Schottky barrier modulation of metal/4H-SiC junction with thin interface spacer driven by surface polarization charge on 4H-SiC substrate

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Fabrication of n-type 4H–SiC/Ni junctions using electrochemical deposition
Schottky barrier modulation of metal/4H-SiC junction with thin interface spacer driven by surface polarization charge on 4H-SiC substrate

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The Au/Ni/Al2O3/4H-SiC junction with the Al2O3 film as a thin spacer layer was found to show the electrical characteristics of a typical rectifying Schottky contact, which is considered to be due to the leakiness of the spacer layer. The Schottky barrier of the junction was measured to be higher than an Au/Ni/4H-SiC junction with no spacer layer. It is believed that the negative surface bound charge originating from the spontaneous polarization of 4H-SiC causes the Schottky barrier increase. The use of a thin spacer layer can be an efficient experimental method to modulate Schottky barriers of metal/4H-SiC junctions. © 2015 AIP Publishing LLC.

Silicon carbide (SiC) has been considered as a prominent wide band-gap semiconductor for high power device applications. Its superior material properties including high breakdown voltage and high thermal conductivity make it possible to overcome the limitations of silicon as the base material for power devices.1–3 It is well-known that SiC is a component wide band-gap semiconductor for high power devices.1–3

It is quite probable to have the 4H-SiC wafer. After cleaning, the deposition of a ~3 nm thick Al2O3 thin film was carried out on one of the two pieces by using atomic layer deposition (ALD) (LUCIDA D100 system, NCD Corporation, South Korea). The Al2O3 film was grown at 200 °C under constant N2 flow (50 sccm) by using trimethylaluminum (TMA) and water (H2O) as precursors. The growth rate was ~1.2 Å per one complete ALD cycle which was composed of 0.2 s pulse of TMA followed by 10 s pause and 0.2 s pulse of H2O followed by 10 s pause. Once all ALD cycles were completed, N2 flow increased to 500 sccm and continued for 3 min as a post process. Then, Au/Ni electrodes (200 nm/500 nm) were deposited through a metal shadow mask on both pieces by using e-beam evaporation at room temperature. Fig. 1(a) shows the cross-sectional high resolution transmission electron microscopy (HRTEM) image of the Au/Ni/Al2O3/4H-SiC junction. In the HRTEM image, the oxide layer is measured to be ~4.3 nm thick, which is somewhat larger than the thickness of the Al2O3 film expected from the ALD process. It is considered that the oxide layer observed in the HRTEM image is a stack of the deposited Al2O3 film and a native oxide known to be ~1.0 nm on 4H-SiC surface.13 It is quite probable to have some native oxide grown during device fabrication, although the wafer surface is cleaned with HF in advance. This very thin native oxide is expected to exist in the Au/Ni/4H-SiC junction as well. Fig. 1(b) shows the cross-sectional HRTEM image of the Au/Ni/4H-SiC junction where the native oxide is barely seen at the interface of the 4H-SiC substrate and the Ni film, implying that it is quite thin.

After the device fabrication was completed, the current-voltage (I-V) curves were measured on the Au/Ni/4H-SiC and Au/Ni/Al2O3/4H-SiC junctions by using a KEITHLEY current amplifier (Model 428) which is capable of amplifying current signals while applying biases simultaneously. As shown in Fig. 2(a), both junctions show the normal rectifying characteristics.
I-V characteristics of an n-type Schottky contact. The Schottky behavior shown in the Au/Ni/Al₂O₃/4H-SiC junction even with the Al₂O₃ spacer layer inserted is considered to be due to the leakiness of the spacer layer itself, associated with direct tunneling or trap-assisted conduction through it. Even though the Al₂O₃ spacer layer is quite transparent in electron transport, it can still be resistive. Hence, the larger junction resistance (above threshold region) observed in the I-V curve of the Au/Ni/Al₂O₃/4H-SiC junction, compared with the Au/Ni/4H-SiC junction, is considered to rely on the additional resistance through the Al₂O₃ spacer layer. One important feature to be emphasized in Fig.2(a) is that the I-V curve of the Au/Ni/Al₂O₃/4H-SiC junction appears to turn on at a voltage substantially higher than the Au/Ni/4H-SiC junction. According to the thermionic-emission theory, the current density of a Schottky contact near threshold at temperature $T$ can be described as $J = A^* T^2 \exp\left(-q\phi_B/k_BT\right) \exp\left(qV/nkB_T\right) - 1$, where $A^*$ is the effective Richardson constant, $q$ is the magnitude of electron charge, $k_B$ is the Boltzmann constant, $\phi_B$ is the Schottky barrier, $V$ is the sample bias, and $n$ is the ideality factor. By fitting the semi-log plot of the measured I-V curves shown in Fig. 2(a) to the thermionic-emission theory with the effective Richardson constant of 4H-SiC (~146 A cm⁻² K⁻²), the Schottky barrier of the Au/Ni/4H-SiC junction is estimated to be 1.51 ± 0.04 eV and that of the Au/Ni/Al₂O₃/4H-SiC junction be 2.06 ± 0.13 eV. It is also relevant here to note that the ideality factor ($n$) of the Au/Ni/Al₂O₃/4H-SiC junction is estimated to be 2.17 ± 0.21 much larger than the ideal Schottky case ($n = 1$). In case of the Au/Ni/4H-SiC junction, the ideality factor is estimated to be 1.18 ± 0.06. The non-ideal behavior of the Au/Ni/Al₂O₃/4H-SiC junction is considered to be associated mainly with the non-uniform thickness of the Al₂O₃ spacer layer, implying the existence of some areas with their local Schottky barriers lower than the surrounding. Several previous works have demonstrated that these low-barrier areas influence I-V curves quite significantly, even though their relative portion in the entire contact is small. They tend to increase the ideality factor of a measured I-V curve and make the Schottky barrier to be estimated lower than the one on the prevailing surrounding area. As Tung pointed out, the energy band profile of low-barrier area on the semiconductor side will be pinched off due to the influence of high-barrier surrounding. If the low-barrier area is small enough, the pinch-off will be enhanced to almost close the low-barrier area. In this case, the low-barrier areas become invisible in terms of carrier transport, and the Schottky junction will show more ideal behavior. Hence, the large ideality factor of our
Au/Ni/Al2O3/4H-SiC junction indicates that some low-barrier areas with non-negligible sizes exist in the junction. The relevant electrical parameters of the Au/Ni/4H-SiC and Au/Ni/Al2O3/4H-SiC junctions including the reverse saturation current density ($J_0$), the ideality factor, and the Schottky barrier ($\phi_B$) extracted from the measured I-V curves are listed in Table I. Fig. 2(b) shows the linear correlation between the Schottky barriers and the corresponding ideality factors extracted from the measured I-V curves. By finding the intercept of the straight line fitted to the measured data with the $n = 1.01$ vertical line, the Schottky barrier excluding the influences of low-barrier areas can be estimated. The estimated Schottky barrier is ~1.64 eV for the Au/Ni/4H-SiC junction and ~2.76 eV for the Au/Ni/Al2O3/4H-SiC junction.

In order to extract the Schottky barriers on the prevailing areas of the two (with and without Al2O3 spacer layer) junctions, C-V curves were measured with an Agilent E4980 LCR meter by applying a reverse bias ($V_R$) ranging from 0 V to 2.2 V. An AC voltage with its amplitude of 50 mV and frequency of 1 MHz was added to the reverse bias for measuring the bias-dependent differential capacitance per unit area $C = dQ/dV$. Fig. 3(a) shows the C-V curves measured on the Au/Ni/4H-SiC (black circles) and Au/Ni/Al2O3/4H-SiC (red circles) junctions. The measured data are plotted as $1/C^2$ vs. $V_R$, with the linearly fitted lines (black lines).

The abrupt depletion approximation, 16,17,25 $1/C^2 = \frac{q}{kT} \frac{d^2}{dV_R^2}$, where $N_d$ is the donor density, $\varepsilon_s$ is the static dielectric constant of the semiconductor, $\varepsilon_0$ is the vacuum permittivity, and $\zeta$ is the difference in energy between the Fermi level and the conduction band minimum in the semiconductor bulk. The doping concentration ($N_d$) can be obtained from the slope of the linearly fitted line by using the relation $N_d = \frac{(2/\varepsilon_s \varepsilon_0)}{[d(1/C^2)/dV_R]}$. The extracted $N_d$ was $(3.34 \pm 0.23) \times 10^{15}$ cm$^{-2}$ for the Au/Ni/4H-SiC junction and $(2.90 \pm 0.10) \times 10^{15}$ cm$^{-2}$ for the Au/Ni/Al2O3/4H-SiC junction. Both are close to the value $2.00 \times 10^{15}$ cm$^{-2}$ provided by the wafer vendor. The Schottky barrier $\phi_B$ can also be extracted from the $1/C^2$ vs. $V_R$ plot by using the relation $\phi_B = -V_I + \zeta + kT/q$, where $V_I$ is the intercept of the fitted straight line with the $V_R$ axis. Using this procedure, the Schottky barrier of the Au/Ni/Al2O3/4H-SiC junction is estimated to be $3.21 \pm 0.082$ eV, while that the Au/Ni/Al2O3/4H-SiC junction is $1.97 \pm 0.027$ eV (Table I). Here, it is noticeable that the Schottky barriers extracted from C-V measurements are larger than the I-V measurement counterparts, even after excluding the influences of low-barrier. The discrepancies between C-V and I-V measured Schottky barriers exceed the amounts expected from the image force lowering which is estimated to be ~29 meV and ~25 meV for the Au/Ni/Al2O3/4H-SiC and Au/Ni/4H-SiC junctions, respectively. It is thought that the capacitive component in the substrate ohmic contact and the stray capacitances associated with the configuration of our measurement system are the main contributors. These additional capacitive components tend to make the measured capacitance of Schottky junction smaller than its actual value. Then, the smaller measured capacitance will bear a larger intercept of the fitted straight line with the $V_R$ axis in the $1/C^2$ vs. $V_R$ plot so that the Schottky barrier is estimated to be higher. The additional capacitive components are expected to be quite similar for both Au/Ni/Al2O3/4H-SiC and Au/Ni/4H-SiC junctions. Therefore, their influences on determining the increase of Schottky barrier with the Al2O3 spacer inserted will be negligible. Similar to the I-V measurements, the C-V measured Schottky barrier of the Au/Ni/Al2O3/4H-SiC junction is much higher by an amount of ~1.24 eV than that of the Au/Ni/4H-SiC junction. Just as a note, the difference of I-V measured Schottky barriers for the two junctions is ~1.12 eV when excluding the influences of low-barrier areas. Related to the inertness to low-barrier areas, there is one important aspect to note for C-V measurements. For both Au/Ni/4H-SiC and Au/Ni/Al2O3/4H-SiC junctions, the oxide layer is much thinner than the depletion region in the 4H-SiC substrate which is estimated to be ~900 nm thick for ~2 × 10$^{15}$ cm$^{-3}$ doping. Accordingly, the

<table>
<thead>
<tr>
<th>Junction</th>
<th>$J_0$ (A/cm$^2$)</th>
<th>Ideality factor</th>
<th>$\phi_B$ from I-V (eV)</th>
<th>$\phi_B$ from C-V (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au/Ni/4H-SiC</td>
<td>$1.06 \pm 0.91 \times 10^{-18}$</td>
<td>1.18 ± 0.06</td>
<td>1.51 ± 0.04</td>
<td>1.97 ± 0.027</td>
</tr>
<tr>
<td>Au/Ni/Al2O3/4H-SiC</td>
<td>$2.26 \pm 2.25 \times 10^{-26}$</td>
<td>2.17 ± 0.21</td>
<td>2.06 ± 0.13</td>
<td>3.21 ± 0.082</td>
</tr>
</tbody>
</table>

FIG. 3. The capacitance-voltage ($1/C^2$ vs. $V_R$) plots (a) measured and (b) obtained by performing finite element electrostatic modeling for Au/Ni/4H-SiC (black) and Au/Ni/Al2O3/4H-SiC (red) junctions with the linearly fitted lines (black lines). The calculation is found to best-fit the measurements with the spontaneous polarization of 4H-SiC assumed to be $3.00 \times 10^{-2}$ C/m$^2$. 

TABLE I. Electrical properties of Au/Ni/4H-SiC and Au/Ni/Al2O3/4H-SiC junctions.

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the Fermi level in the metal electrode will be raised, implying the increase of Schottky barrier. In case of the Au/Ni/4H-SiC junction, the electrostatic potential energy increases only across the thin native oxide (Fig. 4(a)). On the other hand, for the Au/Ni/Al2O3/4H-SiC junction, there will be an additional jump of electrostatic potential energy through the Al2O3 spacer, resulting in a much higher Schottky barrier than the Au/Ni/4H-SiC junction (Fig. 4(b)).

In order to evaluate the idea of dipole layer formation driven by the surface polarization charge, finite element electrostatic modeling was performed to calculate the C-V curves theoretically using a commercial software package FLEXPDE.26 By following the procedure used in Ref. 27, we define the total electron potential energy in the oxide layer and 4H-SiC substrate as $\phi_{en} = \phi(x, y, z) + (\phi_m - \chi)$, where $\phi(x, y, z)$ is the electrostatic potential energy, $\phi_m$ is the work function of the metal electrode (Ni), and $\chi$ is the electron affinity of Al2O3, SiO2, or 4H-SiC. $\phi(x, y, z)$ is determined by solving the Poisson’s equation $\nabla^2 [\phi/(e - q)] = -\rho(x, y, z)/\varepsilon_0\varepsilon$, where $\rho(x, y, z)$ is the net charge density in the oxide layer or 4H-SiC substrate, and $\varepsilon$ is the relative dielectric constant of Al2O3, SiO2, or 4H-SiC. The net charge density is assumed to be zero inside the oxide layers and is given as $\rho(x, y, z) = q[N_d - n_s(x, y, z)]$ in the 4H-SiC substrate, where $n_s$ is the free electron density. The free electron density is calculated as $n_e = N_e \exp[(E_{FS} - \phi_m)/kT]$, where $N_e$ is the electronic effective density of states for 4H-SiC (1.83 x 10^{19} cm^{-3}), and $E_{FS} = -qV_F$ is the Fermi level energy inside the 4H-SiC substrate with an applied reverse bias $V_F$. For the dopant density, the extracted value from the measured C-V curve was used. The negative polarization charge on the 4H-SiC surface was implemented in the calculation as the boundary condition at the oxide/4H-SiC interface. The material parameters used in the modeling are listed in Table II. The differential capacitance was obtained by quantifying the change of the charge $Q_m$ induced on the metal electrode surface as the applied reverse bias varies by a small amount, i.e., $C = \Delta Q_m/\Delta V_F$, where $\Delta Q_m = Q_m(V_F) - Q_m(V_F + \Delta V_F)$. The calculation was repeated by varying the SP of 4H-SiC, and the calculated C-V curves were found to best-fit to the measured ones with the SP of 4H-SiC assumed to be 3.00 x 10^{-2} C/m², as shown in Fig. 3(b). This best-fit SP of 4H-SiC is a bit larger but fairly close to the theoretically predicted 5,8,9 or experimentally estimated values 32,33 ranging between (1.10 – 2.16) x 10^{-2} C/m².

In conclusion, it has been demonstrated experimentally that the Au/Ni/Al2O3/4H-SiC junction with a thin Al2O3 film as spacer layer shows normal rectifying behavior of a Schottky contact, with its threshold voltage significantly higher than the Au/Ni/4H-SiC junction with no spacer. Direct tunneling or trap-assisted conduction is considered to occur through the thin Al2O3 spacer to yield the rectifying characteristics of the junction. The significant threshold voltage increase of the Au/Ni/Al2O3/4H-SiC junction is believed

![FIG. 4. Schematics of layer structure and energy band profile of (a) Au/Ni/4H-SiC and (b) Au/Ni/Al2O3/4H-SiC junctions. The energy band profiles are drawn along the dashed lines. In the Au/Ni/Al2O3/4H-SiC junction, the electrostatic potential energy for electron will jump noticeably across the oxide layer (Al2O3 spacer + native oxide). This electrostatic potential energy jump will be much smaller in the Au/Ni/4H-SiC junction (only native oxide). The jump of electrostatic potential energy causes the increase of Schottky barrier, and the depletion region in the 4H-SiC substrate is enlarged accordingly. The change of depletion region can be detected as the change of measured capacitance.](image-url)

The material parameters used in the modeling are listed in Table II.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_m$(Ni)</td>
<td>5.10 eV</td>
</tr>
<tr>
<td>$Z_{4H-SiC}$</td>
<td>4.05 eV</td>
</tr>
<tr>
<td>$Z_{SiO_2}$</td>
<td>0.9 eV</td>
</tr>
<tr>
<td>$Z_{Al_2O_3}$</td>
<td>1.35 eV</td>
</tr>
<tr>
<td>$\varepsilon_{4H-SiC}$</td>
<td>9.7</td>
</tr>
<tr>
<td>$\varepsilon_{SiO_2}$</td>
<td>3.9</td>
</tr>
<tr>
<td>$\varepsilon_{Al_2O_3}$</td>
<td>9.0</td>
</tr>
</tbody>
</table>

TABLE II. The material parameters used for finite element electrostatic modeling.
to result from the jump in electrostatic potential energy for electron across the dipole layer composed of the negative spontaneous polarization charges bound on the 4H-SiC surface and the compensating positive charges induced on the metal electrode surface. The finite element electrostatic modeling reproduces the measured C-V curves correctly when the SP of 4H-SiC is assumed properly. This assumed SP of 4H-SiC is found to be fairly close to the theoretical and experimental values reported previously. Our results suggest that the SP of 4H-SiC can be an efficient tool to modulate Schottky barriers of metal/4H-SiC junctions, in conjunction with thin interface spacer layers.

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