Leakage Current Conduction Mechanism of Au-Pt-Ti/HfO₂-Al₂O₃/n-InAlAs Metal-Oxide-Semiconductor Capacitor under Reverse-Biased Condition

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Received: 29 August 2019; Accepted: 18 October 2019; Published: 1 November 2019

Abstract: Au-Pt-Ti/high-κ/n-InAlAs metal-oxide-semiconductor (MOS) capacitors with HfO₂-Al₂O₃ laminated dielectric were fabricated. We found that a Schottky emission leakage mechanism dominates the low bias conditions and Fowler–Nordheim tunneling became the main leakage mechanism at high fields with reverse biased condition. The sample with HfO₂ (4 m)/Al₂O₃ (8 nm) laminated dielectric shows a high barrier height φ_B of 1.66 eV at 30 °C which was extracted from the Schottky emission mechanism, and this can be explained by fewer In–O and As–O states on the interface, as detected by the X-ray photoelectron spectroscopy test. These effects result in HfO₂ (4 m)/Al₂O₃ (8 nm)/n-InAlAs MOS-capacitors presenting a low leakage current density of below 1.8 × 10⁻⁷ A/cm² from −3 to 0 V at 30 °C. It is demonstrated that the HfO₂/Al₂O₃ laminated dielectric with a thicker Al₂O₃ film of 8 nm is an optimized design to be the high-κ dielectric used in Au-Pt-Ti/HfO₂-Al₂O₃/InAlAs MOS capacitor applications.

Keywords: high-κ dielectric; leakage current mechanism; interface characteristics

1. Introduction

According to the requirements of high speed, low power dissipation, and low noise application for RF devices used in telecommunication and other modern integrated circuits, increasing interest is focused on new III-V compound devices of InAs/AlSb and InAlAs/InGaAs HEMTs (high-electron mobility transistors), as these devices possess high electron mobility and peak velocity in the channel [1–5]. However, due to the narrow band gap of channels of these HEMTs, the devices suffer from serious current leakage which is considered as the biggest issue of InAs/AlSb and InAlAs/InGaAs HEMTs [6,7]. In this kind of device, InAlAs is most frequently used as the protective layer on the above barrier and as the gate contact semiconductor [1,3], and some reports proposed to deposit a high-κ dielectric film on InAlAs, together with the gate electrode, to become a metal-oxide-semiconductor (MOS) capacitor isolated gate structure, in order to effectively suppress the leakage current. HfO₂ that presents a high dielectric constant is a popular candidate as the high-κ dielectric [8–10], however it does not match well with InAlAs and the poor lattice match would degrade its performance [9]; Al₂O₃ is used frequently as the high-κ dielectric as well [10,11], however its dielectric constant is not high enough, and that will lead to a lower EOT (effective oxide thickness) which is not beneficial for reducing device size. For improvement, the HfO₂-Al₂O₃ laminated dielectric layer is proposed, and in this new device structure, a compromised dielectric constant can be achieved and the leakage current can be effectively suppressed [12–14]. In our previous paper [13], the physical and electrical performance of the new Au-Pt-Ti/high-κ/n-InAlAs MOS capacitors with HfO₂-Al₂O₃ laminated dielectric were studied in detail. However, its leakage current mechanism was not mentioned, and this scheme has been
covered in few other papers. To better understand the generation reason of the leakage current of the Au-Pt-Ti/HfO\textsubscript{2}-Al\textsubscript{2}O\textsubscript{3}/n-InAlAs MOS capacitor, we study the leakage current mechanism of the new devices at different bias condition ranges in detail. As InAs/AlSb HEMTs and InAlAs/InGaAs HEMTs work under negative gate voltage bias conditions, we studied the reverse-bias leakage current mechanism in this paper as in the case of a real application.

2. Experiment

The device structure from bottom to top is a 350 µm semi-insulating InP substrate, a 200 nm InP buffer layer, a 500 nm Si-doped In\textsubscript{0.5}Al\textsubscript{0.5}As semiconductor layer with a doping concentration of $1 \times 10^{17}$ cm\textsuperscript{-3} [15], a 12 nm oxide layer with Al\textsubscript{2}O\textsubscript{3}-HfO\textsubscript{2} dielectrics, and a metal with structure of Ti (20 nm)/Pt (20 nm)/Au (200 nm). The detailed schematic layer structures of the prepared sample can be found in our previous published paper [14]. In order to identify the impact of the thickness of the Al\textsubscript{2}O\textsubscript{3} inserting layer, we manufactured two kinds of samples with an oxide layer of HfO\textsubscript{2} (4 nm)/Al\textsubscript{2}O\textsubscript{3} (8 nm) laminated dielectrics (marked as Sample #1), and HfO\textsubscript{2} (8 nm)/Al\textsubscript{2}O\textsubscript{3} (4 nm) laminated dielectrics (marked as Sample #2), respectively. The detailed fabrication process is listed in Table 1 [16–20].

| Process Step | Process Description | MBE (molecular beam epitaxy) at 470 °C |
|--------------|---------------------|---------------------------------------|
| 1            | InP buffer layer deposition | |
| 2            | InAlAs semiconductor layer deposition | MBE at 350 °C |
| 3            | Surface treatment of InAlAs | 36–38% HCl solution for 1 min and a 7% (NH\textsubscript{4})\textsubscript{2}S solution for 15 min, then dry in N\textsubscript{2} |
| 4            | Al\textsubscript{2}O\textsubscript{3} film deposition | Pass precursor of Al element as TMA (trimethylaluminium) for 0.5 s, then pass N\textsubscript{2} for 2 s in order to transfer the Al-base residue out, then pass precursor of O element as H\textsubscript{2}O for 0.5 s. Repeat the above process steps to obtain the required thickness |
| 5            | HfO\textsubscript{2} film deposition | Pass precursor of Hf element as TEMAH (tetrais ethylmethylamino hafnium) for 1 s, then pass N\textsubscript{2} for 2 s in order to drive off the Hf-base residue, then pass precursor of O element as H\textsubbox{2}O for 1 s. Repeat the above process steps to obtain the required thickness |
| 6            | Post-deposition annealing (PDA) | Heat the film from ambient temperature to 380 °C in N\textsubbox{2} over 15 s, annealing for 60 s, and then cool to ambient temperature over 300 s |
| 7            | Metal | Magnetron sputtering. Size of 150 µm × 150 µm |

3. Measurement and Discussion

The leakage current measurement of the Au-Pt-Ti/HfO\textsubscript{2}-Al\textsubscript{2}O\textsubscript{3}/InAlAs MOS-capacitors under reversed bias condition is shown in Figure 1. It is found that the leakage current density $I$ achieves a significant low value below $10^{-6}$ A/cm\textsuperscript{2} in the bias voltage $V_g$ ranges from $-3$ to 0 V at a temperature of 30 °C for the both Sample #1 and #2. In particular, Sample #1 shows a much lower leakage current, below $1.8 \times 10^{-7}$ A/cm\textsuperscript{2} from $-3$ to 0 V at 30 °C which is three times less than Sample #2 with the leakage current value below $6.5 \times 10^{-7}$ A/cm\textsuperscript{2}. This demonstrates that the thickness ratio of Al\textsubscript{2}O\textsubscript{3} and HfO\textsubscript{2}...
films clearly impact the leakage current. We note that the electric field \( E \) of \( \text{Al}_2\text{O}_3 \) should be higher than that of \( \text{HfO}_2 \), since the dielectric constant of \( \text{HfO}_2 \) is higher than that of \( \text{Al}_2\text{O}_3 \). However, we simply formulate \( E \) by applying \( V/T_{ox} \) (\( T_{ox} \) is oxide thickness) in order to present an intuitive view of the leakage current changing trend. In addition, it is found that the leakage current density \( J \) increases as the temperature increases. This may be explained by the violent electron movements at high temperatures. To better understand the generation reason of the leakage current of the Au-Pt-Ti/\( \text{HfO}_2-\text{Al}_2\text{O}_3/\text{InAlAs} \) MOS capacitor and the reason for the lower leakage current of the sample with the higher thickness ratio of \( \text{Al}_2\text{O}_3 \) and \( \text{HfO}_2 \) films, we will study the leakage current mechanism of the devices at different bias condition ranges and different temperatures in detail.

![Figure 1](image)

**Figure 1.** The leakage current measurement of the Au-Pt-Ti/\( \text{HfO}_2-\text{Al}_2\text{O}_3/\text{InAlAs} \) MOS-capacitors under reversed bias condition at different temperatures. The solid symbol is for Sample #1 with \( \text{HfO}_2 \) (4 nm)/\( \text{Al}_2\text{O}_3 \) (8 nm) laminated dielectrics, and the hollow symbol is for Sample #2 with \( \text{HfO}_2 \) (8 nm)/\( \text{Al}_2\text{O}_3 \) (4 nm) laminated dielectrics.

Schottky emissions often happen in low electrical fields. The energy band diagram for Schottky emissions under the reversed bias condition is shown in Figure 2 [21–24]. Electrons surmount the metal–\( \text{HfO}_2 \) surface barrier first, and then surmount the barrier at \( \text{HfO}_2-\text{Al}_2\text{O}_3 \), and finally fall into the conduction band of \( \text{InAlAs} \) to form the leakage current. It can be verified by linear fitting the curve of \( \ln J \) versus \( E_f^{1/2} \) with a straight line, where \( J \) is the leakage current density and \( E_f \) is the electric field intensity under reversed bias voltage [25,26]. Schottky emission is temperature dependent, and the slope of linear approximation on the curve of \( \ln J \) needs to be consistent at different temperatures, which is the typical feature of Schottky emission [11,25,26]. Therefore, we make the line fit on the measurement curve under different temperatures of 30/50/70 °C in order to identify it correctly by the same scope of the fitting straight line, as shown in Figure 3. According to the analysis, the Schottky emission occurs in the bias range of \( -1.1-0 \) V and \( -1.7-0 \) V for Sample #1 and Sample #2, respectively. As we presented before, Sample #1, with a higher thickness ratio of \( \text{Al}_2\text{O}_3 \) and \( \text{HfO}_2 \) films, shows a reduced leakage current in the Schottky region. This can be explained by its higher barrier height \( \phi_B \). The barrier height \( \phi_{B,n} \) can be extracted from the equation \( \phi_{B,n} = k\ln\left(A^*T_{ox}/J_0\right)/q \) according to the Schottky emission mechanism, where \( k \) is the Boltzmann constant, \( T \) is the temperature, \( q \) is the electron charge, \( A^* \) is the effective Richardson constant as the value of 105600A/K²m², and \( J_0 \) is the saturation current density [15]. The extracted \( \phi_{B,n} \) values are listed in Table 2. The \( \phi_{B,n} \) we extracted was illustrated as in Figure 2. It presents the barrier at \( \text{HfO}_2-\text{Al}_2\text{O}_3 \) where is the top of the barrier. It is worth noting that the \( \phi_{B,n} \) we obtained from the Schottky mechanism should be lower than the ideal barrier height by a value of \( \Delta\phi_B \) as shown in Figure 2. This gap can be explained by the Schottky
As a result, the samples show a clear, increased leakage current by one order of magnitude when the etching process was applied to the dielectric surface in order to make the interface suitable for X-ray Coatings. In addition, it is noted that $\phi_B$ increases as the temperature is increased, while the leakage current is also increased as the temperature is increased (Shown in Figure 1). This is because electrons move more violently at high temperatures, making it easier for the electrons to cross through the even higher barrier between the oxide layer and the gate electrode, to form an increased gate leakage current. As a result, the samples show a clear, increased leakage current by one order of magnitude when the temperature was increased from 30 °C to 70 °C.

Figure 2. Schottky emission energy-band diagram for $V_g < 0$.

![Figure 2](image)

Figure 3. Schottky emission plots for MOS-capacitors at different temperatures. (a) Sample #1 with HfO$_2$ (4 nm)/Al$_2$O$_3$ (8 nm) laminated dielectrics, (b) Sample #2 with HfO$_2$ (8 nm)/Al$_2$O$_3$ (4 nm) laminated dielectrics.

Table 2. Extracted barrier height $\phi_{B,n}$ from the Schottky emission leakage mechanism at different temperatures.

| Temperature | Sample #1 HfO$_2$ (4 nm)/Al$_2$O$_3$ (8 nm) | Sample #2 HfO$_2$ (8 nm)/Al$_2$O$_3$ (4 nm) |
|-------------|---------------------------------|---------------------------------|
| 30 °C       | 1.66 eV                         | 1.62 eV                         |
| 50 °C       | 1.73 eV                         | 1.70 eV                         |
| 70 °C       | 1.83 eV                         | 1.80 eV                         |

As Schottky emission is strongly related to dielectric-semiconductor interfacial conditions, a 60 s etching process was applied to the dielectric surface in order to make the interface suitable for X-ray photoelectron spectroscopy (XPS). An Al sputtering ion beam was applied in the XPS setup.
When the electrical field intensity is large enough, the electrons obtain enough energy to tunnel the potential barrier, which can be verified by fitting the curves of $\ln(J/E_i^2)$ versus $1/E_i$ with a straight line [27–31], becomes the main leakage mechanism. According to the extraction in Figure 5, the F–N emission occurs in the range $-3$–$-1.1$ V and $-3$–$-1.7$ V for Sample #1 and Sample #2, respectively. It indicates that when the electrical field intensity is large enough, the electrons obtain enough energy to tunnel the potential barrier to make F–N tunneling occur. It is noted that the slope of the F–N fitting straight line under different temperatures is not the same. This is because the F–N tunneling is not proportional to temperature [32], which is different from the Schottky emission mechanism. The effective barrier height can be extracted from the F–N fitting curve, and values are shown in Table 3. It is found that the barrier extracted for Sample #1 is higher than that of Sample #2 at 30 °C and 70 °C, resulting in Sample #1 showing a reduced leakage current in the F–N region at room temperature. In contrast, Sample #1 shows a lower barrier height, of 0.18 eV, than Sample #2, showing a barrier height of 0.26 eV with the temperature of 50 °C. This should make Sample #1 present a higher leakage current under the F–N region, which is consistent with the leakage current test result in Figure 1.

![X-ray photoelectron spectroscopy (XPS) measurement of the O1s peak of the dielectric-semiconductor interface](image)

**Figure 4.** (a) X-ray photoelectron spectroscopy (XPS) measurement of the O1s peak of the dielectric-semiconductor interface, (b) comparison of the ratio of various oxide contents on the interface.
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