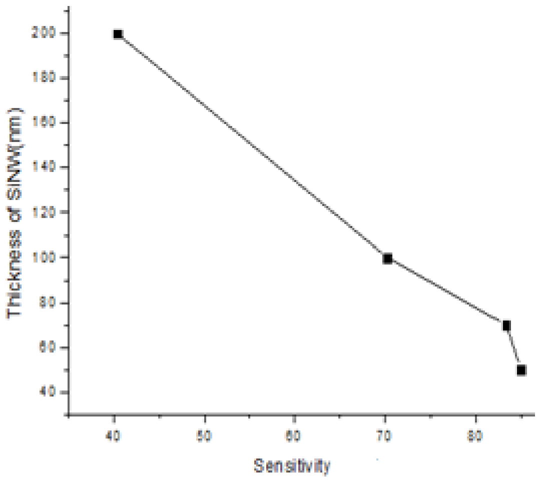

Fig:3 Graph between sensitivity v/s thickness of SiNW(nm)

The increase in sensitivity results from a decrease in thickness, because of the fact that the quantum confinement and surface to volume ratio becomes larger resulting into an efficient gating control of surface charges to conduction. It has been noticed that a Si-NW having a diameter greater than 100 nm works like a planar sensor [5]. When positive charged molecules bind on p-type SiNW surface it results in depletion of the positive carriers, conductance is decreasing.

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