Schottky and ohmic contacts of Pd on *p*-type GaAs distinguished with hydrogen

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Contacts of Pd on *p*-type GaAs with a native oxide layer between them reveal ohmiclike behavior in air or vacuum at room temperature. This behavior is similar to that of contacts annealed at 450 °C for 5 min. To relate the interface electrical properties of the two contacts to their interfacial structures, we propose to measure current-voltage (I-V) and capacitance-voltage (C-V) characteristics in a hydrogen ambient. We show that these two contacts can be distinguished with atomic hydrogen. This method was confirmed with I-V and C-V measurements at low temperatures.

I. INTRODUCTION

Both Schottky and ohmic contacts of metal on semiconductor are essential to semiconductor devices. For Schottky contacts there are various models developed to explain its formation mechanism.[1] However, they do not provide complete satisfactory explanations for all the experimental results, indicating the complexity of correlating electrical properties and interfacial structure. In fact, particular metal/semiconductor combinations may be dominated by their specific interactions. From that perspective, here we report a study of Pd on *p*-type GaAs (Pd/GaAs) contacts. The Pd/GaAs contacts with different interfacial structures, i.e., the as-deposited and high-temperature-annealed contacts, show usually similar ohmiclike behavior[2] when measured at room temperature (RT). After heat treatment at high temperature, about 450 °C, Pd/GaAs contacts are always ohmic.

Palladium reacts easily with GaAs, even during the deposition at RT, resulting in a Pd-Ga-As metallic ternary phase at the Pd/GaAs interface.[3–6] This metallic compound makes an intimate contact with GaAs, forming a Schottky contact. The barrier height for this kind of contact is about 0.88 eV for *n*-type and 0.58 eV for *p*-type GaAs.[7] It is also found that the native oxide layer on GaAs has a retardation effect on the reaction of Pd and GaAs. Depending on surface treatment and deposition conditions, a Pd/oxide/GaAs structure can be obtained at RT. In this case, the difference in barrier height between *n* type and *p* type increases; it is much higher for *n*-type but quite low (ohmiclike) for *p*-type GaAs.[7] Heat treatment causes the usual reaction of Pd and GaAs. Another particular feature of Pd/semiconductor contacts is that hydrogen can affect their electrical properties (hydrogenation).[8] It is already known that hydrogen permeates through the Pd film and accumulates at the interface, where hydrogen induces electrical dipole changing the barrier height,[8] causing a decrease for *n*-type and an increase for *p*-type GaAs.[7]

We will clarify the reason, by experimental results, for that: the electrical properties are similar whereas the interfacial structures are different between the as-deposited and annealed Pd/GaAs contacts. We carry out conventional current-voltage (I-V) and capacitance-voltage (C-V) measurements[9] at RT in air, vacuum, and hydrogen in order to study the variation of the electrical properties with hydrogen. We also measure the electrical properties at RT and low temperatures to find out whether the ohmiclike behavior of the two contacts at RT changes with temperature. By using these measurements, the electrical properties of Pd/GaAs contacts can be related to the structural aspects to more extent than usually.

II. EXPERIMENT

A Zn doped *p*-type GaAs (100) substrate with a carrier concentration of 6×10^{16} cm^3 was used in this study. A conventional ohmic electrode on the back side of the GaAs substrate was prepared prior to the surface treatment.[7] The surface was prepared by conventional etching with sulfuric acid solution. Palladium dots 500 μm in diameter were deposited onto the GaAs surface by the resistive heating method in vacuum with a base pressure of 1×10^{-8} Torr. Details on the preparation of Pd/GaAs samples were reported elsewhere.[7] Annealing was carried out in argon gas flow at 450 °C for 5 min. I-V and C-V methods[9] are used to measure the electrical properties of the as-deposited and annealed samples as a function of temperature and ambient. The barrier height is estimated from the intercept at the current-density axis, and the ideality factor from the slope of the I-V curve. For simplicity, the current at reverse bias will be inverted in the I-V figures. The barrier height is also estimated from the carrier concentration, temperature, and the intercept at the voltage axis of the C-V curve. Helium cryostat provides temperature control between RT and 4.2 K. Hydrogen ambient, with pressures of about 0.5 atm, was provided by flowing hydrogen gas into the evacuated cryostat.

III. RESULTS AND DISCUSSION

Figure 1 shows the RT-measured I-V curves of the as-deposited and annealed Pd/GaAs contacts in air or vacuum. The data in the linear scale, shown as an inserted graph in Fig. 1, indicate that the current changes linearly with bias voltage. We note that both contacts have similar I-V behav-

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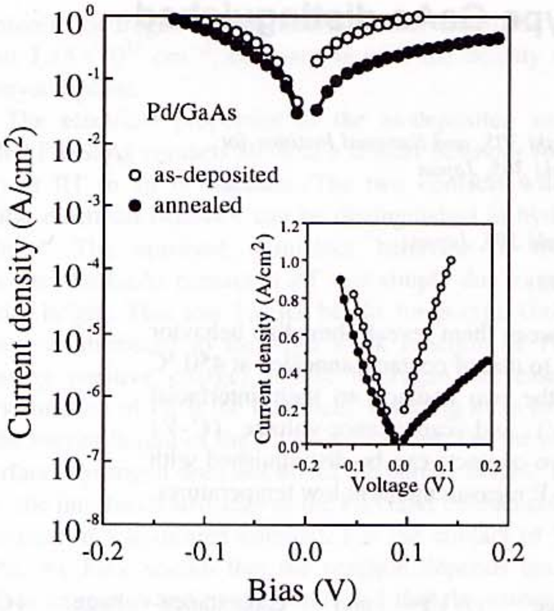

FIG. 1. The *I-V* curves for the as-deposited and annealed (450 °C) Pd/GaAs contacts. The insert shows the data in the linear scale, indicating ohmiclike behavior for both contacts.

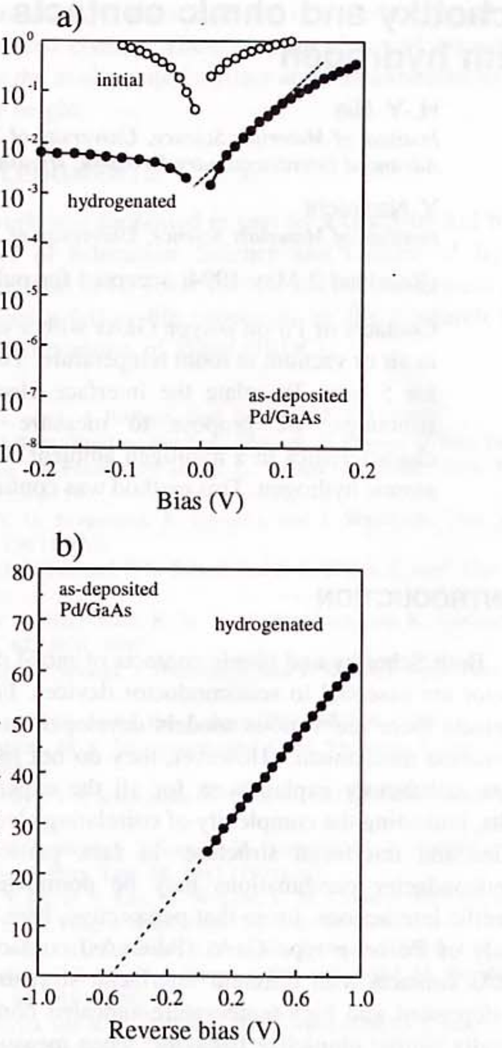

FIG. 2. *I-V* curves in air or vacuum and in hydrogen ambient (a), and the *C-V* curve at reverse bias in hydrogen ambient (b) for the as-deposited Pd/GaAs contact at RT. The current is decreased largely and behaves as a Schottky contact. The dotted line indicates how we analyze the electrical properties in the *I-V* and *C-V* curves. For the annealed (450 °C) contact, no change is detected in hydrogen ambient (not shown).

ior. This ohmiclike behavior precludes the measure of the capacitance for this system. We note that Pd/GaAs contacts become ohmic with heat treatment at temperatures of 400–500 °C.[2] In fact, Pd is usually used for ohmic contact formation to *p*-type GaAs.[10,11] Therefore, for the annealed contact the ohmic behavior can be attributed to the interaction of Pd with GaAs at high temperature. In this paper, we will not discuss the mechanism of ohmic contact formation at high temperature, but we will concentrate on the ohmiclike behavior of the as-deposited Pd/GaAs contact.

The structure of the Pd/GaAs interface has been studied with cross-sectional transmission electron microscopy,[3] x-ray diffraction,[12] and sputtering Auger electron spectroscopy.[7,13] There were oxygen signals at the as-deposited Pd/GaAs interface in sputtering Auger electron spectroscopy. This result is similar to the previously reported one.[7] Therefore, a native oxide layer between Pd and GaAs in the as-deposited Pd/GaAs contact can exist, providing that Pd does not react with GaAs. Occasionally, Pd can react with GaAs during deposition at RT by penetrating through the cracks of the native oxide layer, forming a ternary phase of Pd-Ga-As.[3] Annealing of Pd/GaAs interfaces at about 250 °C results in the ternary phase invariably. No oxygen signal is detected at this reacted interface with sputtering Auger electron spectroscopy.[7] This phase is a metallic compound[3] and results in a Schottky contact with a barrier height of about 0.58 eV for *p*-type GaAs.[7] Therefore, the ohmiclike behavior of the as-deposited contact shown in Fig. 1 may be a consequence of the existence of the native oxide layer between Pd and GaAs.

It is difficult to distinguish the as-deposited from the annealed contacts with the electrical measurements at RT in air or vacuum, although the interfacial structures are obviously different between them. Thus we raise the question of why different interfaces reveal similar electrical properties.

In order to distinguish between these two contacts, we measured them in hydrogen ambient at RT. Shown in Fig. 2 are the results of the *I-V* measurements in air or vacuum (initial) and in hydrogen ambient (a) and the *C-V* curve in hydrogen ambient (b) for the as-deposited Pd/GaAs contact. There appears a remarkable decrease in the currents both at forward and reverse biases after hydrogenation. Moreover, the currents at forward and reverse biases reveal a different variation with bias, indicating that a Schottky contact is formed upon hydrogenation. From the forward *I-V* curve in Fig. 2(a), the barrier height of the hydrogenated contact was estimated to be 0.50 eV with an ideality factor of 1.40. As shown in Fig. 2(b), the capacitance of the as-deposited contact become measurable after hydrogenation. From the capacitance measurement at reverse bias, a barrier height of 0.70 eV is obtained. However, for the annealed Pd/GaAs contact in hydrogen ambient, no change in the *I-V* curve was detected, and also the capacitance was not measurable.

The different response of the electrical properties to hydrogen action between the two contacts is considered to result from the different interfacial structure between them. Hydrogen is known to dissolve into the Pd film and to accumulate at the Pd/oxide interface.[8] It has been reported that the atomic hydrogen induces positive charge at the interface, increasing the barrier height for p-type Schottky contact with a native oxide layer between Pd and GaAs.[7] The electrical properties between the as-deposited and annealed contacts are, therefore, distinguished with atomic hydrogen as an effective probe. The ohmiclike behavior for the as-deposited contact as measured in air or vacuum (Fig. 1) is caused by the low barrier height. However, this low barrier height for the as-deposited contact is not measurable at RT.

Temperature is an important factor in the I-V characteristics of metal/semiconductor contact. In order to estimate the barrier height of the as-deposited Pd/GaAs contact and confirm the difference of the electrical properties between the as-deposited and annealed Pd/GaAs contacts, we carried out measurements at low temperatures. The I-V curves at a low temperature of 100 K for the two contacts are shown in Figs. 3(a) and 3(b). It is clear that the I-V curves at low temperature reveal a remarkable difference between the two contacts. Figures 3(a) and 3(b) show Schottky behavior for the as-deposited but still ohmic behavior for the annealed contacts. The barrier height of the as-deposited contact was estimated from the I-V measurement at 100 K as 0.27 eV with an ideality factor of 1.47. In the thermionic emission theory, the current of a Schottky contact at a certain applied voltage is a strong function of temperature.[9] This behavior was observed in the as-deposited but not in the annealed contacts. The low-temperature I-V curve for the annealed contact has ohmic behavior, and changed only slightly from that at RT. For the as-deposited contact, the capacitance became measurable, as shown in Fig. 3(c), and a barrier height of 0.44 eV was obtained from the C-V measurement. For the annealed contact at 100 K, no capacitance was measurable due to its ohmic behavior. In fact, we found that the capacitance was not measurable even at the lowest temperature obtainable in our cryostat, 4.2 K. Also, the I-V curve was confirmed to be of ohmic behavior at 4.2 K.

The barrier heights estimated, respectively, from the I-V and C-V measurements are different. This difference usually appears in Schottky contacts and becomes remarkable when the ideality factor departs largely from unity.[14] The ideality factor of the as-deposited Pd/GaAs contact is 1.40 at RT and 1.47 at 100 K. This large ideality factor is attributed partly to the existence of the native oxide layer at the interface and to the low barrier height. Therefore, we use the value estimated from the C-V measurement in the following discussion.

Barrier height of a Schottky contact does not change appreciably with temperature. Therefore, we assumed the barrier height of the as-deposited Pd/GaAs contact at RT to be about 0.44 eV, the value obtained at 100 K from the C-V measurement. The barrier height at RT in hydrogen ambient has been estimated from Fig. 2(b) to be 0.70 eV. Thus the increase of the barrier height due to the accumulation of hydrogen at the interface is about 0.26 eV. Following the dipole model for hydrogen at the interface,[8] a concentration

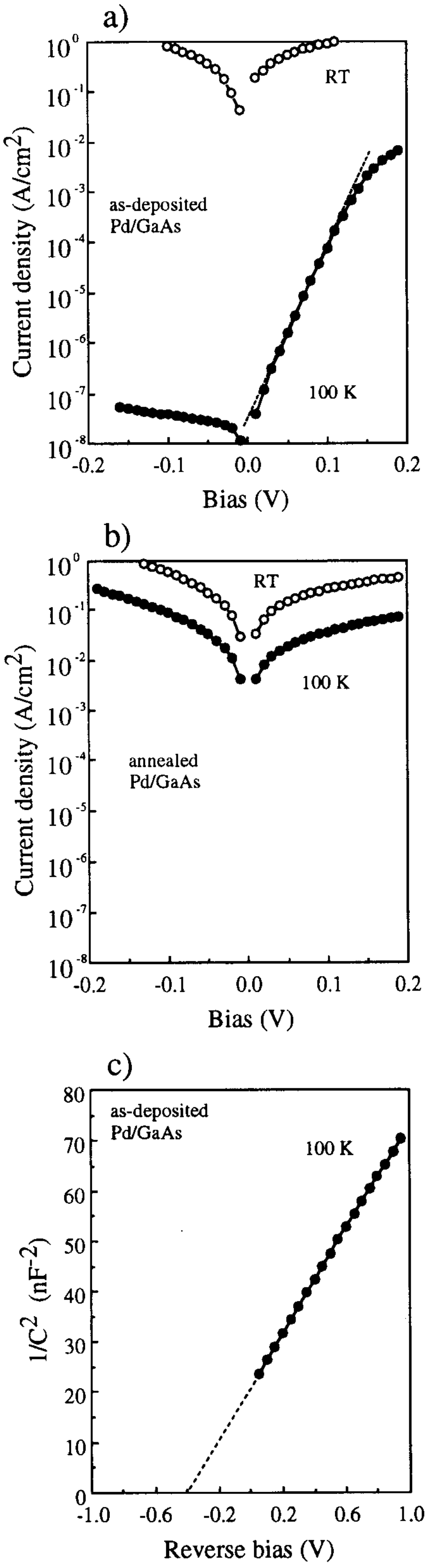

FIG. 3. The I-V curves in vacuum at 100 K for (a) the as-deposited and (b) the annealed (450 °C) Pd/GaAs contacts. The current (a) decreases largely and behaves as a Schottky contact for the as-deposited, (b) but is still of ohmic behavior with a slight decrease for the annealed contacts. The capacitance becomes measurable for the as-deposited (c) but still not for the annealed contacts. The dotted line indicates how we analyze the electrical properties in the I-V and C-V curves.

of atomic hydrogen at the interface was estimated to be about 1.15×10^{15} cm^{-2}, comparable with the density of the Pd crystal plane.

The electrical properties of the as-deposited and annealed Pd/GaAs contacts showed a similar behavior (ohmiclike) at RT in air or vacuum. The two contacts with this similar electrical behavior can be distinguished in hydrogen ambient. The apparent ohmiclike behavior of the as-deposited Pd/GaAs contact at RT was simply due to the low barrier height. This low barrier height for p-type GaAs, in return, is attributed to the high work function of Pd. By inducing positive charge, atomic hydrogen decreases the work function of Pd at the interface,[8] resulting in an increase of the barrier height of the Pd/GaAs contact. For the reacted interface, hydrogen does not affect the barrier height. Therefore, the interfacial structure of the Pd/GaAs contact could be examined in a hydrogen ambient. For the contact of Pd on GaAs, we have shown that the reaction depends upon the surface treatment and temperature, and that the native oxide on GaAs has a retardation effect on the reaction.[7] This unique feature of the Pd/GaAs interface suggests the possibility of controlling the interfacial structure of the Pd/GaAs contact with either surface treatment or heat treatment.

IV. CONCLUSIONS

The as-deposited and annealed (450 °C) Pd on p-type GaAs contacts with a similar ohmiclike behavior at RT in air or vacuum were distinguished and related to their interfacial structures with atomic hydrogen as an effective probe. This method was confirmed by observing the variation of the electrical properties of the two contacts with temperature. We suggested that atomic hydrogen accumulated at the Pd/oxide interface and the resulting induced positive charge there caused an increase of about 0.26 eV in the barrier height of the as-deposited contact. Therefore, the observed ohmiclike behavior of the as-deposited contact at RT is attributed to the low barrier height.

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