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The Influence of La and Zr Doping on TDDB Characteristics of HfO_2 Thin Films

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1. Introduction

HfO_2 gate dielectrics have encountered the following integration related issues: (1) low crystallization temperature; (2) high threshold voltages for n- and p-MOSFETs due to Fermi-level pinning.[1, 2] More recently, La (lanthanum) incorporation into HfO_2 gate dielectrics has been successfully demonstrated to obtain desired device characteristics with low V_T, and increased crystallization temperature without degradation of dielectric constant.[3, 4] On the other hand, compared to HfO_2 gate dielectrics, $HfZrO_2$ (hafnium zirconate) can further achieve a lower NMOS V_T, higher transconductance, lower charge trapping density and interface state density, higher drive current, reduced C-V hysteresis, and improved PBTI reliability.[5] Although time-dependent-dielectric-breakdown (TDDB) reliability is one major concern in advanced technology, it has not yet been fully understood for Hf-based high-κ dielectrics, especially La-incorporated $HfZrO_2$ (HfZrLaO) thin films.

2. Experiments and Results

12-inch *p*-type (100) Si wafers were used as the starting substrate. A thin chemical oxide was formed after the RCA-1 and RCA-2 cleaning procedures. A 2-nm ALD (atomic layer deposition) HfO_2 or $HfZrO_2$ films were deposited, followed by 1-nm ALD LaO capping layer. TaC metal gate was subsequently deposited by PVD as the gate electrode. An annealing in forming gas was then performed for 30 min to achieve a La-incorporated HfO_2 or $HfZrO_2$ thin film, confirmed by TEM (the inset of Fig. 1). The EOT and V_{FB} are extracted through NCSU CVC model. Constant voltage stress (CVS) with a negative bias on the gate is applied to investigate the TDDB characteristics of the HfLaO and HfZrLaO thin films.

The insets in Fig. 1 graphically illustrate the fabrication procedure of the capacitors. Fig. 1 shows the high-frequency (100k Hz) *C-V* characteristics. For HfLaO thin film, the dielectric constant, EOT, and flatband voltage (V_{FB}) are determined to be about 16.3, 0.72 nm, and -0.87 V, respectively. For HfZrLaO thin film, the dielectric constant, EOT, and flatband voltage, are determined to be about 17.2, 0.68 nm, and -0.91 V , respectively.

Fig. 2 shows the J_g-E characteristics at room temperature. The dielectric breakdown fields for HfLaO and HfZrLaO are about 10.5 and 12.5 MV/cm, respectively. The gate leakage densities (J_g) are only about 9.0×10^{-1}, and 1.1×10^{-1} A/cm^2 at V_{FB} - 1 V for HfLaO and HfZrLaO thin film, respectively. Fig. 3 further compares the J_g versus EOT characteristics among various Hf-based gate dielectrics, in which J_g is defined as V_g equals to V_{FB} - 1 V. It is apparent that the HfZrLaO thin film (this work) has a better J_g-EOT performance, suggesting its potential scalability for future advanced gate-dielectric applications.

In this work, time-to-breakdown (T_{BD}) is defined when hard breakdown (HBD) occurs. The normalized Weibull distributions of two different capacitor areas match to a single line in Fig. 4, meaning that the breakdown is intrinsic and it can be explained by percolation model.[10] Fig. 5 (a) and (b) show the TDDB Weibull distributions of different capacitor areas under various stress voltages at room temperature. A very similar Weibull slope (β) is obtained for all distributions. The parallel Weibull distributions shown in Fig. 5 (a) and (b) indicate that under this study the TDDB failure mechanism of two kinds of samples should be independent of stress voltages and capacitor areas. Fig. 6 (a) and (b) show the Weibull distributions at various temperatures. For HfLaO thin film, it is observed that β increases as temperature increases in Fig. 6 (a). This phenomenon has been ascribed to temperature-sensitive defects that may be redistributed within high-κ layer at elevated temperatures.[12] On the other hand, for HfZrLaO thin film, a very similar β is also obtained for all distributions in Fig. 6 (b).

The activation energy (ΔH_0) is determined from the Arrhenius plot of the 63% CDF of T_{BD}, as shown in Fig. 7 (a) and (b). The extracted ΔH_0 values of HfLaO and HfZrLaO are in the range of 0.51~ 0.54 and 0.54 ~ 0.60 eV, respectively. Fig. 8 shows the TDDB dependence on electric field, in which the thermochemical breakdown *E*-model has been employed and can be expressed as the following equations[11, 12]

$$\ln(T_{BD}) \propto \frac{\Delta H_0}{k_B T} - \gamma E_{ox} \tag{1}$$

$$\Delta H_0 = \Delta H_0{}^* - p_0\left(\frac{2+\kappa}{3}\right)E_{ox} \tag{2}$$

By utilizing Eqs. (1)-(2), the field acceleration parameter (γ) as well as other parameters can be obtained. From Fig. 9, V_g = 2.03 V (or 6.1 MV/cm) and V_g = 1.87 V (or 5.6 MV/cm) are projected to yield 10-year TDDB lifetime at normal operation of 85 ℃ for HfLaO and HfZrLaO thin film, respectively. Table I summarizes some important parameters of this work.

3. Conclusions

MOS capacitors incorporating La-incorporated HfO_2 or $HfZrO_2$ gate dielectrics were fabricated and extensively investigated. The HfZrLaO thin film shows a better J_g-EOT performance, indicating its potential scalability for future advanced gate-dielectric applications. At 85 ℃, the maximum voltage projected to have 10-year TDDB lifetime are V_g= 2.03 and 1.87 V for HfLaO and HfZrLaO thin film, respectively. The excellent electrical properties and TDDB characteristics indicate that this La-incorporated $HfZrO_2$ (HfZrLaO) gate dielectric has outstanding scalability for future high-κ gate-dielectric applications.

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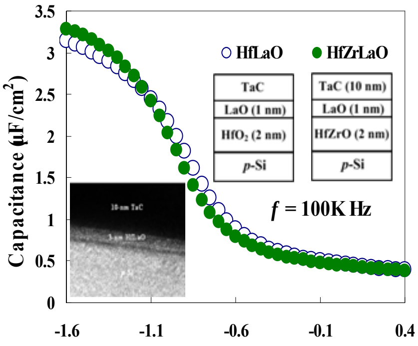

Fig. 1. *C-V* characteristics of the samples. The insets show the structures of the samples and TEM graph.

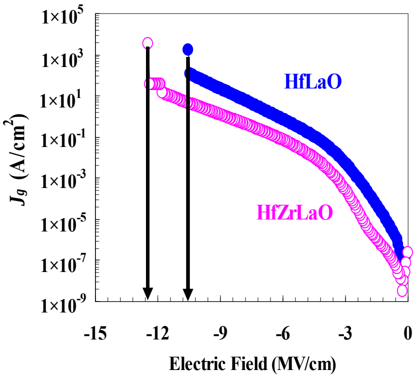

Fig. 2. *J-E* plot for breakdown characteristic of two kinds of samples.

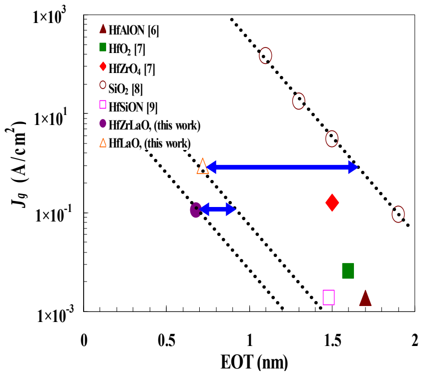

Fig. 3. Comparison of J_g-EOT for SiO$_2$ and Hf-based high-κ dielectrics.

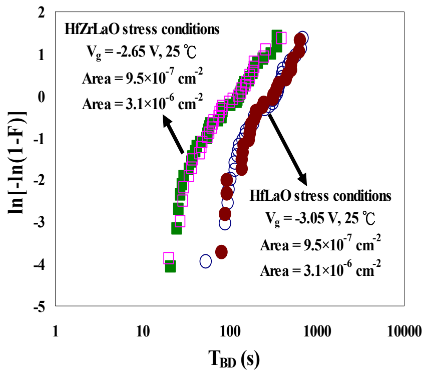

Fig. 4. Normalized Weibull distributions of two kinds of samples.

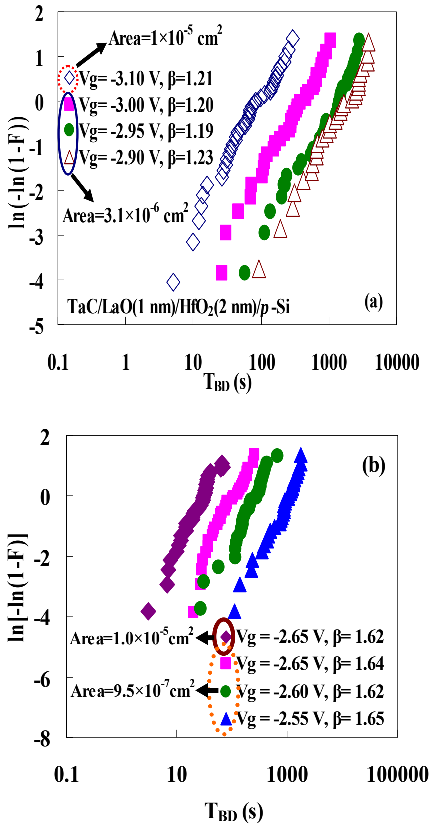

Fig. 5. The TDDB Weibull distributions of (a) HfLaO and (b) HfZrLaO thin films with various areas and different stress voltages.

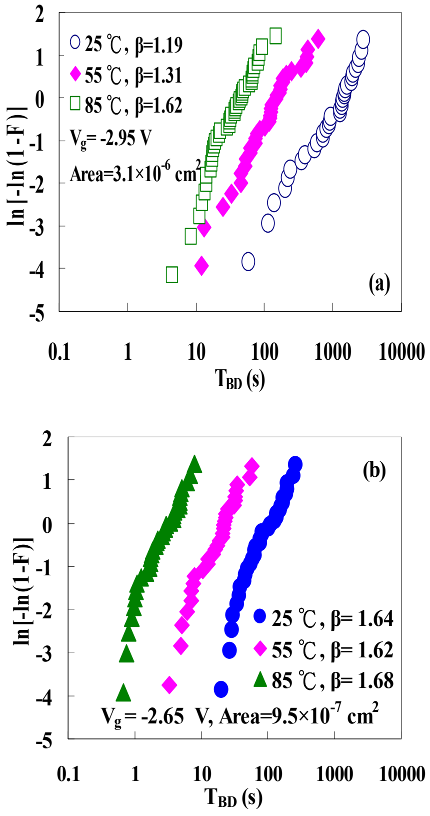

Fig. 6. The TDDB Weibull distributions of (a) HfLaO and (b) HfZrLaO thin films at different temperatures.

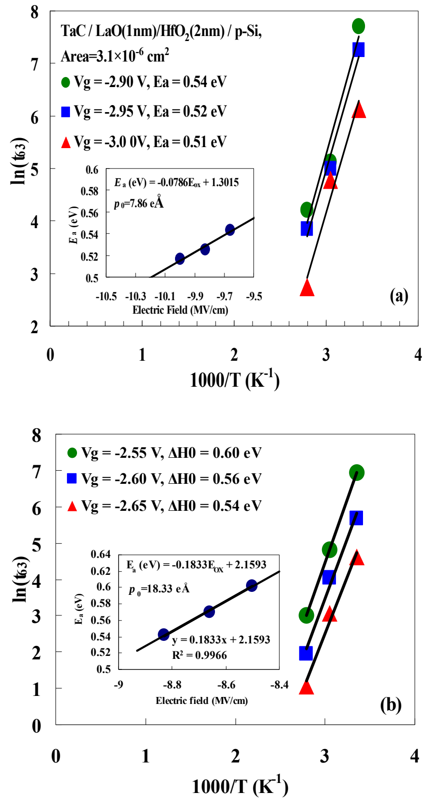

Fig. 7. Arrhenius plot of T_{BD} for (a) HfLaO and (b) HfZrLaO thin films. The insets are the dependence of TDDB activation energy on oxide field.

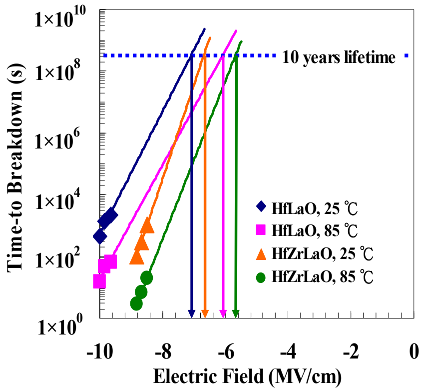

Fig. 9. T_{BD} is plotted as a function of electric filed.

Table Ⅰ. Some important parameters of HfLaO and HfZrLaO gate dielectrics

Oxide	HfLaO	HfZrLaO
EOT (nm)	0.72	0.68
J_g (A/cm^2)	9.0×10^{-1}	1.1×10^{-1}
$E_{BD,acc.}$ (MV/cm)	10.5	12.5
ΔH_0 (eV)	0.51~0.54	0.54~0.60
γ (cm/MV)	4.3~4.5	5.9~7.0
$E_{10\text{-year}}$ at 85℃ (MV/cm)	6.1	5.6