Interface-aware high-k dielectric designing for deep sub-nm EOT Ge gate stack

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[Introduction] Intensive investigation has been done on the gate stack formation on Ge and prominent interface passivation has been demonstrated by high quality GeO₂-based dielectrics [1-4]. However, it is still challenging to achieve deep sub-nm EOT with maintaining good interface because the use of a high-k dielectric layer might also degrade the interface [5]. In this work, we provide a high-k dielectric designing strategy, which can help us to find the interface aware high-k on Ge.

[Experiment] The ternary high-k deposition in this work was carried out by rf co-sputtering of two binary oxide targets on Ge(111) substrate. Prior to the high-k deposition, Ge substrate was cleaned by HF-last wet chemical process and passivated by an ultra-thin yttrium doped GeO₂ (Y-GeO₂) interfacial layer (IL) [4]. After the deposition of high-k/IL/Ge stack, the entire gate stack was annealing in N₂/O₂ (0.1%) ambient at 500°C.

[Results and discussion] Conventional high-k oxides like HfO₂ is reported to have interface defect state on Ge intrinsically [5], therefore, we decide to give up the conventional high-k oxides and design the interface aware high-k out of the periodic table. Firstly, metal oxide (MOₙ) species are selected from the periodic table according to two reaction criteria as schematically shown in Fig. 1. As long as the MOₙ does not undergo the first reaction,

\[ \text{MO}_n + n/2\text{Ge} \rightarrow \text{M} + n/2\text{GeO}_n \]  

the corresponding MOₙ can exist stably on Ge. And, if the MOₙ does not undergo the second reaction,

\[ \text{MO}_n + (1 + n/2)\text{Ge} \rightarrow \text{MGe} + n/2\text{GeO}_n \]  

there should be no defect state formation due to the Ge-M metallic bond. There are only limited amount of cation species which survive both criteria, like Y, Sc, Al and some of the rare-earth (RE) oxides. Unfortunately, most of them have medium k-value. Thus, a second step is needed to create a high-k out of medium-k components. The ternary RE scandates formation might be a solution. It is because the ternary RE scandates is reported to have higher packing density than their binary compounds as shown in Fig. 2 [6]. (The density of RE scandates are high than a linear combination of their binary compounds). According to the Clausius-Mossoti equation [7], the densely packed oxides can enhance the k-value. We experimentally examined the dielectric properties of YScO₃ as an example. It is found that YScO₃ increases its k-value to 17 (12 and 14 for Y₂O₃ and Sc₂O₃, respectively) and the band gap is kept at 6 eV, which is a big advantage in terms of EOT scalability. The critical merit of YScO₃ over the conventional oxides is that it does not form any defect states at the interface intrinsically. With such a merit, we can further reduce the Y-GeO₂ IL thickness to scale down the EOT without significant disturbance on the interface properties as shown in Fig. 3. It forms a sharp contrast with the conventional high-k dielectrics like HfO₂. It is notable that this high-k designing strategy also brings us other successful combinations such as GdScO₃, and better dielectric properties are still expectable from an optimization of the components.

[Conclusion] We have proposed an interface aware high-k designing strategy for deep sub-nm EOT Ge gate stack. YScO₃/Y-GeO₂/Ge stack is demonstrated with good interface and EOT scalability.


![Fig. 1](image1.png) Schematic of two reaction criteria for the stable and defect free MOₙ on Ge. The stable MOₙ (noted by the green line) is mandatory for the interface aware high-k formation.

![Fig. 2](image2.png) Densities of RE scandates and their binary components. It is notable that the densities of RE scandates are higher than a linear combination of their binary components.

![Fig. 3](image3.png) Dₐ at E(0.2 eV) as a function of EOT in HfO₂ and YScO₃/Y-GeO₂/Ge stacks. Note that the thicknesses of both high-k are fixed at 2 nm while the EOT is changed by Y-GeO₂ IL thickness.