Impact of ALCVD and PVD Titanium Nitride Deposition on Metal Gate Capacitors

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Abstract

In this paper it will be shown that the deposition method is an important parameter for the electrical properties of the metal gate. Indeed, ALCVD(Atomic Layer Chemical Vapor Deposition) TiN metal has a 5.3eV workfunction, suitable for PMOS devices. The PVD sputtered (Physical Vapor Deposition) TiN has a lower workfunction around 4.8eV and is mid-gap like. The PVD TiN capacitors have a higher effective oxide charge than the ALCVD capacitors as extracted from capacitance measurements and from workfunction calculations.

PVD TiN also exhibits process-induced damage as seen from leakage measurements.

1. Introduction

As the gate length of CMOS devices is scaled down to the sub-100 nanometer range, poly depletion, poly high sheet resistance and boron penetration through the SiO\(_2\) gate oxide become an issue. On the other hand, new metal gate electrodes and high-k dielectrics are investigated as a replacement for polysilicon and SiO\(_2\). Significant effort has been put into finding a suitable high-k gate dielectric[1-3] in order to meet the ITRS requirements for gate leakage[4]. Furthermore, a thicker high-k dielectric could minimize the boron penetration.

The use of a metal gate is required to solve the poly depletion and high resistivity of polysilicon.

The gate stack should meet some requirements. The gate electrode has to be stable in contact with the gate dielectric (SiO\(_2\) or high-k material) during a conventional CMOS flow and needs a proper workfunction and high reliability. The optimal metal workfunction should coincide with the valence band edge and with the conductance band edge of Si for PMOS and NMOS respectively[5]. The metal gate/dielectric stack has to show low charge density and material/process compatibility (both thermodynamically and chemically).

In this paper, ALCVD and PVD sputtered TiN/SiO\(_2\) capacitors were characterised with respect to workfunction, charge density and reliability. A comparison between the deposition methods is made.

2. Device Fabrication

Metal Oxide Semiconductor capacitors on p-type substrate were used for electrical characterisation. The active area was defined by using a modified LOCOS isolation scheme. Thermally grown SiO\(_2\) was chosen as a gate dielectric, with thicknesses ranging from 2.5nm to 25nm.

After the gate oxidation, the TiN metal is deposited either by PVD reactive sputtering, 100nm thick(10" Ti target, 8kW, 75 sccm of N\(_2\), 25 sccm Ar) or 10nm thick ALCVD TiN(TiCl\(_4\) and NH\(_3\) as precursors at 350°C). Gate electrode was defined by optical lithography and metal dry etching. Samples were finally annealed in forming gas at 420°C for 30 minutes to passivate interface states.

Additional reference samples with p-type and n-type polysilicon gates were prepared similarly.

3. Capacitance Measurements

By using conventional CV measurements, MOS parameters such as flat band voltage, \(V_{FB}\), oxide thickness, \(T_{OX}\), surface doping, \(N_{AD}\), and effective charge density \(N_{eq}\) can be extracted.

3.2. High frequency CV

High Frequency CV measurements(HFCV) are used to extract the flat band voltage and the electrical effective oxide thickness. These parameters are extracted with the NCSU program[6]. Figure 1 compare the HFCV data for
PVD and ALCVD TiN gate capacitors with the 10nm oxide thickness and the corresponding simulated curves.

The experimental data show that the workfunction of ALCVD is different from PVD. The $V_{FB}$ values are 0.38V and 0.04V for the ALCVD and PVD respectively. The higher $V_{FB}$ value for the ALCVD TiN is an indication of higher workfunction than for the PVD TiN as detailed in section 4. The oxide thickness extracted is 10.14 nm for ALCVD and 9.65 nm for PVD electrodes.

The ALCVD data fits better to the simulated data. This is an indication of high effective charge induced by the PVD process since assumptions about the presence of these defects were not included in the fit of the data with the NCSU program. Furthermore, oxide consumption was also observed in the PVD gate electrodes.

3.3. Quasi-static Measurements

To check the effective charge density, Quasi-Static CV measurements (QSCV) were performed. Figures 2 shows the measurements for the ALCVD and PVD TiN with the 10nm thick oxide.

The voltage shift from HFCV to QSCV measurements is mainly due to the effective oxide charge, which cannot follow the high frequency signal. The effective charge densities are extracted at the $V_{FB}$ value. For ALCVD TiN it is about 2.8x10$^{11}$cm$^{-2}$. The PVD TiN gate capacitors show higher charge density from the QSCV measurements, above 3.6x10$^{11}$cm$^{-2}$. A probable source of oxide charge is sputtering damage.

4. Workfunction Extraction

In order to extract the metal/semiconductor workfunction difference, $\phi_{MS}$, the flat band voltage of a MOS capacitor needs to be measured:

$$V_{FB} = \phi_{MS} + \frac{Q_{OX}T_{OX}}{k_{OX}e_0}$$

(1)

Assuming that the $Q_{OX}$ is independent of the oxide thickness $T_{OX}$, the graph of $V_{FB}$ as a function of $T_{OX}$ should intercept the y-axis at $\phi_{MS}$. As the $\phi_{MS}$ value is the workfunction difference between the metal and the semiconductor can be calculated in the flat band voltage (vacuum level as reference) as shown in figure 3, the metal workfunction $\phi_m$ is:

$$\phi_M = \left( \chi + \frac{E_g}{2} \pm \phi_B \right) - \phi_{MS}$$

(2)

where the plus sign is used for p-type substrate and the minus sign is used for n-type, $\phi_B$ is the Fermi potential, $E_g$ is the band gap, $\chi$ the electron affinity of the semiconductor and $q$ is the electron charge.
The values of $V_{FB}$, extracted from the capacitors with oxide thicknesses ranging from 5 to 25nm, were used to calculate the metal workfunction with (1) and (2). Figure 4 shows the $V_{FB}$ vs. $T_{OX}$ data for ALCVD and PVD TiN together with those of p-type and n-type polysilicon control samples. The ALCVD data are very close to those of p-type polysilicon capacitors.

ALCVD TiN has a workfunction of 5.3eV (p-type like) and the PVD TiN is around 4.8eV (mid-gap like). The higher workfunction of the ALCVD TiN can be attributed to the deposition process in which more nitrogen is bonded to titanium. The ALCVD TiN is a suitable material for PMOS transistors.

From the slope of the lines in figure 4, the effective charge density can be calculated. It is $3.8 \times 10^{11}$ cm$^{-2}$ for the ALCVD TiN and $4.0 \times 10^{11}$ cm$^{-2}$ for the PVD TiN. These values are consistent with the values extracted from the QSCV measurements.

Polysilicon samples show even lower charge densities than the metal gate capacitors. Further optimization of the forming gas anneal step is needed for the TiN metal gate capacitors.

5. Leakage Measurements

To confirm the workfunction of the two different materials, leakage measurements with substrate injection polarity were considered. The 10nm oxide thickness samples were used. The current density was measured as function of gate voltage for both materials. The tunnelling barrier for ALCVD TiN should be higher (high workfunction difference) and therefore the onset voltage of the leakage current should be higher. The expected shift in the leakage currents should be approximately the workfunction difference between the materials.

Figure 5 shows the leakage measurements for ALCVD and PVD TiN capacitors. The leakage current presents a 0.5V shift, which is about the workfunction difference between the materials.

This result confirms that the ALCVD TiN has a higher workfunction than PVD TiN.

5.1. Process-induced Damage

Systematic leakage measurements were done on the 5nm thick oxide capacitors to check for deposition process-induced damage. Leakage measurements, with substrate injection as mentioned above, were performed. Different areas were used and 30 dies were measured on each wafer for reasonable statistics. Area scaling and yield (breakdown) of the capacitors were checked.

Figure 6 shows the leakage current spread for all areas at 7.5V from the PVD and ALCVD TiN.

The gate leakage in ALCVD TiN was uniform and scaled with area as seen in figure 6. On the other hand, the PVD material show a large area dependence in the leakage. No area scaling is observed. The high leakage...
current from the PVD TiN samples is due to lower oxide thickness (0.5 nm oxide consumption occurs in the PVD sputtered gates). This spread can be a result of low quality or weak spots in the dielectric, mainly process damage. In this case, the sputtering seems to be responsible for the damage.

6. Conclusions

In this work, the ALCVD and PVD TiN gate electrodes were characterised regarding workfunction, effective oxide charge density and process-induced damage. The ALCVD has a 5.3eV workfunction, suitable for PMOS transistors. The PVD TiN shows 0.5eV lower workfunction than the ALCVD. This shows that the deposition method is important for workfunction determination. Leakage measurements confirm the workfunction difference of the materials.

The effective oxide charge density was extracted from QSCV/HFCV measurements and from workfunction calculations. The ALCVD gate capacitors show lower charge densities than the PVD capacitors. Improvements in the forming gas anneal treatment are needed.

The spread in leakage current from the PVD TiN shows that significant oxide damage occurs. The CVD deposition type is preferable for metal gate devices due to the best reliability results.

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8. References


