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Palladium Gate All Around - Hetero Dielectric -Tunnel FET based highly sensitive Hydrogen Gas Sensor

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ABSTRACT

The paper presents a novel highly sensitive Hetero-Dielectric-Gate All Around Tunneling FET (HD-GAA-TFET) based Hydrogen Gas Sensor, incorporating the advantages of band to band tunneling (BTBT) mechanism. Here, the Palladium supported silicon dioxide is used as a sensing media and sensing relies on the interaction of hydrogen with Palladium-SiO_2-Si. The high surface to volume ratio in the case of cylindrical GAA structure enhances the fortuities for surface reactions between H_2 gas and Pd, and thus improves the sensitivity and stability of the sensor. Behaviour of the sensor in presence of hydrogen and at elevated temperatures is discussed. The conduction path of the sensor which is dependent on sensors radius has also been varied for the optimized sensitivity and static performance analysis of the sensor where the proposed design exhibits a superior performance in terms of threshold voltage, subthreshold swing, and band to band tunneling rate. Stability of the sensor with respect to temperature affectability has also been studied, and it is found that the device is reasonably stable and highly sensitive over the bearable temperature range. The successful utilization of HD-GAA-TFET in gas sensors may open a new door for the development of novel nanostructure gas sensing devices.

1. Introduction

Hydrogen gas (H_2) participates as a clean energy in fuel cells and energy carrier and thus acts as a strong candidate to replace fossil fuels that are at the edge of exhaustion. But the smaller size of H-atoms attributes to the risk of leakage and thus creates a need for the detection of H_2 gas for fuel monitoring. Moreover, H_2 is an extremely flammable gas as it can burn at a concentration of 4% in air and have a large window (4–75% v/v H_2) of flammability in comparison with methane, ethane, natural gas, etc. Thus, H_2 gas sensors have perpetual demand for automotive, environmental monitoring, petroleum refining process, and medical industries [1,2]. These gas sensors mainly work as transducer devices that detect the presence of H_2 gas, measure its concentration, and produce an electrical signal that is further calibrated with the magnitude of H_2 gas concentration. Out of various gas sensors such as catalytic sensors, semiconductor sensors, electrochemical sensors and infrared sensors; semiconductor sensors have numerous benefits and can be used for an extensive range of gases including toxic, combustible, etc. Further, the low cost, high sensitivity, stability, fast response time, wide operation temperature range and reliability make it highly applicative for detection of variety of gases [3–5].

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Palladium (Pd) has a very high selectivity towards H_2 gas. Pd based gas sensor rely on the fact that after absorption of H_2 gas, a chemical species called palladium hydride is formed, which has a comparatively high electrical resistance. Apart from high selectivity, out of several catalytic metals, the sensitivity of Pd for hydrogen is highly appreciable because of the sites located at Pd–SiO_2 interface (in case of MOS architecture based FETs such as MOSFET and TFETs) along with the surface reactions, participating in the catalytic reactions. It is also reported that at room temperature and atmospheric pressure, Pd can absorb up to 900 times its volume of hydrogen [6,7]. When H_2 molecules interact with Pd surface, the H_2 molecules dissociate on the surface of metal to form atomic hydrogen and some of the dissociated H-atoms diffuse through the Pd surface. The probability of dissociation of H_2 on Pd is almost unity, or H_2 dissociates very meritoriously on Pd. Within few nanoseconds, the diffused H-atoms reaches to the interface of Pd and SiO_2 or the H-atoms gets adsorbed at the SiO_2–Pd interface. The H-atoms reaching the metal-insulator interface gets polarised and forms surface dipole layer. This dipole layer in turns modulates the work function, conductivity, etc. and thus affects the device electrical properties. The high sensitivity of Pd for H_2 is mainly attributed to the great polarisation of H-atoms at the Pd–SiO_2 interface rather than the large diffusion of H-atoms through Pd [8,9].

The key focus of earlier research work had been to enhance sensitivity and selectively (for a particular gas) and is done by either exploring suitable sensitive films or by various device design engineering schemes. For high sensitivity and selectivity, numerous films such as metal compounds [10–12], polymers [13], organic compounds [14], hydrated salts [15] and catalytic metals [16–18] were used. In the novel device design, dual gate MOSFET; nanowire MOSFET, conventional TFET, etc. has already been taken into consideration. Till now in order to fulfill the requirement of sensing H_2 gas, silicon nanowire based H_2 gas sensor was proposed by Cao A et al. [2]. Further, to obtain appreciable sensitivity, the surface of SiNW FET sensor was functionalised with catalytic layers of Pd nanoparticles by Bongsik Choi et al. [19], for enhancing the selectivity and thus the sensitivity. Moreover, various gas sensors using metal oxide nanowires such as SnO_2, ZnO and In_2O_3 have been reported previously. A lot of work in the field of semiconductor gas sensors has been carried out with MOSFETs. But there is a need to investigate TFET as a gas sensor, as TFET is highly suitable for low power digital CMOS applications. The novel properties of TFET such as low leakage current, lower subthreshold swing (lower than 60mV/decade); immunity against short channel effects makes it an outstanding candidate for low power devices in the semiconductor industry [20–23]. Apart from these remarkable features, TFET suffers from few shortcomings such as low I_{ON}, ambipolar current and high threshold voltage. So to overcome these drawbacks, various engineering schemes were introduced such as hetero gate dielectric engineering, gate metal work function engineering, heterojunction devices, gate drain underlap/overlap TFETs, etc. In heterogate-dielectric (HD) scheme, a high-k material is locally inserted (near the source side) in the gate dielectric to enhance the ON-current [24]. The presence of high-k dielectric results into a higher band bending due to increasing surface potential (at a constant gate bias) [25–27]. This boosted band bending leads to reduction in tunneling barrier width, which further increases the generation rate and hence, on-current. In this work, the concept of palladium gate based Tunnel FET for H_2 gas sensing applications has been proposed. In addition, hetero gate dielectric engineering scheme and gate all around architecture has also been incorporated to further enhance the sensitivity of the hydrogen gas sensor.

2. Structural descriptions and simulation methodology

Table 1 indicates the structural parameters of all four devices based gas sensor which are compared for the improved sensitivity. For GAA-TFET and HD-GAA-TFET, cylindrical geometry is considered. In the case of HD-GAA-TFET, the channel consists of two regions; region 1 (near the source $L_1 = 20$ nm) and region 2 (near the drain $L_2 = 30$ nm). Region 1 consists of high-k dielectric (optimized value is 21 corresponds to HfO_2) and region 2 is of low-k dielectric (SiO_2, k = 3.9) whereas, in the case of GAA TFET, the entire channel consists SiO_2. In both the cases, radius (R) is 10 nm. To reduce ambipolarity effect, source and drain are doped asymmetrically in the case of TFET. Uniform doping profile has been considered in each case. The source and drain junctions are abruptly doped for an effective BTBT and the interface of high-k and SiO_2 is taken as abrupt. (see Fig. 1)

All simulations have been performed using ATLAS device simulator. The models activated during simulation of TFET Gas Sensor are as follows: concentration and field dependent mobility model, Shockley-Read-Hall for carrier recombination, non-local BTBT, band gap narrowing and Fermi-Dirac statistics. For conventional MOSFET based gas sensor, models invoked for simulation are: - Shockley-Read-Hall for carrier recombination, Lombardi CVT mobility model, concentration and field dependent mobility model and boltzmann transport statistics. The most important model for Tunnel FET simulations is the band-to-band tunneling (BTBT) model. A non-local model is chosen in this work instead of local model, to incorporate the effect of electric field at each point in the tunneling path. In local models such as Kane's model the triangular barrier

Table 1
Default structural parameters for all the devices based gas sensors.

Device	Parameters			
	Channel length (nm)	Source doping (cm^{-3})	Drain doping (cm^{-3})	Channel/Substrate doping (cm^{-3})
Conventional MOSFET	50	$n^+ -10^{19}$	$n^+ -10^{19}$	$p -10^{16}$
Conventional TFET		$p^+ -10^{20}$	$n^+ -5\times10^{18}$	$p -10^{16}$
GAA TFET		$p^+ -10^{20}$	$n^+ -5\times10^{18}$	$p -10^{16}$
HD-GAA- TFET	$50 = 20 + 30$ $L = L_1 + L_2$	$p^+ -10^{20}$	$n^+ -5\times10^{18}$	$p -10^{16}$

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