How to secure both sufficient passivation and long term reliability in Ge gate stack -The key is to keep a proper network structure of oxides-

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[Introduction] The current research on Ge gate stack has pointed out that GeO_2 might be the best passivation for Ge interface [1-4]. However, a good initial passivation of Ge interface does not secure the long term reliability because the optimum bond configuration does not mean it's strong against electric stress field (E_{stress}). In this work, we point out that, both the initial passivation and long term reliability are dependent on the network of the oxide, and the way to secure both is to tune a flexible and strong network structure.

[Theoretical consideration] We have found recently that the GeO_2 network structure can be modified by transition metal oxide doping (e.g. Y-GeO_2), which results in a drastic improvement of material robustness of GeO_2 [4, 5]. In fact, when an oxide is discussed in terms of its material robustness against thermal or chemical decomposition, the underlying physics is how much energy is consumed to dissociate the network of the oxides. We use the term "network strength" in this work to identify this energy, and its value is simple assumed as follows,

$$\text{Network strength}=N_{av}\times\varepsilon_{single\ bond} \tag{1}$$

Here, N_{av} and $\varepsilon_{single\ bond}$ is the average coordination number of every atom in the oxide and the single M-O bond strength, respectively as shown in **Fig. 1**. Examples are given with different network strength (HPO-GeO_2, 10%Y-GeO_2 and Y-rich germinate, respectively). It is also important to note that the N_{av} value of the oxide is strongly related to the rigidity of the network, which is an intrinsic criterion on whether good initial passivation can be achieved by an oxide.

[Results and discussion] We have experimentally investigated the interface states density (D_{it}) and pre-existing trap density (N_t) in gate stacks with different network structure using aforementioned dielectrics. Note that the pre-existing N_t is estimated from the flat band voltage (V_{FB}) shift under a low electric stress field ($E_{stress}=V_{ox}/EOT=4$ MV/cm) and the D_{it} is measured by LT-GV method. As shown in **Fig. 2**, both initial D_{it} and N_t are increased a lot in very rigid network (high N_{av}). It is because the ions in a flexible network can adjust their position to let all the possible M-O bonds to form. While in a very rigid network, higher coordination put more constraint on the ions, exceeding their degree of freedom, which results in bond breaking and trap sites formation either at the interface or in the bulk. However, the situation is inversed when these gate stacks are under high E_{stress} (9 MV/cm) as shown in **Fig. 3**. It is found that the gate stack with very soft network (low N_{av} in HPO-GeO_2) shows significant D_{it} generation under 9 MV/cm. While the enhancement of strength (larger N_{av} in 10%Y-GeO_2) here can suppress the D_{it} generation. It is because higher energy is needed to break the bonds and displace the ions in the relatively strong network than the very soft one. Similar trend can be found in bulk trap generation rate as reflected from the gate leakage current (data not shown). Thus, the moderate N_{av} secures initial passivation and long term reliability.

[Conclusion] The key to obtain a good initial passivation and long term reliability of Ge gate stack lies in the tuning of N_{av} of the network (not rigid but strong enough). And it is demonstrated by Y-GeO_2 with suitable Y composition.

[Reference] [1] A. Toriumi *et al*, *IEDM*, 646, (2011). [2] S. Takagi *et al*., *IEDM*, 372, (2012). [3] C. H. Lee *et al*., *IEEE TED*, **58**, 1295 (2011). [4] C. Lu *et al*., *APL*, **104**, 092909 (2014). [5] C. Lu *et al*., *JAP*, **116**, 174103 (2014).

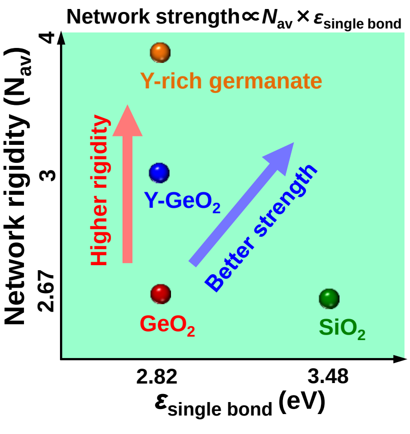

Fig. 1 Schematic on the definition of network strength and rigidity. GeO_2, 10%Y-GeO_2 and Y-rich germinate are examples with different N_{av} value and network strength.

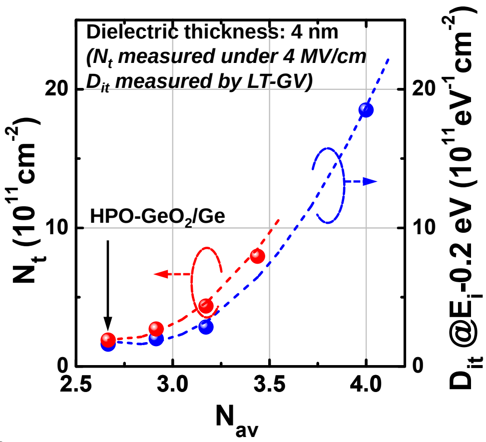

Fig. 2 N_t for electron and D_{it} near mid gap in dielectric/Ge gate stack as a function of N_{av}. Note that the N_t is estimated from the V_{FB} shift by:

$$N_t=\Delta V_{FB}C_{ox}/q$$

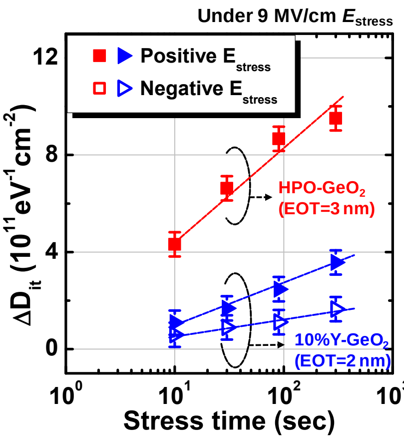

Fig. 3 D_{it} increase in HPO-GeO_2 and 10% Y-GeO_2/Ge stacks as a function of time under positive or negative 9 MV/cm E_{stress}. Note that HPO-GeO_2 break down under 9 MV/cm negative E_{stress}