Impact of YScO₃ on Ge gate stack in terms of EOT reduction as well as interface control

Cimang Lu, Choong Hyun Lee, Tomonori Nishimura, Kosuke Nagashio, and Akira Toriumi

> Department of Materials Engineering, The University of Tokyo JST-CREST 7-3-1 Hongo, Tokyo 113-8656, Japan Phone: +81-3-5841-1907 E-mail: cimang@adam.t.u-tokyo.ac

Abstract

Ternary metal oxide $YSCO_3$ is shown to be a promising dielectric thin film for sub-nm EOT gate stack formation on Ge thanks to a high-permittivity about 17. The improvement of the permittivity is attributable to a structural change in M-O coordination polyhedron.

1. Introduction

As Ge is emerging as a new channel material in replacement of Si, intensive investigation is being carried out in search of a desirable gate dielectric on it. Although several metal oxides have been identified as "friendly" on Ge [1-3], their medium-permittivity cannot satisfy the aggressive EOT scaling of the gate stacks. On the other hand, the conventional high-k metal oxides, like HfO₂, yield poor interface properties on Ge [4]. In this work, we propose the ternary metal oxide YScO₃ as a Ge "friendly" dielectric with high-permittivity, which is attributable to a structural change in M-O coordination polyhedron.

2. Experimental details

00 After p-Ge substrate was chemically cleaned with methanol, HCl, and HF solutions, YScO₃ films with various thicknesses were deposited on it by co-sputtering of Y_2O_3 and Sc₂O₃ targets. Y:Sc ratio was controlled to be 1:1 by sputtering power and confirmed by XPS measurements. Thermal treatment of YScO₃/Ge stack was carried out at 500°C in 1 atm O₂ ambient for different time. To characterize the electrical properties, Au and Al were deposited by vacuum evaporation for the gate electrode and substrate contact of MOSCAPs, respectively.

3. Results and discussions

To examine the uniformity of the deposited film, the top surface morphology of a (4 nm)YScO₃/Ge stack was measured by AFM. **Fig. 1(a)** shows the AFM image of the as-deposited YScO₃ surface. The smooth and featureless morphology indicates a good uniformity of YScO₃ film without any phase segregation. **Fig. 1(b)** shows the RMS roughness of the YScO₃ surface as a function of annealing temperature. The RMS roughness of as-cleaned Ge substrate is also shown as a reference. As-deposited YScO₃ surface has an RMS value about 0.3 nm, which is close to that of Ge substrate. The low RMS value is maintained up to 600°C, indicating a high thermal robustness of the



Fig. 1(a) AFM image of as-deposited YScO₃ (4 nm thick) surface. Note that the image size is $2 \times 2 \mu m$. (b) RMS roughness of YScO₃ as a function of annealing temperature. It is notable that the uniformity of the film is maintained up to 600°C.

YScO₃ film.

Due to the unsatisfying electrical property of the direct $YScO_3/Ge$ interface, thermal oxidation was carried out to form an ultra-thin GeO_2 IL in the $YScO_3/Ge$ stack. Meanwhile, Y^{3+} and Sc^{3+} cations are expected to intermix into this IL, as schematically shown in **Fig. 2(a)**. This IL formation was confirmed by XPS observation. **Fig. 2(b)** shows the GeO_2 IL thickness and chemical shift as a function of oxidation time in a (1.5 nm)YScO_3/Ge stack. The IL thickness increases slightly with the oxidation time as expected. The chemical shift of GeO_2 IL is relatively lower comparing to pure GeO_2 , which is attributable to the second-nearest effect of intermixed Y^{3+} or Sc^{3+} cations [3, 5].



Fig. 2(a) Schematic of ultra-thin GeO_2 IL formation by thermally oxidizing YScO_3/Ge stack. (b) GeO_2 IL thickness and chemical shift as a function of oxidation time.

Since both Y^{3+} and Sc^{3+} exhibit "friendly" character when intermixed in the GeO₂ IL, it is expected that a

defect-free GeO₂ IL is formed with the coexistence of Y^{3+} and Sc³⁺ according to the thermodynamic criteria [6]. **Fig. 3** shows the bidirectional *CV* curves of (1.5 nm)YScO₃/IL/Ge gate stack measured at room temperature. The negligible hysteresis and frequency dispersion indicate a low D_{ii} , which is in agreement with the thermodynamic expectation [6]. The EOT of this gate stack is scaled down to about 0.7 nm in this experiment.



Fig. 3 Bi-directional *C-V* curves of (1.5 nm)YScO₃/IL/Ge gate stack measured at room temperature. EOT of this gate stack is estimated to be about 0.7 nm.

The EOT scalability is mainly attributed to the relatively high permittivity of YScO₃. **Fig. 4(a)** shows the EOT of the gate stacks as a function of the YScO₃ physical thickness. From the slope of the linear fit, k value of about 17 is derived, which is higher than both Y_2O_3 (~12) and Sc_2O_3 (~14). It is interesting from the material selection viewpoint that, by a proper combination of two medium-k materials, it is possible to form a real high-k without changing the interface properties. Furthermore, it was reported that the band-gap of YScO₃ is 5.98 eV [7], which is almost the same with its binary components. **Fig. 4(b)** shows the leakage current of YScO₃/IL/Ge gate stacks as a function of EOT. Despite the aggressive EOT scaling, the leakage current of the gate stacks are relatively low thanks to the high-permittivity and sufficient band-gap.



Fig. 4(a) EOT of $YScO_3/IL/Ge$ stacks as a function of the physical thickness of the $YScO_3$. The curves for Y_2O_3 and Sc_2O_3 are shown in the dotted lines for comparison. (b) Gate leakage current of $YScO_3/IL/Ge$ stacks as a function of EOT.

To understand the improvement in the permittivity of $YScO_3$, the microscopic structure is investigated. Y_2O_3 and

 Sc_2O_3 have a similar structure, featuring the M-O₆ octahedron unit. However, by forming YScO₃, a structural change occurs with the Y-O coordination number increase to 8 [8], as schematically shown in **Fig. 5(a)**. It has been pointed out in the previous research that the permittivity of the ionic oxides follows a semi-empirical rule as follows [9]:

$$k = N_c Z_a N_e / 6E_t, \qquad (1)$$

where N_c, Z_a, N_e and E_t stand for the cation coordination number, anion valency, effective number of valence electron per anion and the direct band-gap, respectively. By increasing the N_c, the increase of k value can be expected without the shrinkage of band-gap. The changing of the Y-O coordination polyhedron also leads to a dense-packing of YScO₃ comparing to its binary compound as evident in **Fig. 5(b)**, which shows that the density of $YScO_3$ is higher than the linear combination of the Sc_2O_3 and Y_2O_3 . Since the higher packing-density of YScO3 is equivalent to a relatively low gibbs free energy [10], it also explains the thermal stability of the $YScO_3$ as discussed in Fig 1. It is interesting to note in Fig. 5(b) that some of the other rare-earth scandates (LnScO₃) show the similar dense-packing feature of YScO₃ [11], which hints us that more desirable high-k materials might be found among LnScO₃.



Fig. 5(a) Schematic of structural change of $YScO_3$ from its binary compounds. (b) Densities of some $LnScO_3$ and that of their binary compounds [11].

3. Conclusions

 $YScO_3$ is found to be a desirable high-k material on Ge due to its "friendly" character with GeO₂ IL and a high permittivity about 17. The improvement in the permittivity is attributable to the structural change in M-O coordination polyhedron.

References

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