



A bottom-gate silicon nanowire field-effect transistor with functionalized palladium nanoparticles for hydrogen gas sensors



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ABSTRACT

The highly sensitive operation of a bottom-gate silicon nanowire (SiNW) field-effect transistor (FET)-based hydrogen (H₂) sensor is demonstrated by controlling the working regime of the sensor. It is observed that the deposition of palladium (Pd) nanoparticles on the SiNW surface for the selective absorption of H₂ can result in a significant enhancement of the electrostatic properties, such as the sub-threshold swing and on-current, of the SiNW FET-based H₂ sensor. By comparing the experimental results with the numerical simulation, we conclude that the improvement of the electrostatic properties of the sensor is due to the coupling effect between the electrostatic potentials in the Pd nanoparticle and bottom gate. Based on these results, highly sensitive detection of H₂ gas could be achieved in the subthreshold regime where the gating effect induced by absorbed H₂ gas is the most effective.

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1. Introduction

Silicon nanowires (SiNWs) are being actively explored for various sensor applications, such as pH sensors [1,2], biosensors [1–3], vapor sensors [4], and gas sensors [5–7], because of the high sensitivity resulting from their high surface/volume ratio. In addition, the reason for SiNWs being preferable is that they are readily compatible with the existing semiconductor processing technologies as they have easy control of electrical properties, facile surface functionalization with chemical linkers to molecules and mechanical and chemical robustness for various field of usage [2,8]. The typical structure of SiNW sensors is based on a bottom-gate field-effect transistor (FET) capable of converting chemical interaction into electrical signals [1,5,6]. The carrier density in the channel of SiNW sensors is generally modulated through the electrostatic potential applied to the bottom gate to enhance the sensitivity by controlling the working regime to the subthreshold regime, in which a maximal sensitivity can be achieved [9]. Therefore, the exposed SiNW channel surface of bottom-gate SiNW FET sensors is employed for the detection of various biological and chemical

species according to the functionalization of the SiNW surface [1,5].

Recently, hydrogen (H₂) sensors have been developed for a wide range of industrial applications, such as hydrogenation, petroleum refining processes, and hydrogen cooling systems [10,11]. Moreover, because H₂ has been considered to be a strong candidate as a future fuel and energy carrier, the utilization of H₂ sensors in the fuel cell applications, including leakage tests and fuel monitoring, has received increased attention [10,11]. In response to these demands, SiNW FET-based H₂ sensors are being developed since they can be easily fabricated by well-developed complementary metal-oxide-semiconductor (CMOS) compatible processes and their electrical properties can be easily tuned by doping [11]. However, because pristine SiNWs do not show appreciable sensitivity to H₂ [11], the surfaces in SiNW FET sensors should be functionalized with catalytic layers such as palladium (Pd) nanoparticles for the selective absorption of H₂ [5,11]. Therefore, a detailed investigation of the effect of Pd nanoparticles on the electrical properties of SiNW FET-based H₂ sensors is required to understand and optimize the device sensitivity, but insufficient studies have been performed to date. In addition, this type of investigation would be important in predicting the electrostatics of SiNW FET-based sensors for the detection of various gases in which diverse metal nanoparticles are used as catalysts.

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In this study, therefore, we conducted an in-depth analysis of the electrostatics of a SiNW FET-based H_2 sensor functionalized with Pd nanoparticles. Importantly, it was observed that the electrostatic potential of Pd nanoparticles functionalized on the surface of a SiNW could be coupled to that of the bottom gate of the SiNW FET-based H_2 sensor, resulting in a significant enhancement in the electrical properties of the sensor. Based on these results, the highly sensitive detection of H_2 gas could be achieved by adjusting the bottom-gate potential to control the working regime of the sensor to the subthreshold regime.

2. Device structure and I - V characteristics

A schematic of the SiNW FET-based H_2 sensor examined in this study is shown in Fig. 1(a). Detailed information regarding the fabrication of a bottom-gate SiNW FET was presented in our previous work [12]. The phosphorous doped n-type SiNW ($2 \times 10^{18} \text{ cm}^{-3}$) was fabricated on a 6" silicon-on-insulator (SOI) wafer using conventional CMOS technology. The boron doped p-type substrate underneath the 375 nm thick buried oxide in SOI wafer was used as a bottom gate. For the selective and sensitive detection of H_2 gas with the bottom-gate SiNW FET, the SiNW surface was functionalized with Pd nanoparticles by depositing a very thin Pd film (thickness $\sim 1 \text{ nm}$) using an electron beam evaporator. It is known that the deposition of a very thin metal film, which is deposited on a silicon oxide surface, will be formed in the form of nanoparticles instead of a continuous thin film because the metal atoms tend to agglomerate due to the low surface energy of the oxide (the native oxide in our case) [13]. Fig. 1(b) shows the scanning electron microscopy (SEM) images of the Pd nanoparticles deposited on the SiNW with the width (W_{NW}) of 70 nm, the length (L_{NW}) of 10 μm , and the height of 80 nm.

The transfer characteristics of the SiNW FET-based H_2 sensor with and without Pd nanoparticles on the SiNW surface were measured using an Agilent 4156C in an ambient condition (Fig. 2(a)). To avoid device-to-device variations, the same SiNW FET was characterized before and after the deposition of Pd layer. The SiNW FET without Pd nanoparticles showed a large subthreshold swing (SS) of 2.02 V/dec and a low on-current (I_{ON}) of 82 nA because the gate control of the device was weak due to the thick gate dielectric layer in the bottom-gate FET structure (375 nm). Herein, I_{ON} is defined as the drain current (I_{DS}) at the overdrive voltage, 15 V, and the overdrive voltage is defined as $V_{\text{BG}} - V_{\text{T}}$, where the V_{BG} is the bottom gate voltage and the threshold voltage (V_{T}) is defined by the current constant method (0.2 nA). Interestingly, we observed that the presence of Pd nanoparticles on the SiNW could significantly improve the transfer characteristics of the sensor. After the deposition of Pd nanoparticles, the SiNW FET showed significant enhancements in I_{ON} and SS from 82 to 329.20 nA and from 2.02 to 0.34 V/dec, respectively. It should be noted that this finding is in contrast to previously reported results for H_2 sensors featuring a two-terminal SiNW structure [5]. For two-terminal SiNW H_2 sensors, it has been observed that I_{ON} tends to decrease after the deposition of Pd nanoparticles, which can be explained by the electron depletion at the Pd nanoparticle–SiNW interface due to the high work function of Pd nanoparticles [5]. However, our results show the opposite trend, i.e., an increase in I_{ON} and a steeper SS, indicating that the gate control over the SiNW channel could be improved via a coupling effect between the bottom gate and floating Pd nanoparticles. Moreover, the enhancement in the electrical properties became more prominent as W_{NW} was decreased, as shown in Fig. 2(b). Similar results have been observed for SiNW biosensors in which the presence of an electrolyte in the SiNW results in a significant enhancement in the transfer characteristics of bottom-gate SiNW FETs due to a coupling effect between the electrostatic potentials in the electrolyte and bottom gate [14,15].

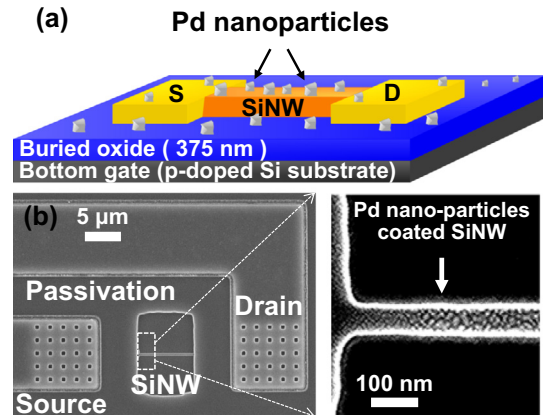


Fig. 1. (a) Schematic of a SiNW FET with a bottom-gate structure for H_2 sensing. For the detection of H_2 , Pd nanoparticles were deposited on the surface of the SiNW. (b) SEM images of the fabricated device with deposited Pd nanoparticles.

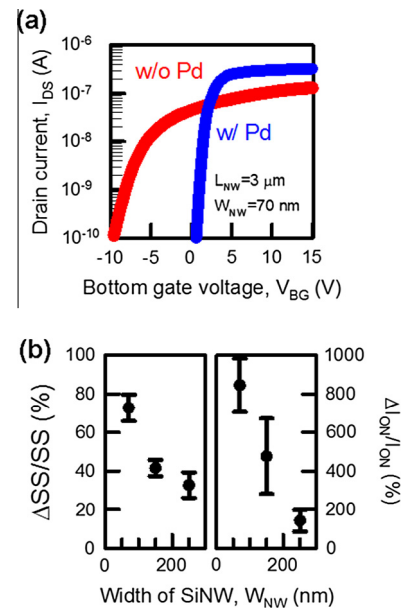


Fig. 2. Electrostatic characteristics of a SiNW FET sensor functionalized with (w/) and without (w/o) deposited Pd nanoparticles. (a) The $I_{\text{DS}}-V_{\text{BG}}$ characteristics of the sensors w/ and w/o Pd nanoparticles at $V_{\text{DS}} = 50 \text{ mV}$. (b) Variation in $\Delta\text{SS}/\text{SS}$ and $\Delta I_{\text{ON}}/I_{\text{ON}}$ as a function of W_{NW} . ΔSS and ΔI_{ON} are defined as the differences in the respective characteristics between the sensors w/ and w/o Pd nanoparticles.

3. Simulation result and discussion

In fact, the direct measurement of gate capacitance is the best way to investigate the enhanced gate control afforded by Pd nanoparticles, but it is difficult to measure the extremely low gate capacitance at the aF-fF level because it is shadowed by a large background parasitic capacitance [16]. Therefore, a 3D TCAD simulation was performed in order to confirm the effect of Pd nanoparticles on the electrical characteristic of the bottom-gate SiNW FET examined in this study [17]. To simplify the simulation, we considered a thin Pd layer, which was defined to be in a floating state to describe the role of Pd nanoparticles on the SiNW surface. The length, width, height of the SiNW in the simulation were set to 1 μm , 70 nm, and 80 nm, respectively, to make the simulation results comparable to the experimental data. The thickness of the native oxide layer covering the SiNW was set to 3 nm, and the SiNW was assumed to be n-type doped, with $N_d = 2 \times 10^{18} \text{ cm}^{-3}$. The simulated cross-sectional electron current density along the

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