Impact of Alkali-Earth-Elements Incorporation on V_{fb} Roll-Off Characteristics of La_2O_3 Gated MOS Device

T. Koyanagi[a], K. Kakushima[b], P. Ahmet[a], K. Tsutsui[b],
A. Nishiyama[b], N. Sugii[b], K. Natori[a], T. Hattori[a], and H. Iwai[a]

[a]Frontier Research Center, Tokyo Institute of Technology,
[b]Interdisciplinary Graduate School of Science and Engineering,
Tokyo Institute of Technology,
4259, Nagatsuta, Midori-ku, Yokohama 226-8502, Japan

The impacts of Mg, MgO, CaO, SrO or BaO incorporation on La_2O_3 MOS devices have been examined. Roll-off behavior in the flat-band voltage (V_{fb}) of the MOS capacitors on equivalent oxide thickness (EOT) has been observed. The roll-off characteristic has been suppressed with Mg incorporation. On the other hand, with MgO, CaO, SrO or BaO incorporation, the characteristic has been enhanced. Interface-state density (D_{it}) has slightly increased and leakage-current density (J_g) has unchanged with the incorporation.

Introduction

Degradation to the electrical characteristics with equivalent oxide thickness (EOT) scaling has been one of the major problems in high-k gated MOSFETs. La_2O_3, which can achieve an EOT below 1 nm with fairly nice interface (1), also suffers from this problem. Recently, it has been reported that the incorporation of Mg into La_2O_3 films can suppress the generation of fixed charges and eventually improves mobility (2). In this paper, the incorporation of Mg, MgO, CaO, SrO or BaO, alkali-earth-elements, has been investigated and its impact on electrical characteristics is discussed.

Experiment

The fabrication procedure of metal oxide semiconductor (MOS) capacitors is shown in Figure 1(a). After SPM cleaning and HF treatment, La_2O_3 layers ranging from 2 to 4 nm in thicknesses were deposited on a *n*-Si(100) wafer with a 400-nm-thick SiO_2 isolation regions by e-beam evaporation at a deposition rate of 0.2 ~ 0.4 nm/min at a pressure of 10^{-6} Pa. Either Mg, MgO, CaO, SrO or BaO layer was successively evaporated onto the formed La_2O_3 layer as the same way with the La_2O_3 layer, and subsequently a 60-nm-thick W layer was *in situ* deposited by RF sputtering. To avoid the absorption of any moisture or carbon-related contamination, the wafers were not exposed to air during the depositions. The W layer was patterned by reactive ion etching (RIE) using SF_6 chemistry to form gate electrodes. The wafers were then post-metallization annealed (PMA) in a rapid thermal annealing (RTA) furnace in forming gas (FG)(N_2:H_2= 97%:3%) ambient at 500 ^{o}C for 30 min. Finally, an Al layer was deposited on the backside of the substrate as a bottom contact by thermal evaporation. The schematic illustration of the gate stack structure at as-deposited state is shown in figure 1(b). Capacitance-voltage (*C*-*V*) and leakage current density-voltage (J_g-*V*) characteristics were measured using an Aglilent E4980A precision LCR meter and 4156C semiconductor parameter analyzer, respectively.

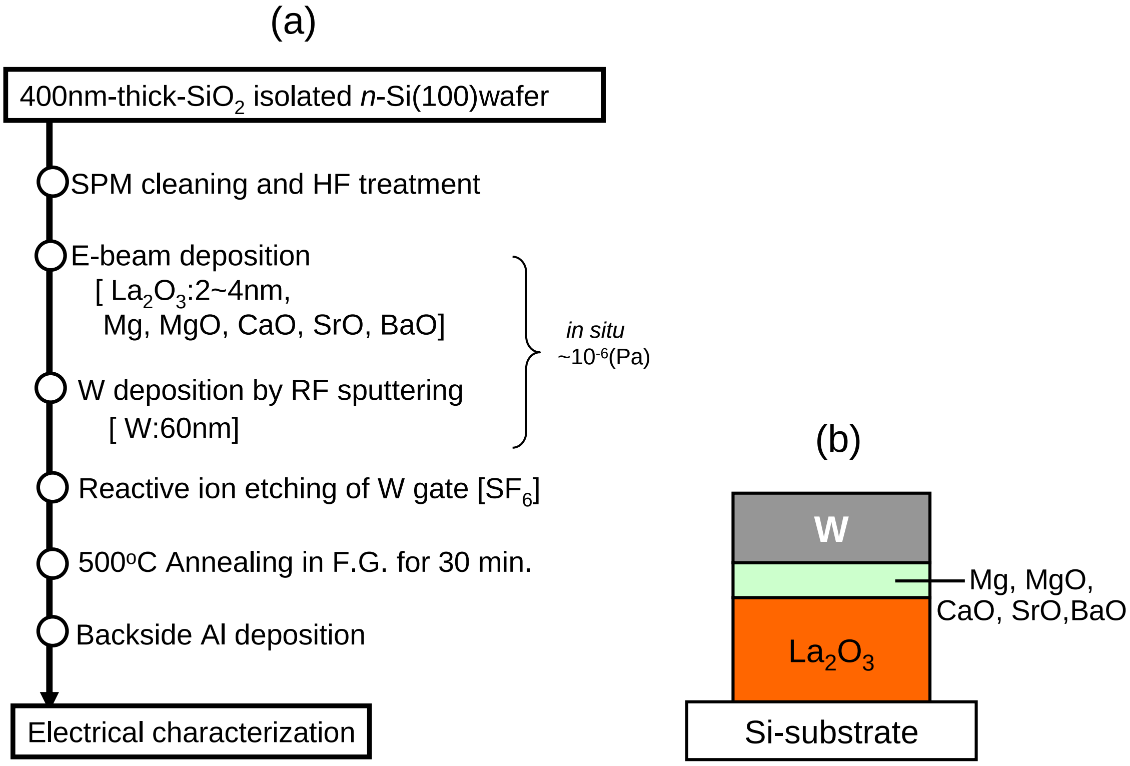

Figure 1.(a) Fabrication process flow of MOS capacitors. (b) Schematic illustration of the MOS structure in as-deposited condition.

Result and Discussion

Behaviors in V_{fb}-EOT Plots

Figure 2 shows flat-band voltage (V_{fb}) dependence on EOT of the capacitors. W/La_2O_3/Si gate stack structure MOS capacitors were fabricated. The thickness of La_2O_3 layer was changed from 2 to 4 nm. Negative shift (roll-off) and positive shift (roll-up) of V_{fb} are observed at EOT region of 1.3 nm to 0.9 nm and 0.9 nm to 0.6 nm. The V_{fb} roll-off and roll-up are considered to be caused by fixed charges. La-silicate is reactively formed by heat treatment and the fixed charges are considered to be located at the La_2O_3/La-silicate interface and inside the La-silicate layer. It is reported that the fixed charges inside the La-silicate layer is increased as the W atoms diffuse into the La-silicate layer (3). The number of fixed charges can be roughly estimated by defining the fixed charge density inside the La-silicate (ρ) and the fixed charge density at the La_2O_3/La-silicate interface (σ). Assuming that the thickness of La-silicate is constant at the EOT region from 2.0 nm to 0.9 nm as shown in figure 3, V_{fb} can be expressed as

$$V_{fb} = -\left(\frac{\sigma\, t_{La2O3}}{\varepsilon_{La2O3}} + \frac{\rho\, t_W t_{La2O3}}{\varepsilon_{La2O3}} + \frac{\rho\, t_W^{\;2}}{2\varepsilon_{LaSilicate}} \right) + \phi_{ms}\,, \qquad [1]$$

where ε_{La2O3} and $\varepsilon_{Lasilicate}$ are the permittivity of La_2O_3 and La-silicate, respectively. t_{La2O3} and t_W are the thicknesses of La_2O_3 and the distance of W atoms diffused into the silicate layer. ϕ_{ms} is the work function difference of the metal and the Si substrate. Using this equation, the number of the fixed charged inside La-silicate ($N_{LaSilicate}$) and the number of the fixed charges at La_2O_3/La-silicate interface (N_{int}) can be well fitted to be 7.6 x 10^{19} cm^{-3} and 3.7 x 10^{12} cm^2, respectively, as shown in figure 2.

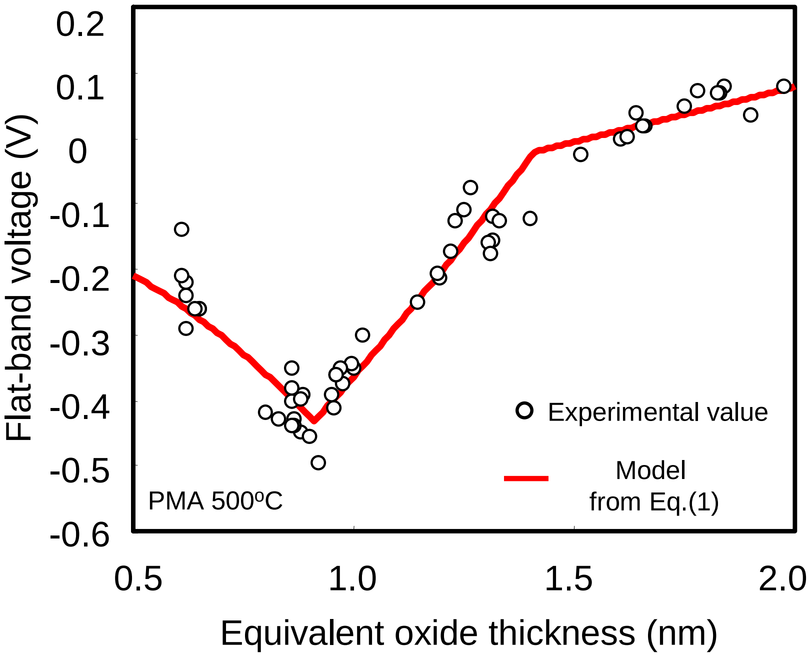

Figure 2. V_{fb} dependence on EOT of $W/La_2O_3/Si$ gate stack structure MOS capacitors.

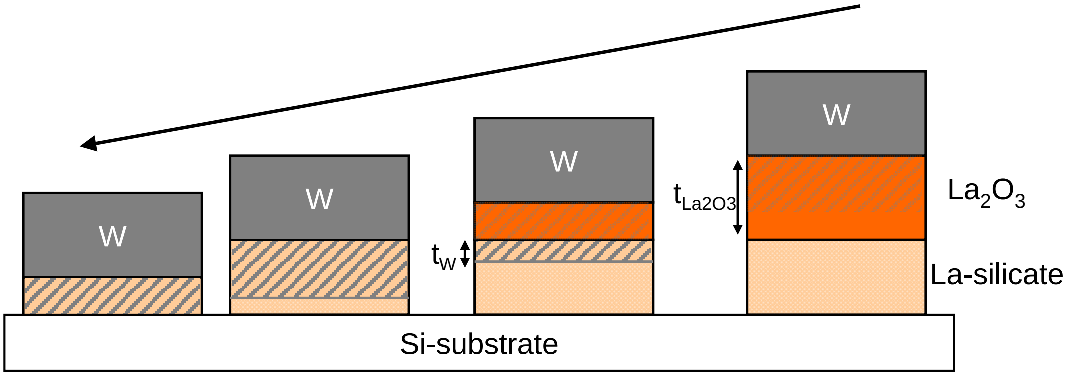

Figure 3. Schematic illustration of the variation of La_2O_3 and La-silicate layer.

Suppression of V_{fb} roll-off with Mg incorporation

W/Mg/La_2O_3/Si gate stack structure MOS capacitors were fabricated with Mg capping thickness of 1.0 nm. The thickness of La_2O_3 layer was changed from 2 to 4 nm. Figure 4 shows V_{fb} dependence on EOT of the capacitors with and without Mg capping layer. The negative shift in V_{fb} is well suppressed with the Mg capping presumable owing to the suppression of the fixed charge generation.

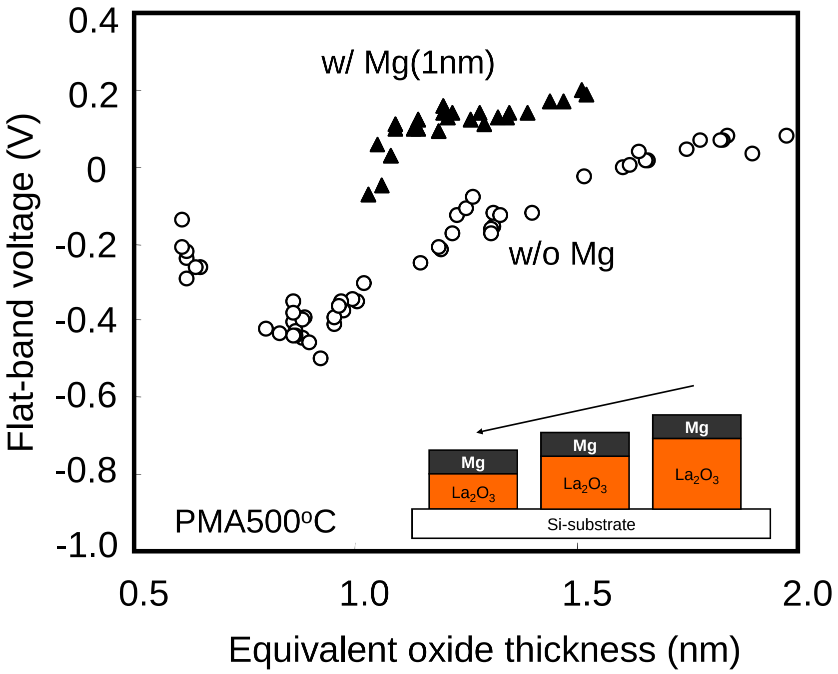

Figure 4. V_{fb} dependence on EOT with and without Mg incorporation.

Enhancement of La-silicate Growth with Alkali-Earth-Elements Incorporation

W/BaO/La_2O_3/Si gate stack structure MOS capacitors were fabricated. A 2-nm-thick La_2O_3 layer was capped by 1.0 and 1.5-nm-thick BaO. Figure 5 shows *C-V* characteristic of the capacitors. EOT increases with increasing BaO incorporation. The EOT decrease indicates that more La-silicate was formed at Si/La_2O_3 interface by BaO capping after PMA. It is reported that ionic oxygen conductivity is increased with alkali-earth-elements incorporation (4). It is considered that the La-silicate was formed by oxygen supplying because of the high ionic conductivity. Therefore, the amount of alkali-earth-elements incorporated into La_2O_3 should be minimized to avoid EOT increasing. Figure 6 shows result of x-ray photoelectron spectroscopy (XPS) analysis of W/BaO/La_2O_3/Si gate stack structure MOS capacitors. The thickness of La_2O_3 layer and BaO layer are 2 nm and 1 nm, respectively. The increase of amount of La-silicate with BaO incorporation is observed.

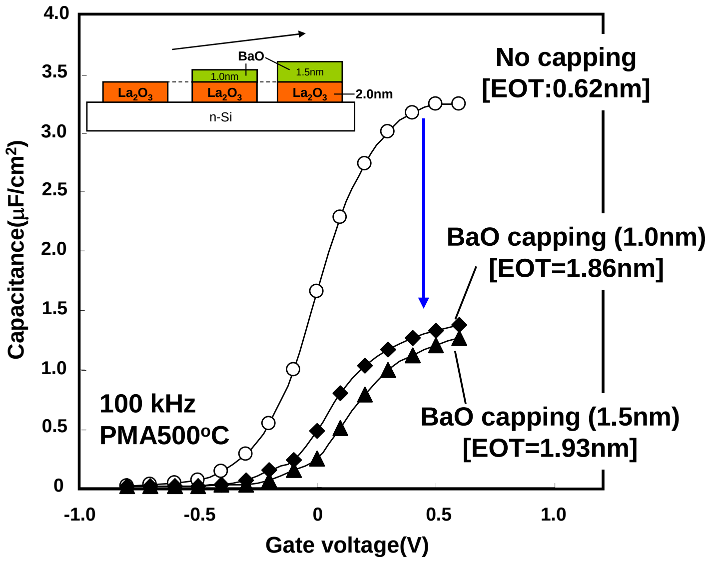

Figure 5. *C-V* characteristics with and without BaO incorporation.

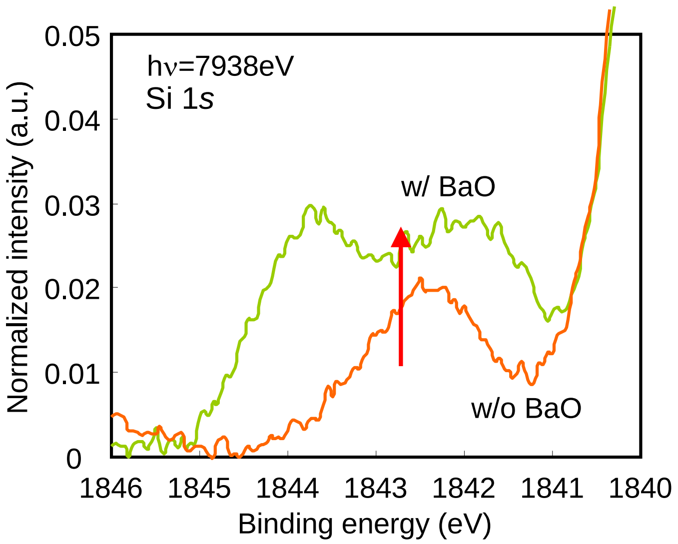

Figure 6. Result of XPS analysis of W/BaO/La_2O_3/Si gate stack structure MOS capacitors.

V_{fb} roll-off Enhancement with MgO, CaO, SrO or BaO Incorporation

The V_{fb} roll-off characteristics of La_2O_3 capacitors with either MgO (1nm), CaO (0.7nm), SrO (1nm) or BaO (0.3nm) capping were shown in figure 7. One can observe enhancement in the roll-off characteristics with alkali-earth oxide incorporation. As the ionic oxygen conductivity is higher with alkali-earth-elements silicate, it is considered that La-silicate growth was enhanced by supply of oxygen atoms due to the high ionic conductivity so that the number of fixed charges, which is generated by diffusion of W atoms in La-silicate is also increased. The enhancement of V_{fb} roll-off is caused by the increased fixed charges.

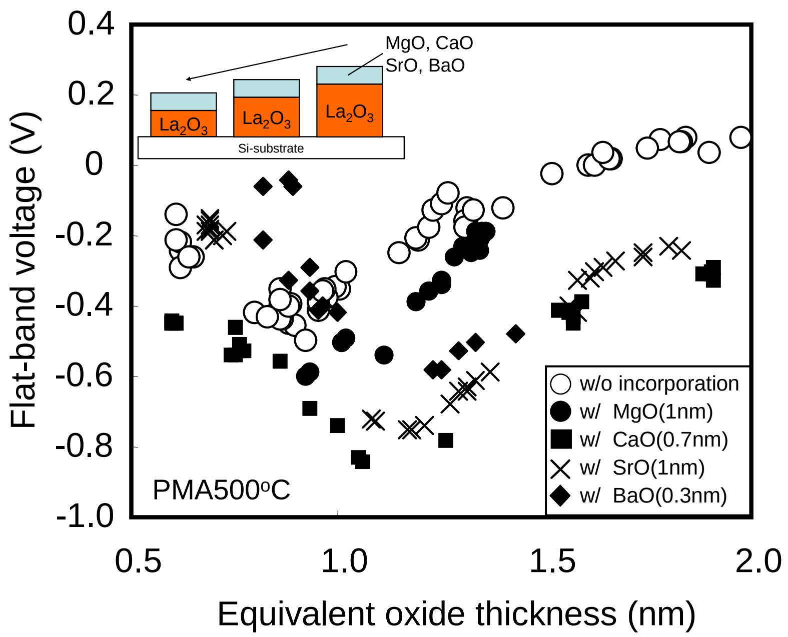

Figure 7. V_{fb} roll-off characteristics of La_2O_3 capacitors with either MgO (1nm), CaO (0.7nm), SrO (1nm) or BaO (0.3nm) capping.

J_g on EOT with Alkali-Earth-Elements Incorporation

Figure 8 shows the EOT dependence of J_g change with or without the alkali-earth-elements incorporation, measured at gate voltage (V_g) = 1.0 V. J_g slightly increases with MgO incorporation. However, no notable change was observed with alkali-earth-elements incorporation.

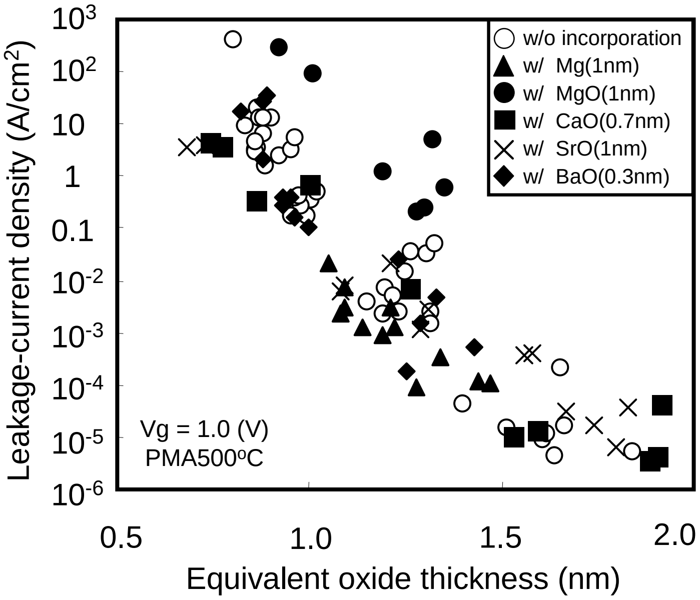

Figure 8. EOT dependence of J_g change with or without the alkali-earth-elements incorporation.

D_{it} on EOT with Alkali-Earth-Elements Incorporation

Figure 9 shows the EOT dependence of interface-state density (D_{it}) with and without alkali-earth-elements incorporation, measured by conductance method. With MgO incorporation, D_{it} is slightly decreased. On the other hand, D_{it} is slightly increased with the other elements incorporation.

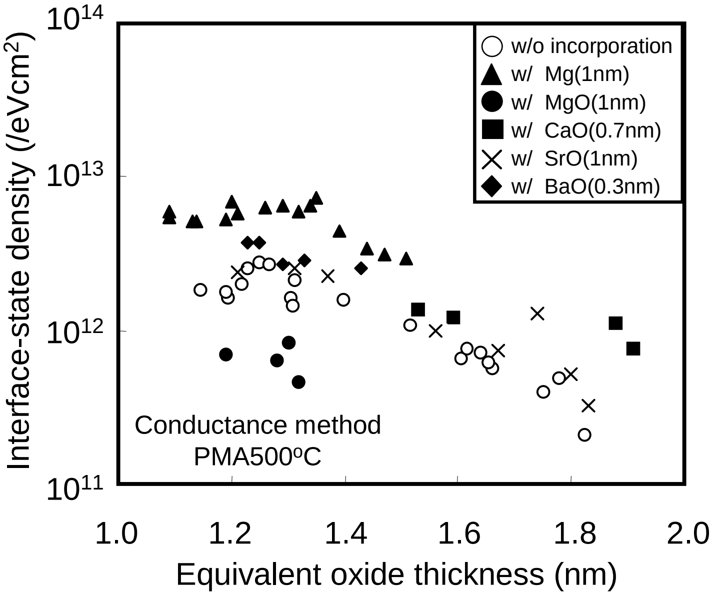

Figure 9. EOT dependence of D_{it} with and without alkali-earth-elements incorporation.

Conclusion

The impact of alkali-earth-elements incorporation into La_2O_3 gated MOS device on electrical characteristics have been conducted. The V_{fb} roll-off and roll-up have been observed. Mg incorporation can well suppress the negative shift of V_{fb} at EOT value above 1.0 nm indicating the suppression of increase of fixed charges. The other elements incorporation enhanced the negative shift of V_{fb}. It is considered that fixed charges inside La-silicate layer were increased with the incorporation. No notable change in leakage-current density and interface-state density has been observed with the incorporation.

Acknowledgement

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