Characterization of the semi-insulating properties of AlHfO$_{3.5}$ for power devices

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Abstract. Physical and electrical characterization of hafnium aluminates gate dielectrics was carried out to investigate their semi-insulating characteristics as passivating layer for power devices. The deposited films were annealed in pure nitrogen to simulate the thermal budget during a conventional CMOS processing. C-V measurements were performed having as a result a high-frequency behavior of the flat band voltage ($V_{FB}$) and values greater than or equal to zero. On the other hand, the leakage phenomenon was modeled with a simplified electrical model using a leakage admittance $Y_L$ whose influence was predominant at the accumulation region. Using X-ray reflectometry (XRR), the average thickness obtained was 15.5nm and a leakage process was inferred to occur for AlHfO$_{3.5}$ due to the observed phase separation and crystallization that occurs after annealing in pure N$_2$.

1. Introduction

Semi-insulating materials have been considered to replace the silicon dioxide passivation layers in power devices such as thyristors and power transistors [1-3]. An example is the semi-insulating polycrystalline silicon (SIPOS) that can be used to increase the breakdown field without increasing the on-state series resistance [1-3]. In this case, the potential drop across the layer is controlled by the high volume concentration of the charged states. Two important electrical properties of the semi-insulating films are the shift of the flatband voltage due to the charging effect and the leakage process, which means a shunt parasitic resistances coexisting with a series resistance associated to the substrate [3-6]. Aluminates are possible candidates to be used as semi-insulating materials since they have bulk states at high concentrations to be charged in order to promote the increase of the breakdown field [3,7,8].

Literature points out the increase of the leakage current density for hafnium aluminates as the thermal budget of annealing is increased. This effect occurs due to the phase decomposition and crystallization of the hafnium aluminates. On the other hand, thermodynamic stability from interfacial layer leads to well-behaved electrical characteristics and low interface state density ($D_{it}$) [9]. For Capacitance-Voltage (C-V) characteristics, a decrease of the accumulation capacitance is reported due to the presence of the leakage current [9-11].

In this work, hafnium aluminates were electrically characterized according to the flatband voltage and the leakage current through the MOS structure.

2. Experimental

At first, the samples underwent an IMEC clean. AlHfO$_{3.5}$ was deposited by Atomic Layer Deposition on Si(100) substrate with equal molar concentrations of aluminum and hafnium. Layers were deposited in an ASM Pulsar 3000 connected to a Polygon 8300 Platform on Si substrate, on which a
1 nm thick chemical oxide has been grown [14]. Following, the sample was also annealed using an ASM Levitor 4300 at 1000°C during 60s in N₂ and, it was subsequently immersed into a boiling isopropyl alcohol for 1h. Finally, aluminum was deposited (200 nm thick) through a mechanical mask to define MOS capacitors with area of 2x10⁻² cm² and they were sintered at 420°C in ultrapure N₂+10%H₂ during 30min.

MOS capacitors were electrically characterized with the aid of HP 4280 C at 1MHz or Agilent E4980A Precision LCR Meter at 1MHz in order to obtain parameters from C-V characteristics, including series resistance (Rₛ) and effective charges in the dielectrics (Qₛ/q).

Grazing Incidence X-Ray Diffraction (GIXRD) was employed to the films using an X-ray beam with λ = 0.1542 nm at an incidence angle of 0.7º. X-ray reflectometry (XRR) was employed to obtain the physical thickness of the films. The XRR curves have a typical wavy appearance known as Kiessig fringes [13-16]. These fringes appear due to the interference effect of the beams reflected at the air/dielectric and dielectric/silicon interfaces [15,16]. The periodicity of these undulations is related to the thickness, while the fall rate is influenced by the roughness of both interfaces [13,14,17]. Based on the periodicity of the peaks in the XRR curves, an estimation of the thickness, valid for homogeneous films, was made using the relation

\[ T_{XRR} = \frac{2\pi}{\Delta q} \]  

In addition, the XRR curves were fitted using the PARRAT32 code. This computational program uses Parrat formalism [18] along with the Névot-Croce factor that takes into account the surface roughness effect upon the reflectivity [19] and the variation of the electronic density in depth. Mathematically they are expressed as:

\[ R_j = \frac{r_{j,j+1} + R_{j,j+1} \exp(i\gamma_j k_{c,j+1})}{1 + r_{j,j+1} R_{j,j+1} \exp(i\gamma_j k_{c,j+1})} \]  

\[ r_{j,j+1} = k_{c,j+1} - k_{c,j} \exp(-2\sigma_j k_{c,j} k_{c,j+1}) \]  

\[ k_{c,j} = \sqrt{k_{c,0}^2 - 4\rho_j} \]  

The reflectivity of the system is given by \( R = |R_0|^2 \), \( R_{N+1} = 0 \); \( R_N = r_{N,N+1} \). In equation (3), \( t_j \) and \( k_j \) are the thickness and wave number of the j-th layer, while \( \rho_j \) is the complex value of the electron density and \( \sigma_j \) is the roughness of the j-th layer.

3. Electrical Modeling

C-V curves were modeled by the electrical circuits shown in figure 1, where \( C_0 \) is the film capacitance, \( Y_c \) is an admittance that represents a leakage process and \( R_s \) [1, 20] the series resistance associated to the silicon substrate [8].

Based on equal impedances of the electrical circuits shown in Fig. 1a and 1b, an expression for the corrected capacitance in the accumulation (\( C_a \)) and the admittance \( Y \) across the leakage current path are given by [20].

\[ C_a = \frac{C_{ma} \left( (\omega C_{ma})^2 + G_{ma}^2 \right)}{(\omega C_{ma})^2 + (G_{ma} - R_s (\omega C_{ma})^2 + G_{ma})^2} \]  

\[ Y = \sqrt{\omega C_s - \omega C_a + \omega C_{ma} \left( 1 + \frac{G_{ma}}{(\omega C_{ma})^2} \right) \right) \]  

Where \( C_{ma} \) is the measured capacitance, \( G_{ma} \) is the measured conductance and \( \omega = 2\pi f \). In addition, the effective charge in the dielectrics (\( Q_s/q \)) is given by:
\[ Q_{SS} = \left( -0.6 - \frac{kT}{q} \ln \left( \frac{N_A}{n_i} \right) - V_{FB} \right) \frac{C_r}{A_g} \]  \hfill (6)

Where \( N_A \) is the substrate doping, \( n_i \) is the intrinsic concentration of carriers, \( V_{FB} \) is the flatband voltage, \( A_g \) is the area of the capacitor and \( kT/q = 0.0259V \) at room temperature.

Figure 1. (a) MOS electrical model and (b) \( C_{ma} \) and \( G_{ma} \) measured by the LCR Meter in the accumulation.

4. Results and Discussion

Figure 2 shows the GIXRD for a typical AlHfO\(_{3.5}\) film. It is noteworthy that, after annealing in N\(_2\) by RTP, the matrix film passes to contain both crystalline Al\(_{2.4}\)O\(_{3.6}\) and HfO\(_2\) phases, indicating phase separation and crystallization.

X-ray reflectometry (XRR) was employed to obtain the physical thickness of the films. Although the films were supposed to be single layer, they could not be fitted using the single layer model, being necessary a four-layer one. The XRR curve shown in figure 3 was fitted with the aid of the PARRAT32 code using the procedure mentioned in the experimental. The AlHfO\(_{3.5}\) film was 15.5nm in physical thickness and it was slightly different of that computed using the simplified equation \( T_{XRR}=2\pi/\Delta q_z \). The surface roughness of these films was lower than 0.6nm.

Figure 3. Typical XRR for the AlHfO\(_{3.5}\) film and the fitting.
As already mentioned, for the AlHfO$_{3.5}$, phase separation and crystallization takes place, promoting the formation of HfO$_2$ and Al$_{2.4}$O$_{3.6}$ crystalline phases. Also, non-homogeneous electronic density distribution in the dielectrics gave rise to the formation of several regions which can be viewed as fitting sub-layers, each of them with arbitrary electron density to obtain the real thickness using the PARRAT32 code.

Figure 4. Typical experimental and corrected C-V curves for AlHfO$_{3.5}$.

Figure 4 shows the typical experimental and corrected C-V curves for AlHfO$_{3.5}$, where the correction of the capacitance was performed with the aid of the Equation (4). At first, it is important to highlight that the C-V experimental curve in figure 4 shows a slight decrease of the measured accumulation capacitance when the gate voltage decreases, which indicates an intense leakage process occurring [9-11].

Table 1 shows an average accumulation capacitance ($C_a$) almost three times lower compared to the corrected one, which means an intense leakage process occurring for AlHfO$_{3.5}$. Equation (5) allows one to appreciate this qualitative observation, this is to say, the higher the $G_{ma}$ parameter, the higher the leakage conductance ($Y_C$). This fact can be correlated to the GIXRD analysis since AlHfO$_{3.5}$ presented phase separation and crystallization, which is a well-known morphological appearance associated with higher leakage current density as reported in literature [20].

Table 1 also shows the obtained effective charge ($Q_{SS}/q$) and the flatband voltage ($V_{FB}$) for the AlHfO$_{3.5}$ film. It was observed positive flatband voltage and negative $Q_{SS}/q$ parameters indicating a negative charging effect in the dielectrics. As a result, AlHfO$_{3.5}$ is a possible candidate to be used as passivating material for power devices because of two important semi-insulating properties: high flatband voltage due to the charging effect and a intense leakage process [3].

|       | A1       | A2       | A3       | A4       | Average value |
|-------|----------|----------|----------|----------|---------------|
| $C_a$ (pF) | 1883.6   | 7044.2   | 4493.8   | 5144.7   | 4600±1500    |
| $C_{ma}$ (pF) | 836    | 934      | 1100     | 1120     | 998±110      |
| $G_{ma}$ (μS) | 5880   | 15010    | 12140    | 13340    | 11600±2800   |
| $N_A$ (cm$^{-3}$) | 8.4E+13 | 3.9E+14 | 7.8E+14 | 6.8E+14 | (4.8±2.5)E+14 |
| $V_{FB}$ (V) | 0.25  | 0.40     | 0.05     | -0.01    | 0.17±0.15    |
| $Q_{SS}/q$ (cm$^2$) | -5.9E+11 | -2.6E+12 | -1.2E+12 | -1.3E+12 | -(1.4±0.6)E+12 |

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5. Conclusions
The hafnium aluminate was electrically and physically characterized in order to investigate its semi-insulating characteristics as passivating layer for power devices. The deposited films were annealed in pure nitrogen to simulate the thermal budget during a conventional CMOS processing. Phase separation and crystallization took place, promoting the formation of HfO$_2$ and Al$_{2.4}$O$_{3.6}$ crystalline phases. Also, non-homogeneous electronic density distribution in the dielectrics gave rise to the formation of several regions which can be viewed as fitting sub-layers, each of them with arbitrary electron density to obtain the real thickness using the PARRAT32 code. In addition, it was observed an average accumulation capacitance ($C_{ma}$) almost three times lower compared to the corrected one, which means an intense leakage process occurring for AlHfO$_{3.5}$. Also, a positive flatband voltage and a negative $Q_{SS}/q$ parameter were observed indicating a negative charging effect in the dielectrics.

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