Article

Ohmic Contact of Pt/Au on Hydrogen-Terminated Single Crystal Diamond

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Abstract: In this study, contact properties of platinum/gold (Pt/Au) on the surface of hydrogen-terminated single crystal diamond (H-SCD) were studied with several treatment conditions. The electrodes of Pt (20 nm)/Au (100 nm) were deposited on H-SCD surface by electron beam evaporation technique. Then, the specific contact resistance ($\rho_c$) of the as-fabricated sample was measured by the circular transmission line model, which showed good ohmic properties with the value of $5.65 \times 10^{-4} \Omega \cdot \text{cm}^2$. To identify the thermal stability of Pt/Au/H-SCD, the sample was annealed in hydrogen ambient from 200 to 700 °C for 20 min at each temperature. As the temperature increased, $\rho_c$ demonstrated better thermal stability. In addition, the barrier height was evaluated to be $-0.67 \pm 0.12 \text{eV}$ by X-ray photoelectron spectroscopy (XPS) technique.

Keywords: diamond; platinum; ohmic contact; annealing; XPS

1. Introduction

Diamond exhibits excellent properties [1–4], such as wide bandgap (5.47 eV), high breakdown field (>10 MV·cm⁻¹), high thermal conductivity (22 W·cm⁻¹·K⁻¹), high carrier saturation velocity ($10^7$ cm·s⁻¹), low dielectric constant (5.7), high carrier mobility of electron (4500 cm²·V⁻¹·s⁻¹) and hole (3800 cm²·V⁻¹·s⁻¹), etc., demonstrating a potential application in the field of electronic devices such as Schottky diodes [5–8], field-effect transistors (FETs) [9–12], and other electronic devices [13,14]. However, the immaturity of doping processes greatly limits the development of diamond-based electronic devices. Hydrogen-terminated single crystal diamond (H-SCD) [15–18] presents a potential solution to this challenge due to the formation of a two-dimensional hole gas (2DHG) layer on the diamond surface with high carrier density of $10^{13}$ cm⁻² and high carrier mobility of 200 cm²·V⁻¹·s⁻¹. Besides, H-SCD epitaxial layers can be used to fabricate diamond-based devices. Along with the improvement in the performance of diamond-based devices, an excellent ohmic contact between the electrode metal layer and the diamond film is vital. So far, many investigations of ohmic contact between metal and diamond have been reported. Metals such as gold (Au) [19], palladium (Pd) [20], and iridium (Ir) [21], were used as contact material for H-SCD diamond, which showed good ohmic properties. The properties like high melting point and good chemical stability indicate platinum (Pt) as a good material for ohmic contacts. Therefore, it can be considered as a promising candidate to form ohmic contact with diamond film. Nevertheless, few investigations of Pt/Au/H-SCD ohmic contact were reported.
In this work, contact properties of Pt/Au/H-SCD were investigated with various treatments. The annealing processes with different temperatures were performed to determine the thermal stability of the ohmic contact, and specific contact resistance (pc) was evaluated by circular-transmission line model (C-TLM). Furthermore, XPS measurement was utilized to identify the barrier height at the interface of Pt/Au/H-SCD.

2. Experiment

$\text{Ilb-type (100)-oriented high-pressure high-temperature (HPHT) SCD with the dimension of} 3 \text{ mm} \times 3 \text{ mm} \times 0.5 \text{ mm was used as the substrate. The schematic of the fabrication processes of the Pt/Au/H-SCD is shown in Figure 1. The diamond substrate was cleaned in an acid mixture solution of H}_2\text{SO}_4:\text{HNO}_3:\text{HClO}_4 = 31.2:36:11.4 \text{ at 250 °C for 1 h, and then in a mixed alkali solution of NH}_4\text{OH:H}_2\text{O}_2:H_2\text{O} = 4:3:9 \text{ at 80 °C for 10 min to remove nondiamond impurities. Then, 200 nm undoped, homoepitaxial SCD was grown by microwave plasma CVD (MPCVD, AX5250S, Cornes Technologies Ltd., Tokyo, Japan) to produce the H-SCD. During diamond growth processes, the total gas flow, CH}_4/H_2 \text{ ratio, pressure, temperature, and power were 500 sccm, 1%, 100 Torr, 900 °C, and 1 kW, respectively. After growth, hydrogen plasma was kept for 10 min to form the hydrogen termination, and the sample was cooled down in pure hydrogen ambient. Thereafter, the photolithography technique was used to pattern C-TLM configuration with 200 μm diameter inner circle electrodes, and the outer electrodes spacing varied from 5 to 30 μm. Finally, Pt (20 nm)/Au (100 nm) electrodes were deposited on the H-SCD surface by electron beam evaporation technique (EB, VPC-1100, ULVAC, Billerica, MA, USA). Moreover, ohmic contact was studied by annealing at 35 Torr pressure and hydrogen ambient for 20 min, with temperatures ranging from 200 to 700 °C.}$

![Figure 1. The fabrication process of Pt/Au/H-SCD.](image)

3. Result and Discussion

The single crystal diamond surface morphology was evaluated by an atomic force microscope (AFM, Innova, Bruker, Billerica, MA, USA) with the scan range 5 μm, which showed a smooth surface with the root mean square (RMS) roughness around 0.6 nm [22,23]. Along with that, the Hall measurement of the diamond was performed at room temperature, with the carrier density, square resistance, and mobility of $1.4 \times 10^{13} \text{ cm}^{-2}$, 12.4 kΩ, 35.4 cm² V⁻¹ s⁻¹, respectively. Besides, X-ray diffraction (XRD, X’Pert Pro MRD, PANalytical B.V., Almelo, The Netherlands) was carried out to determine the quality of the epitaxial diamond film, which is shown in Figure 2a. The XRD rocking curve of (004) orientation exhibits a relatively low full-width-at-half-maximum (FWHM) of 42.3 arcsec.
which shows a good crystalline quality of diamond film [20,24]. As shown in Figure 2b, the scanning electron microscopy (SEM, Quanta FEG250, FEI, Hillsboro, OR, USA) image of C-TLM configuration fabricated on H-SCD is very neat, indicating a good fabrication process.

For the C-TLM configuration, the total resistance $R_T$ (acquired by $V/I$) can be expressed by Equation (1) [25], where $R_s$ is the sheet resistance, $L_T$ is the transfer length, $r_n$ and $r_0$ are the radius of outer circle and inner circle, respectively. On the other hand, $\rho_c$ can be calculated by Equation (2) [25].

In order to study the thermal stability of Pt contact on diamond film, an annealing process was carried out. As we know, the desorption of carbon–hydrogen dangling bonds would occur to the H-SCD surface after long-time annealing at high temperature, and the carbon–hydrogen bonds were passivated during annealing at hydrogen ambient for a protection [26]. Accordingly, the Pt/Au/H-SCD sample was subjected to annealing treatment at several temperatures ranging from 200 to 700 °C in hydrogen ambient for 20 min. The specific contact resistance values of Pt/Au/H-SCD with different annealing temperature are shown in Figure 3. For the as-fabricated sample, $\rho_c$ was $5.65 \times 10^{-4}$ Ω·cm$^2$, illustrating good ohmic properties even without the annealing process. As temperature increased, $\rho_c$ approached $9.80 \times 10^{-5}$ Ω·cm$^2$ at 700 °C, which was lower than that of the as-fabricated sample. And, it is clear that $\rho_c$ changed no more than one order of magnitude with the variation of the temperature, demonstrating excellent thermal stability of the ohmic contact.

$$R_T = \frac{R_s}{2\pi} \ln \left( \frac{r_n}{r_0} \right) + \frac{R_s}{2\pi} \frac{2}{r_0} L_T$$  \hspace{1cm} (1)

$$\rho_c = R_s L_T^2$$  \hspace{1cm} (2)

![Figure 2. (a) XRD image of H-SCD, (b) SEM image of C-TLM structures fabricated on H-SCD.](image)

![Figure 3. The specific contact resistance values of Pt/Au/H-SCD with different annealing temperature.](image)
As displayed in Figure 4a, the $I$-$V$ properties were measured at room temperature for the as-fabricated sample, with the 5 μm space electrodes between two C-TLM pads. Subsequently, the sample was annealed with temperatures ranging from 200 to 700 °C. It is evident that the $I$-$V$ plots exhibit good ohmic properties for all the curves. There was no degradation of the ohmic properties with different annealing temperatures. As the annealing temperature increased, the linear slope increased, indicating the decrease of resistance between the measured Pt electrodes, which could be attributed to the improvement of the interface performance by the annealing process. Besides, when the annealing temperature was increased higher than 200 °C, the current saturation occurred, which could be ascribed to the 10 mA overcurrent protection setting. Figure 4b shows the $R_T$ versus the spacing $d$ for Pt/Au/H-SCD contact annealed at 700 °C. The fitted curve shows a good linear characteristic, which indicates good behavior of ohmic contacts.

![Figure 4](image-url)  
(a) $I$-$V$ characteristics of as-fabricated and annealed Pt/Au/H-SCD with the same C-TLM pattern, (b) Linear fitting diagram for the Pt/ Au/H-SCD contact at 700 °C annealing.

To determine the barrier height of Pt/Au contact on the H-SCD at room temperature, XPS technique was performed. Since the diffusion of Au and Pt metal is very difficult at room temperature, the contact interface was only Pt and diamond. The schematic diagram of XPS for barrier height measurement is shown in Figure 5a. To form the Pt/H-SCD contacts, the Pt layer was evaporated by electron beam technique. Furthermore, it is essential to measure the photoelectrons from both the diamond and metal electrode during XPS determination. Accordingly, the discontinuous thin Pt metal layer should be formed on the diamond surface, to collect the photoelectrons from the diamond surface among the metal islands [27]. In our work, thin Pt metal layer was 3 nm and thick Pt layer was 70 nm. For the XPS determination, X-ray beam was focused on the 3 nm thin Pt to study C 1s and Pt 4f peaks. After that, the X-ray beam was focused on the 70 nm thick Pt to determine the Pt 4f peaks for calibrating. Moreover, the SEM image of the 3 nm Pt metal is shown in Figure 5b. As the Pt metal layer was extremely thin, it is clear that the deposited Pt layer was not a uniform film but consisted of small platinum islands. The XPS spectrum of Pt 4f and C 1s are shown in Figure 6. The binding energies for 3 nm Pt 4f/7/2 and 70 nm Pt 4f/7/2 were 69.82 ± 0.02 eV and 69.80 ± 0.02 eV, respectively, whereas the binding energy for the C 1s was 283.25 ± 0.02 eV. And, the barrier height of Pt/H-SCD can be calculated by the following formula [28].

$$\Phi_{BH} = E_{C\, 1s}^{3\, nm\, Pt/diamond} - \Delta E_{diamond} - \left( E_{C\, 1s}^{3\, nm\, Pt/diamond_{metalcore}} - E_{C\, 1s}^{70\, nm\, Pt/diamond_{metalcore}} \right)$$  \hspace{1cm} (3)

The C 1s binding energy for the 3 nm thin Pt/H-SCD is represented as $E_{C\, 1s}^{3\, nm\, Pt/diamond_{metalcore}}$. And, the value of $\Delta E_{diamond}$ is 283.90 ± 0.10 eV, with respect to the previous report [29]. $E_{C\, 1s}^{3\, nm\, Pt/diamond_{metalcore}}$ and $E_{C\, 1s}^{70\, nm\, Pt/diamond_{metalcore}}$ means the binding energy for the 3 nm thin Pt/H-SCD and 70 nm thick Pt/H-SCD, respectively. Accordingly, $\Phi_{BH} = (283.25 ± 0.02) - (283.90 ± 0.10 - [(69.82 ± 0.02) - (69.80 ± 0.02)]) = -0.67 ± 0.12$ eV.
Figure 5. (a) Schematic diagram for the measurement of barrier height of Pt/H-SCD (100) by XPS, (b) SEM image of the 3 nm Pt deposited on the diamond film.

Figure 6. (a) XPS spectrums of Pt peaks (red line for 3 nm Pt, black line for 70 nm Pt), (b) XPS spectrums of C 1s peaks for the as-fabricated sample.

The band diagram of Pt/H-SCD is shown in Figure 7. Since the barrier height value of Pt/H-SCD was \(-0.67 \pm 0.12\) eV, the valance band at the diamond surface interface bent up. So, the holes could flow to the metal layer freely, in other words, the electrons could be easily injected to the H-SCD by the applying voltage, indicating excellent ohmic behavior of Pt contact on the diamond film.

Figure 7. Schematic of band diagram for Pt/H-SCD contact.
4. Conclusions

In summary, ohmic contact of Pt/Au/H-SCD was realized and investigated under different annealing temperatures in hydrogen ambient. The value of $\rho_c$ was evaluated to be $5.65 \times 10^{-4}$ $\Omega \cdot \text{cm}^2$ for the as-fabricated sample. The variation in $\rho_c$ was not more than one order of magnitude as the annealing temperature changed, demonstrating good thermal stability. Finally, the barrier height was determined to be $-0.67 \pm 0.12$ eV by XPS analysis.

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