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Effect of the metal gate on the breakdown characteristics and leakage current of Ta_2O_5 stack capacitors

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The effect of metal gates (Al, W, TiN) deposited by evaporation (Al) and sputtering (W, TiN) on the breakdown characteristics and leakage currents of 15 nm Ta_2O_5 stack capacitors has been investigated. Leakage currents, breakdown fields and mechanisms of conductivity are discussed in the terms of possible reactions between the Ta_2O_5 and the electrode material, as well as electrode-deposition-introduced defects acting as electrically active centers. The top electrode affects the electrical characteristics of the capacitors and sputtered W is found to be the best. During the deposition of TiN and Al, reactions that degrade the properties of the Ta_2O_5 occur. The high leakage current is attributed to radiation defects generated in the Ta_2O_5 during sputtering of the TiN, and a damaged interface due to a reaction between the Al and Ta_2O_5, respectively. W deposition is not accompanied by the introduction of detectable damage leading to a change of the properties of the initial as-grown Ta_2O_5, (the leakage current is 5 to 8 orders of magnitude lower, as compared to Al and TiN-gate capacitors).

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1. Introduction

The introduction of high-*k* dielectrics into DRAM fabrication requires switching the gate electrode from poly-Si to metal, due to the incompatibility of the most high-*k* materials with poly-Si [1,2]. An important characteristic of a potential gate material is its chemical compatibility with Ta_2O_5 (the metal's inability to reduce Ta_2O_5). Since the type of metal electrode can also have a strong influence on the leakage currents, the choice of the metal gate for Ta_2O_5 capacitors is of crucial importance for dynamic memory manufacture. Many materials (including double-gate alloys) are under investigation, but compatible metal(s) have not been selected yet for Ta_2O_5-based capacitors. Recently [3,4], we reported that stoichiometric and amorphous Ta_2O_5 films can be obtained by thermal oxidation of Ta films on Si. The $Al/Ta_2O_5/Si$ capacitors exhibited excellent dielectric and electrical characteristics. The purpose of this work is to study the influence of the metal gate (Al, W, TiN) on the leakage currents, conduction mechanisms and breakdown fields of 15 nm thermally grown Ta_2O_5 on Si.

2. Experimental

Ta_2O_5 films (15 nm) were grown on p (100) Si, 15 Ωcm by thermal oxidation of rf sputtered Ta films. The oxidation temperature was low enough (873 K) to minimize the oxidation of the substrate and to prevent tantalum silicide formation. Electrical measurements were performed on a set of MOS structures with three top electrodes (Al, W, TiN); gate area 10^{-4} cm^2. Al electrodes were evaporated; W and TiN gates were deposited by rf sputtering. C-V and I-V measurements were carried out to determine the permittivity, electrical and insulating properties of the films. The breakdown electric field E_{bd} was defined as the average applied field at which the current density through the dielectric exceeded 10^{-6} A.

3. Results and discussion

The values of the measured dielectric constant, ε_{eff} ranged from 5.7 to 9.5, varying with the gate material. The dielectric constant of the bulk Ta_2O_5, ε_t was obtained from ε_{eff} by the double layer model [2,3] assuming a 2 nm SiO_2-like interfacial layer, as determined by XPS and TEM [3-5]. ε_t was 12.2, 8.5 and 6.1 for the layers with electrodes of Al, W and TiN respectively. The effect of the top electrode on ε_{eff} is attributed to a reaction between the gate and Ta_2O_5, and/or gate deposition process induced defects, resulting in a change of ε_{eff}. The oxide charge, Q_f was high for all samples (~9-20x10^{11} cm^{-2}), which is typical of as-grown non-annealed layers. This high value presumably masks an eventual weak dependence of Q_f on the electrode material, including various compositional structures of the interface at the top electrode. This means also that the high Q_f is a feature of the oxidation rather than electrode deposition–induced traps in Ta_2O_5. The midgap density of the interface states, D_{it} was 2.5, 5.5 and 9×10^{10} cm^{-2}eV^{-1}, for Al, W and TiN electrodes, respectively. Juxtaposing the Q_f and D_{it} data, one can see that the damage introduced during TiN electrode deposition is basically of the form of interface states, (the created defects are in the interfacial region rather than in the bulk of the Ta_2O_5). C-V hysteresis is small but detectable, 0.1-0.15 V, regardless of the top electrode. The density of slow states Q_{sl} was in the range

~$1.7\text{-}2.5\times10^{11}$ cm^{-2} respectively. The slow states are thought to originate from non-perfect Ta-O and Si-O bonds, as well as Ta- and Si-suboxides located near the interface with the Si [3,4]. Generally, the presence of oxygen vacancies and a number of suboxides in the interfacial region is a phenomenon of the system Ta_2O_5/Si itself, and is not due to electrode deposition effects.

Fig. 1 gives a comparison of the leakage current for capacitors with different electrodes. The current density (J) under negative bias was much higher for samples with TiN and Al gates as compared with W ones, indicating that both the TiN/ Ta_2O_5 and the Al/ Ta_2O_5 interface have high defect densities. The capacitors with W gates yielded a 5 to 8 orders of magnitude lower leakage current density at V = -1V than for Al and TiN gates, respectively. The natural explanation for Al-electroded capacitors is that the Al reacts with Ta_2O_5 to form a thin Al_2O_3 (or Al suboxide) layer, which may produce unwanted traps at the top electrode interface, giving a high current. The formation of an intermixed TiO_x layer is assumed for the TiN gate process. As expected [6], unlike the Al electrode, W does not reduce the Ta_2O_5. A certain discrepancy exists between the data from C-V and I-V measurements, namely: Al-electroded capacitors have the best C-V parameters, while W electrodes consistently show the best I-V curves. Since the C-V curves reflect the characteristics of the interface at the Si, while the I-V curves feel the gate interface region. The results permit us to attribute this behavior again to radiation induced defects in the surface layer at the metal/Ta_2O_5 interface during the deposition of the electrode. Such a kind of damage is missing during the evaporation of Al. The deposition-created damage is stronger for the case of TiN than for W. The behavior of the curves corresponding to the W electrode does not enable us to invoke any of the commonly observed conduction mechanisms. We will focus only on the curves of capacitors with Al and TiN gates.

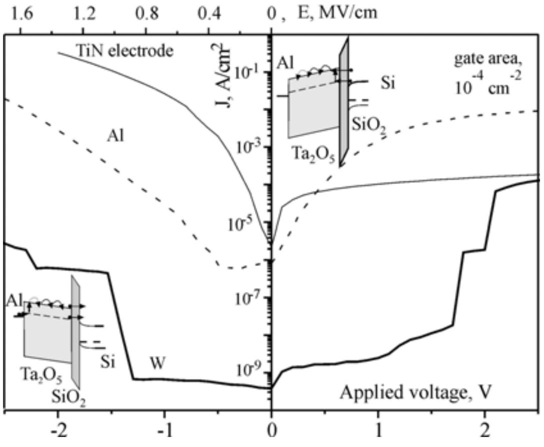

Fig. 1. J-V curves of capacitors with different gates.

The J(E) characteristics of these capacitors in Poole-Frenkel (PF) and Schottky plots are shown in Fig. 2. The dynamic dielectric constant, k_r was deduced from the slopes of the straight lines. k_r should be equal to the optical dielectric constant (typically ~3.8-5) to ensure that conduction is through a PF or Shottky mechanism. The coefficient r in the PF J(E) relation gives information on the trapping centers; ($1 \le r \le 2$). r = 1 corresponds to the normal PF effect, and r = 2 to the modified one. The conduction mechanism in Al-capacitors is governed by a nearly normal (PF) effect (r = 1.1; k_r = 4.8) at E of ~ 0.3 to 1.7 MV/cm and the agreement with the ellipsometrically determined refractive index is accurate (Fig. 2a). The current was constant up to 0.3 MV/cm. A slightly modified Poole-Frenkel effect (r = 1.2, E ~ 0.06-0.5 MV/cm) can also be invoked for a TiN gate. These results indicate that the type and the density of traps are changing with both the electrode material and the deposition conditions, causing small variations in the degree of compensation. The slope of 2.5 for a TiN electrode at medium and high fields is not consistent with the PF process. The current mechanism is of Schottky type in the range 0.5-1.4 MV/cm, (Fig.2b); k_r, = 3.8. Therefore, both the PF process and Schottky emission are dominant conduction mechanisms in capacitors with Al and TiN gates. The absence ofa well pronounced effect of the gate material indicates that the impact of the bulk-limited mechanism is stronger. The current for the W-gate case was nearly constant up to the appearance of breakdown events. This result strongly suggests that by appropriate choice of both the electrode material and its deposition process, a transition from one conduction process to another occurs.

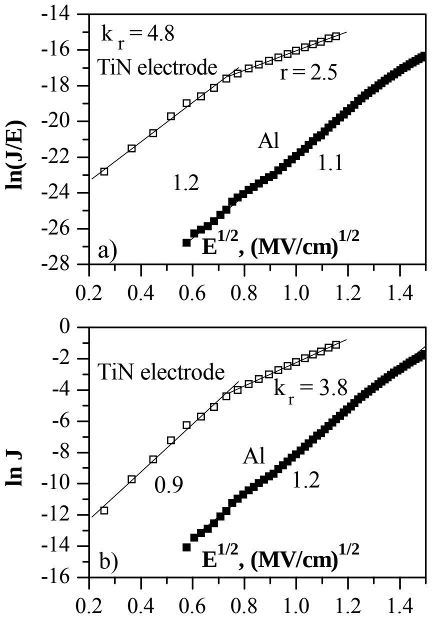

Fig. 2. a) Poole-Frenkel and b) Schottky plot of the I-V curves for TiN and Al-gate capacitors.

The mechanism is critically related to the density of charged traps in the films, and these traps can mask the effect of the electrode work function. We propose that the process starts with electron injection from Al, or TiN, into traps in the Ta_2O_5 close to the gate interface, and further that the conductivity is governed by a PF mechanism, i.e. the leakage current is caused by trap-assisted transport from cathode to anode through the bulk traps. The nature of these traps is structural imperfections and radiation induced defects caused by the electrode deposition, rather than intrinsic Ta_2O_5 traps due to the oxidation. This is supported by the behavior of W-gate capacitors, which do not exhibit PF conductivity. The change of the mechanism for TiN capacitors from bulk (low and middle fields) to electrode limited (high fields) is strange, and at a first glance it is not consistent with the indication of a noticeable generation of defects during TiN deposition. This behavior can be attributed to the quality of the top electrode-interface region itself (in one case electrons tunnel from the gate into the traps located close to/in this region, and in the other case they overcome the gate barrier by Schottky emission) defined by the density and energy distribution of the traps created during gate deposition. If the trap concentration close to the electrode is small, the electrons could not tunnel through them into Ta_2O_5 conduction band. In this case, Schottky emission is more relevant at high fields; especially for the TiN case, this means that the sputtered-induced traps are not basically in the form of traps at the gate, but rather of interface states at Si, as indicated by the C-V data.

At positive bias, when the electrons are injected from the Si, the curves saturated at ~ 10^{-4} A/cm^2, with the exception of Al-gate capacitors having a saturation level of 10^{-2} A/cm^2. There was virtually no change in the magnitude of conductivity with a change in the polarity of the applied voltage for W capacitors, up to the beginning of soft breakdown events, indicating that the process defining the breakdowns is bulk rather than electrode limited. The behavior of the curves is closely related to the parameters of the interfacial layer at Si, and its breakdown. The obvious dependence of the curves on the gate means that the gate deposition process initiates reactions which affect not only the region near the gate but also the layer at the Si giving a contribution to the interface defects. The rapid increase of the current at ~ 1.7-2 V for W-capacitors may be due to the breakdown of the interface layer. For TiN-capacitors, such an increase is not observed. In this case the electrons injected from Si tunnel through the SiO_2 to the bulk traps in the Ta_2O_5, which are present close to the interface with the SiO_2, i.e. the conduction is a combination of direct or a double layer barrier tunnelling in SiO_2 and a PF effect in the Ta_2O_5. This can explain the existence of a higher leakage current in TiN capacitors (and is consistent with the high density of interface states), compared to W ones, and the absence of an abrupt current increase as well. Al-gate capacitors demonstrated intermediate characteristics between those of W and TiN structures, reflecting the specific properties of the near-interface region at the Si in this case. Since the thickness of the SiO_2 is the same for capacitors with all three electrodes, the different levels of the current under reverse bias should be attributed to traps created even in the interface layer at the Si during gate deposition. In this context, the curves in the case of a W gate reflect the intrinsic properties of this interfacial region, defined by the oxidation process itself.

Fig. 3 illustrates the breakdown characteristics in dependence on the type of the gate. The highest E_{bd} corresponds to the W-gate capacitors. The magnitude of the peak at 9-12 MV/cm, was 40 %, and breakdown did not occur up to ~ 6 MV/cm applied field. The samples with Al electrodes also showed relatively good characteristics: most capacitors broke down at ~ 1.5 MV/cm, (35% of the failures) and in the field range ~ 9.5-10.5 MV/cm. Among the three electrodes, the characteristics of the TiN ones were the worst: the greatest fraction of capacitors broke down in the field range up to 1 MV/cm. independently of the presence of the breakdowns at higher fields. The results are in a good correlation with C-V and I-V data and confirm that indeed the sputtered W gate provides capacitors with a good quality.

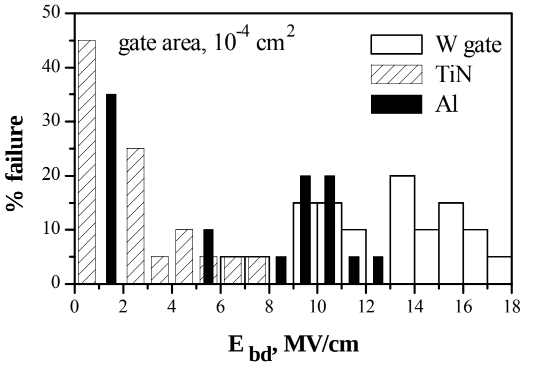

Fig. 3 Breakdown histograms of capacitors with various gates.

Evidently W deposition is not accompanied by the introduction of detectable damage leading to a change in the properties of the initial as-grown Ta_2O_5 as in the case of TiN where the low values of E_{bd} are attributed to a film damaged by the TiN deposition. In this sense, the E_{bd} characteristics of W-capacitors are closest to the intrinsic breakdown of Ta_2O_5.

3. Conclusions

Based on the results, one would tend to conclude that the *unavoidable introduction of metal electrodes* in advanced generations of high-*k* dielectric based DRAMs *introduces its own set of manufacturing and capacitor quality challenges*, and requires the development of specific technological schemes. We have shown that some reduction of the Ta_2O_5 during deposition of the top electrode can occur. This may be attributed both to the gate deposition technique and the chemical reactions between the Ta_2O_5 and electrode material. The former dominates in the case of a TiN gate, (radiation induced defects in the Ta_2O_5 during the sputtering of TiN), and the second is typical of Al-electroded capacitors, (Al reacts with Ta_2O_5 to form Al-oxides). The final result in both cases is a damaged Ta_2O_5/top electrode interface, which affects the parameters of the capacitors, and mainly the leakage current. No severe reaction occurs between the W and underlying Ta_2O_5 during W sputtering. The electrode deposition induced defects act as electrically active centers, causing a much higher current for Al and TiN gate capacitors as compared to W ones. These defects are also responsible for the strong dependence of the conduction mechanism on the electrode material, and are the critical factor controlling the conductivity. *Their effect can be strong enough to mask that of the electrode work function*. The results imply that the sputtering technique is a beneficial technology for W deposition, ensuring a stable contact to Ta_2O_5 and tolerable leakage currents, while radiation induced damage of the Ta_2O_5 during the deposition makes this method less favourable in the TiN case. Although some reaction between the Al electrode and the Ta_2O_5 obviously occurs, the resulting electrical properties are still acceptable. The more general conclusion is that *the choice not only of the gate material but the gate deposition technique remains a critical concern for high-k oxides*.

Acknowledgements

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