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Impact of Zirconia addition for ALD Hafina in HKMG Device Fabricated GF vs. GL

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1. Introduction

Hf-based dielectrics suffer from mobility degradation, charge trapping and poor reliability **[1]**. Doped high-k with rare-earth element via dielectric cappings (LaO, DyO, etc.) has been demonstrated as a practical solution to achieve low V_T nMOSFETs **[2-3]** for advanced technologies. Hafina (HfO_2) and Zircon ia (ZrO_2) have very similar physical and chemical properties **[4]**. Among all the binary materials $HfZrO_x$ films were shown to present higher reliability and mobility than HfO_2 thin films **[5-6]**. In this stud y, we investigated an extensive physical characterization of $HfZrO_x$ dielectrics as a fun ction of Zr concentration ratio (Zr%). Furthermore, Hf ZrO_x MOSCAPs we re fabricated to understand the impact of ZrO_2 addition for ALD HfO_2 on device properties by changing the Zr% and ZrO_2 position in gate stack with Gate First (GF) and Gate Last (GL) process flow comparison.

2. Experimental

The MOSCAP sample fabricatio n flow is shown in **Fig. 1**. The single (HfO_2 or ZrO_2) or bi-layer ($HfZrO_x$) high-k dielectric were deposited by ALD on the th ermal grown SiO_2. The different Zr% eff ect and ZrO_2 position in HfO_2 were study. GF and GL process were compared in this work. Thin La_2O_3 caps was deposited for nMOSCAP effective workfunction (EWF) tuning und er GF process. The different N/P metal were used for GL EWF tuning.

3. Results and Discussion

The **Fig. 2(a)** shows band gap (E_g) analysis by spectroscopic ellipsometry, the band gap of $HfZrO_x$ decreased when ZrO_2 addition with HfO_2. Preliminary result of Plan-View TEM fo r HfO_2 (**Fig. 2(b)**) and $HfZrO_x$ (**Fig. 2(c)**), respectively. The $HfZrO_x$ grain size shows sma ller than HfO_2. We believe that the change in grain-size plays a role in reducing charge trapping in HfO_2. In **Fig. 3, c**ross section HR-TEM image of HfO_2/SiO_2 (**Fig. 3(a)**) and $HfZrO_x/SiO_2$ with different ZrO_2 position at Top (**Fig. 3(b)**), Center (**Fig. 3(c)**) and Bottom (**Fig. 3(d)**) after annealing at 1050°C. A uniform contrast indicates a compositional uniformity. Both Hf-based dielectric are polycrystalline with similar bulk dielectric thickness and interface oxide thickness. ZrO_2 was mixed into HfO_2 for three different ZrO_2 position samples, due to the differences in the lattice constants of ZrO_2 and HfO_2 are very small, and the equivalent valence and almost equivalent ionic radii of Zr^+ and Hf^+ cations. **Fig. 4** shows HfO_2, $HfZrO_x$ and ZrO_2 k value comparison which were extracted from EOT vs. ph ysical thickness plot. ZrO_2 addition on HfO_2 can increase k value. As in **Fig. 5** , the XP spectra of Si2p of the sample for HfO_2 and dif ferent ZrO_2 position in $HfZrO_2$. $ZrSiO_x$ silicate was identified. Bottom ZrO_2 in HfO_2 shows higher $ZrSiO_x$ signal. **Fig. 6** shows TDDB lifetime of $HfZrO_x$ gate stack as a function of V_g. $HfZrO_x$ gate stack device lifetime is longer than HfO_2 device and better Weibull slop. In **Fig. 7**, gate stack d epth profile for dif ferent ZrO_2 position of $HfZrO_x/SiO_2$ gate stack obtained from angle resolved x-ray photoelectron spectroscopy (AR-XPS). The po sition of the Zr3d peak in the profiles was found to b e accurately reproduced. Greater accuracy in this region would be exp ected if a larger number of data points ar e used. **Fig. 8** shows ZrO_2 position ef fect for $HfZrO_x$ gate stack MOSCAP under GL process flow. For both of n/pMOSCAP $HfZrO_x$ gate stack, when ZrO_2 addition position in HfO_2 is higher, the device leakage current is lower. **Fig. 9** shows GF vs. GL process flow with different ZrO_2 position for MOSCAP device comparison. **Fig. 10** shows sa mples A~E nMOSCAP characteristics comparison between different ZrO_2 position in HfO_2 gate stack with top La_2O_3 capping layer under GF flow. Compared to HfO_2, the higher J_g was observed for $HfZrO_x$ samples (B~E). This is due to smaller band gap (**Fig . 2(a)**) and lower conduction band offset for $HfZrO_x$ than that of HfO_2. Sample B shows better EOT scaling , Sample E shows worse J_g and lar ger V_{fb} shift to band edge for EWF tuning. In **Fig. 11(a),** ZrO_2 position effect for $HfZrO_x$ gate stack nMOSCAP device under GF pro cess with top La_2O_3 capping layer. The MOSCAP C-V shows larger V_{fb} shift and higher J_g (in **Fig. 11(b)**) for ZrO_2 position on (top+bottom) of HfO_2 layer. The ZrO_2-HfO_2-ZrO_2 gate stack may enhance top and bottom unstable interface formation with metal gate and SiO_2 layer than HfO_2. In **Fig. 12,** ZrO_2 position effect for HfZrOx gate stack nMOSCAP device under GF process with different La_2O_3 capping layer position EOT-V_{fb} plots were compared. The ZrO_2 position effect for bottom La_2O_3 cap lay er device is more significant th an top La_2O_3. **Fig. 13** shows EOT dependence of (a) V_{fb} and (b) J_g for $HfZrO_2$ nMOSCAP with changing Zr% in high-k film for GL process. Zr% increased can shift V_{fb} to band edge and increase J_g. In **Fig. 14**, Schematic of the ZrO_2 position impact for $HfZrO_x$ MOSCAP on GL. The V_{fb} is dominated by Metal/High-k different interface dipole and the J_g is dominated by HK/IL interface $ZrSiO_x$ formation (as s how in **Fig. 5**). The decomposition of ZrO_2 are unstable on a thin SiO_2 layer during annealing at 900°C. ZrO_2 position to SiO_2 interface layer can impact the silicate-like compound formation , then increase device leakage current.

4. Conclusions

Compared to the difference of changing ZrO_2 within $HfZrO_x$ dielectric showed: (1) For GF process, the ZrO_2 position effect on V_{fb} for bottom La_2O_3 cap layer device is more significant than device with top La_2O_3 . (2) For GL pro cess, the Zr% and ZrO_2 position impact for $HfZrO_x$ MOSCAP shows the V_{fb} is dominated by Metal/High-k different interface dipole and the J_g is dom inated by HK/IL interface $ZrSiO_x$ formation..

Acknowledgements

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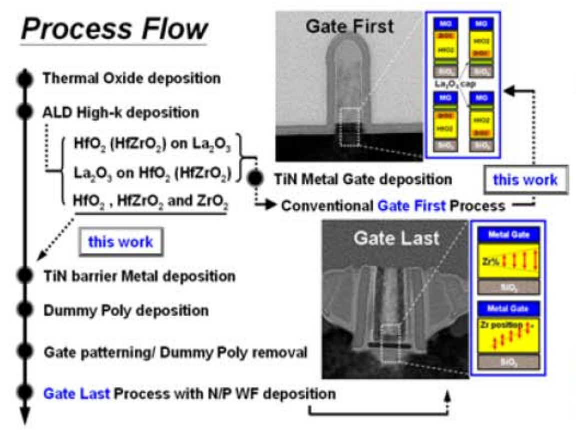

Fig. 1 Gate First (GF) and Gate Last (GL) fabrication process of high-k gate stack MOSCAP in this work.

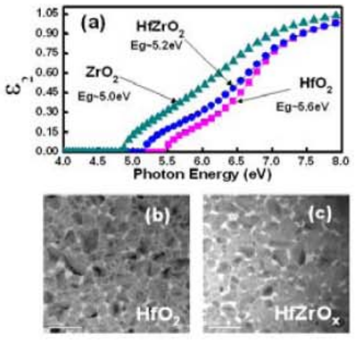

Fig. 2 (a) Band gap (E_g) decreased when ZrO_2 addition with HfO_2. Preliminary result of Plan-View TEM for (b) HfO_2 and (c) $HfZrO_x$. the $HfZrO_x$ grain size shows smaller than HfO_2

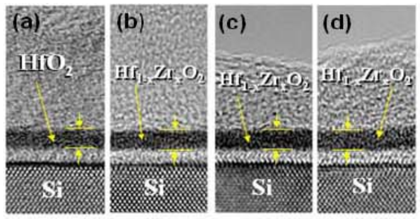

Fig. 3 Cross section HR-TEM image of (a) HfO_2/SiO_2 and $HfZrO_x/SiO_2$ with different ZrO_2 position (b) Top (c) Center (d) Bottom after annealing at 1050ºC. A uniform contrast indicates a compositional uniformity

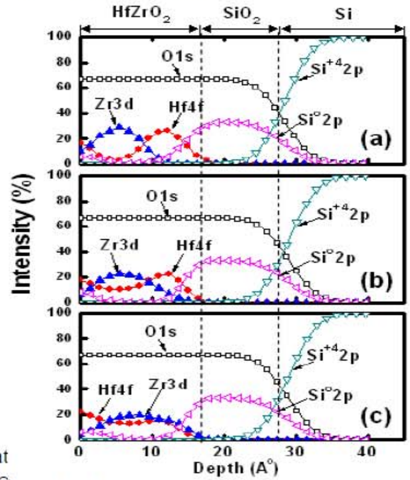

Fig. 7 Maximum Entropy entropy depth profile for different ZrO_2 position of $HfZrO_x/SiO_2$ Gate Stack obtained from AR-XPS (a) Top ZrO_2 (b) Center ZrO_2 (c) Bottom ZrO_2 .

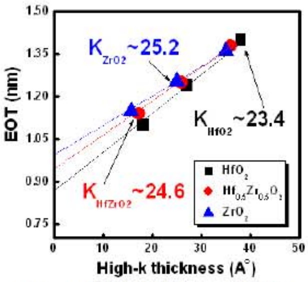

Fig. 4 HfO_2, $HfZrO_x$ and ZrO_2 k value comparison which were extracted which were extracted from EOT vs. High-k physical thickness plot.

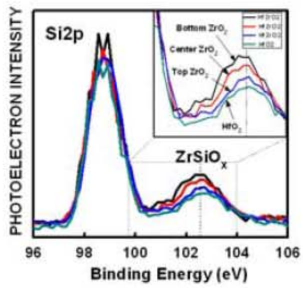

Fig. 5 XP spectra of Si2p of the sample for HfO_2 and different ZrO_2 position in $HfZrO_2$. $ZrSiO_x$ silicate was identified.

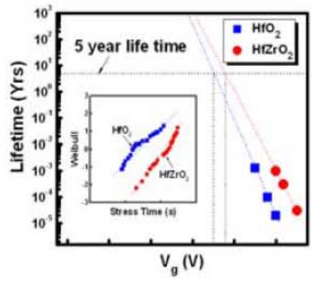

Fig. 6 TDDB lifetime of $HfZrO_x$ gat stack as a function of V_g. $HfZrO_x$ lifetime is longer than HfO_2 device and better Weibull slop.

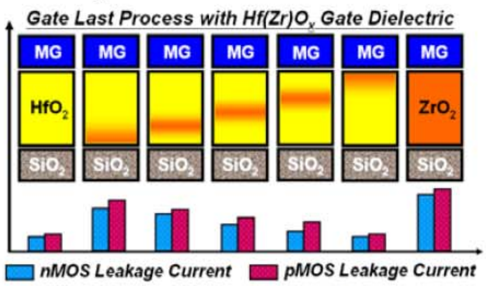

Fig. 8 The ZrO_2 position effect for $HfZrO_x$ gate stack n/pMOSCAP J_g comparison under GL process flow.

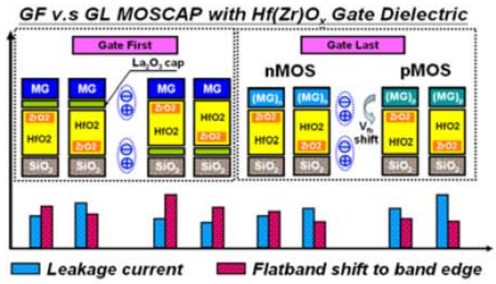

Fig. 9 GF v.s GL process flow with different ZrO_2 position in HfO_2 for MOSCAP device comparison.

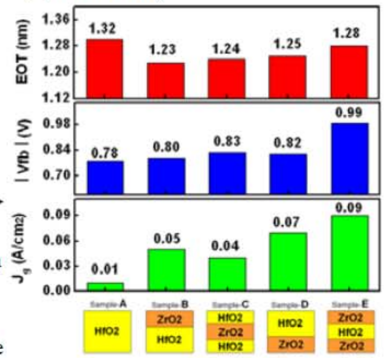

Fig. 10 nMOSCAP device characteristics comparison between different ZrO_2 position in HfO_2 gate stack under GF process with top La_2O_3 capping layer.

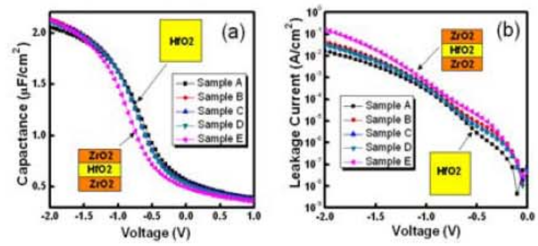

Fig. 11 (left) ZrO_2 position effect for $HfZrO_x$ gate stack nMOSCAP device under GF process with top La_2O_3 capping layer. The nMOSCAP characteristics (a) C-V shows larger V_{fb} shift and higher J_g (as shown in (b)) for ZrO_2-HfO_2-ZrO_2 gate stack sample compared with HfO_2

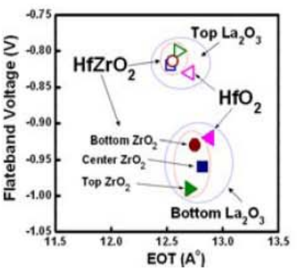

Fig. 12 ZrO_2 position effect for $HfZrO_x$ gate stack nMOSCAP device under GF process with different La_2O_3 capping layer position EOT-V_{fb} plots was compared.

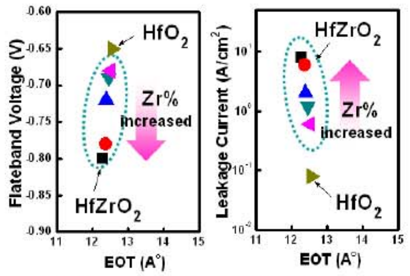

Fig. 13 EOT dependence of (a) V_{fb} and (b) J_g for $HfZrO_2$ nMOSCAP with changing Zr% in high-k film for GL process. Zr% increased can shift V_{fb} to band edge and increase J_g.

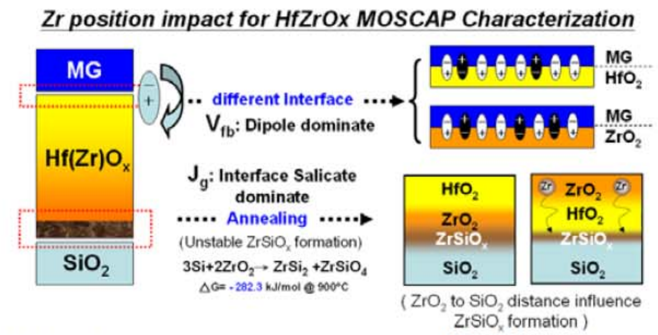

Fig. 14 Schematic of the ZrO_2 position impact for $HfZrO_x$ MOSCAP on GL. The V_{fb} is dominated by Metal/High-k different interface dipole and the J_g is dominated by HK/IL interface $ZrSiO_x$ formation. The decomposition of ZrO_2 are unstable on a thin SiO_2 layer during annealing at 900ºC. ZrO_2 position to SiO_2 interface layer can impact the silicate-like compound formation , then increase device leakage current.