Comprehensive analysis of hydrogen sensing properties of a Pd-gate metal-semiconductor high electron mobility transistor

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The electric and hydrogen sensing properties of an interesting Pd-gate metal-semiconductor-type high electron mobility transistor are comprehensively studied. The dipolar layer formed by adsorbed hydrogen atoms at the semiconductor of Pd–AlGaAs interface is equivalent to a two-dimensional layer. The concentration of available hydrogen adsorption sites at the metal-semiconductor interface is equivalent to a two-dimensional layer. Furthermore, the simulated curves are in excellently agreement with the experimental results. © 2007 American Institute of Physics.

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Recently, hydrogen has been recognized as an energy source medium that has the potential to overcome problems associated with fossil fuels. However, hydrogen is highly combustible with a lower explosion limit of 4.65% in air. Thus, the effective hydrogen monitoring is required for process control of hydrogen-based energy systems. A chemical hydrogen sensor is, in short, a device that transforms a chemical state into an electrical signal. The output signal is based on the change in work function of a gas sensitive material which is caused by the reaction or interaction with the target gas molecules. Once hydrogen sensors with a catalytic Pd-gate metal have become the interesting searching principles in the field of solid-state sensors. Although these electric signals are measured for various types of detectors, it is currently believed that these changes are attributed to the adsorption of atomic hydrogen resulting in the formation of a dipolar layer at the catalytic metal-semiconductor (or metal-insulator) interface. In this work, a Pd–AlGaAs metal-semiconductor (MS)-type high electron mobility transistor (HEMT) hydrogen sensor is fabricated and comprehensively studied. The principle is based on the fast diffusion of hydrogen through the catalytic Pd metal and a connected change of the surface potential at the Pd–AlGaAs interface which shifts the threshold voltage of the studied HEMT. This effect is observable even at room temperature. The image charge effect is also considered in this study. The theoretically simulated electric and hydrogen sensing properties are obtained by using the two-dimensional device simulator integrated systems engineering (ISE).

The studied hydrogen sensor was grown by a low-pressure metal organic chemical vapor deposition system on a (100) oriented semi-insulated GaAs substrate. The detailed epitaxial structure consisted of a 5000-Å-thick GaAs undoped buffer layer, a 150-Å-thick undoped In0.15Ga0.85As channel, a 45-Å-thick undoped Al0.25Ga0.75As spacer, a 100-Å-thick doped buffer layer, a 150-Å-thick n+-Ga0.76As cap layer. The mesa etching was first employed to etch the samples into the substrate with a H3PO4 :H2O2 :H2O solution at room temperature. Schottky contact layer, and a 600-Å-thick n1+Ga0.76As cap layer. The mesa etching was first employed to etch the samples into the substrate with a H3PO4 :H2O2 :H2O (1:1:20) solution at room temperature to isolate devices. Then, the drain-source Ohmic contacts were formed by evaporating Au/Ge/Ni metals on the n1+GaAs cap layer and alloying in nitrogen gas at 380 °C for 20 s. The chemically etched surfaces were prepared by removing the native oxide with a solution of HF:H2O1:1 and the gate recess process was used by a solution of H3PO4 :H2O2 :H2O (3:1:500). Finally, the gate Schottky contacts with a gate length of 1.4 μm were achieved by depositing the catalytic Pd metal on the Al0.25Ga0.75As Schottky contact layer.

It is well known that the hydrogen sensing mechanism can be expressed by the reaction kinetics as follows. As the introduced hydrogen gas touches with the catalytic Pd-gate metal, hydrogen molecules are dissociated as hydrogen atoms and these hydrogen atoms are adsorbed on the metal surface. Some of hydrogen atoms diffuse through the thin catalytic Pd metal film and adsorbed on the metal-semiconductor interface. These adsorbed hydrogen atoms will be polarized to form a dipolar layer, which results in an opposite potential drop with respect to the applied voltage.

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This potential change $\Delta V$ can be determined by the hydrogen coverage at the interface as:

$$\Delta V = \frac{p n_i}{\varepsilon_s},$$  \hspace{1cm} (1)

where $p$ is the equivalent dipole moment induced by the adsorbed hydrogen atoms at the interface, $n_i$ the amount of adsorbed atoms per unit area or adsorbed sites at Pd-semiconductor interface, and $\varepsilon_s$ the dielectric permittivity of Al$_{0.24}$Ga$_{0.76}$As. Figure 1 illustrates the adsorbed atoms at the Pd-semiconductor interface $n_i$ as a function of hydrogen concentration. Clearly, good linear relationship between the adsorbed atoms $n_i$ and hydrogen concentration is observed at lower hydrogen concentration (below 500 ppm H$_2$/air). However, this linear phenomenon is relatively diverged because the interface sites are almost filled and the dynamic interface equilibrium will be established. Thus, a saturation trend is found as exposing to higher-concentration hydrogen gases. Furthermore, the concentration of available hydrogen adsorption sites at the Pd–AlGaAs interface under 9970 ppm H$_2$/air gas is approximately $10^{14}$ cm$^{-2}$. This saturated value is also in agreement with previous observations.

As the hydrogen atoms traveled through the Pd metal and adsorbed at the Pd–AlGaAs interface, the formation of dipoles together with their image charges in the Pd metal can be observed. This image effect will cause the lowering of Schottky barrier height. Figure 2(a) is the schematic illustration of the studied device upon exposing to hydrogen gases. Because the electrostatic potential perpendicular to a dipole is zero, these dipoles will only slightly change the electrostatic energy. Also, it is believed that the hydrogen atoms adsorb at the semiconductor side of metal-semiconductor interface. By using the ISE simulator, the dipolar layer formed by adsorbed hydrogen atoms at the Pd–AlGaAs interface is equivalent to a two-dimensional layer. Two important factors determine this equivalent layer. One is the concentration of available hydrogen adsorption sites at the metal–semiconductor interface $n_i$ (as shown in Fig. 1) and the other is the effective distance $d$ from the metal-semiconductor interface to adsorbed hydrogen atoms. In Fig. 2(b) the experimental and simulated drain saturation currents $I_{DS}$ are plotted as a function of gate-source voltage $V_{GS}$ under 980 ppm H$_2$/air gas at room temperature. By considering the influence of effective distance $d$, the $d$ value is varied from 1 to 5 Å. Also, the amount of adsorbed hydrogen atoms at the interface $n_i$ is kept as $9.5 \times 10^{13}$ cm$^{-2}$. Clearly, as the $d$ value is set as 3 Å, the simulated curve is almost matched to the experimental curve. In addition, the corresponding drain saturation current is increased with increasing the effective distance $d$. Figure 3 shows the simulated and experimental typical common-source output current-voltage ($I-V$) characteristics of the
device are firstly determined and simulated using the two-dimensional device simulator ISE. According to the hydrogen sensing mechanism, the dipolar layer formed by adsorbed hydrogen atoms at the semiconductor of Pd–AlGaAs interface is equivalent to a two-dimensional layer. The saturated value of the amount of adsorbed hydrogen atoms at the interface $n_i$ is estimated as $1 \times 10^{14}$ cm$^{-2}$. This value is in agreement with previous observations. The concentration of available hydrogen adsorption sites at the metal-semiconductor interface $n_i$ is $9.5 \times 10^{13}$ cm$^{-2}$ and the effective distance from the metal-semiconductor interface to adsorbed hydrogen atoms $d$ is about 3 Å. The simulated curves in $I$-$V$ characteristics are almost matched to the experimental results.

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**FIG. 3.** Simulated and experimental results of typical common-source output $I$-$V$ characteristics at room temperature in air and under 50.2 and 980 ppm H$_2$/air gases, respectively.

**FIG. 4.** Hydrogen current-response curves upon the introduction and removal of different concentration hydrogen gases at 52 °C. The applied voltages are biased at $V_{GS}=-0.3$ V and $V_{DS}=1.2$ V.