Stability of Ferroelectric Phase in Epitaxial Hfo$_2$-based Films

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Recently, ferroelectric HfO_2–based thin films with noncentrosymmetric orthorhombic phase receive remarkable attention for ferroelectric devices using thin films, because they remain large remnant polarization in small thickness[1]. To stabilize metastable orthorhombic ferroelectric phase, substitution of some ions such as Zr, Y and Al have been reported. However, these substituted ferroelectric HfO_2 film in previous reports was polycrystalline film that consists of not only ferroelectric phase but also paraelectric phase. This gives insufficient insight for determining the factor to stabilize ferroelectric phase. In this study, we report on the stability of ferroelectric phase by the investigation of thickness dependent phase stability for $0.07YO_{1.5}$-$0.93HfO_2$ (YHO7) and $0.5ZrO_2$-$0.5HfO_2$ (HZO) films using epitaxial films. Based on the obtained data we discuss on the stability of ferroelectric phase in epitaxial HfO_2-based films.

Figure 1 shows X-ray diffraction pattern of HZO films with the film thickness ranging from 2.2 to 16.1 nm. The peak originating from high symmetry phases, tetragonal or orthorhombic phases was observed at higher *2θ* position than YSZ *111* peak for 2.2 and 4.9 nm-thick HZO films. While the peak originating from low symmetry phase, monoclinic phase, was observed at lower *2θ* position than YSZ *111* peak for 10.2 and 16.1 nm-thick HZO films. Figure 2 shows X-ray diffraction *2θ - Psi* mappings near {*110*} of 4.9 and 10.2 nm -thick HZO films. Although *110* peak from orthorhombic phase was obtained for 4.9 nm-thick HZO film, *011* and *110* peaks from monoclinic phase were obtained for 10.2 nm-thick HZO film. This suggests that 4.9 nm-thick HZO film is ferroelectric orthorhombic phase, while 10.2 nm-thick one is paraelectric monoclinic phase. Therefore, film thickness to obtain ferroelectric phase is found to be thin for HZO films comparing with YHO7 film in which ferroelectric orthorhombic phase was obtained even for 15 nm-thick one. In my presentation, we will discuss the factor to stabilize ferroelectric phase through the results of epitaxial film research.

Acknowledgments
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Reference
[1] T. S. Boscke *et al*., Appl. Phys. Lett. 99, 102903 (2011).

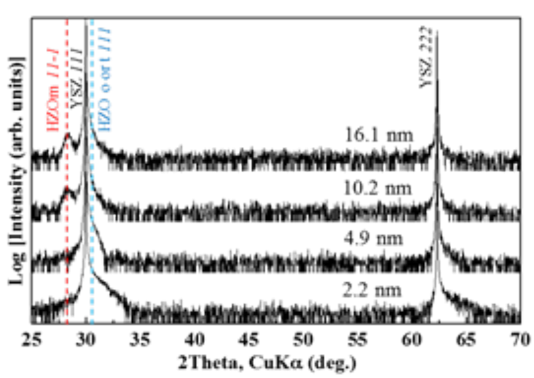

Fig.1 XRD θ - 2θ profiles of HZO films with various film thickness.

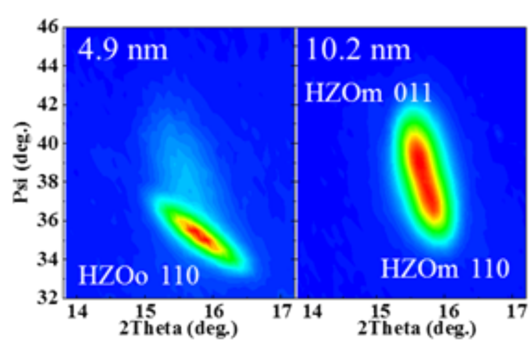

Fig. 2 XRD 2θ - *Psi* mappings near *{110}* of 4.9 and 10.2 nm-thick HZO films.