Epitaxial single crystalline oxide is a potential candidate for high-k gate dielectrics in sub-45 nm CMOS transistors, in which generation the channel engineering such as strain in Si becomes more important. Strain effect of epitaxial oxide on Si channel would be greater than that of amorphous oxide. We demonstrated the direct growth of CeO₂ on Si (111) with the equivalent oxide thickness as small as 0.38 nm [1]. The purpose of this study is to clarify the strain in Si, on which CeO₂ is epitaxially grown, by evaluating lattice spacings in CeO₂ and Si.

CeO₂ (10 nm) was grown on a Si (111) substrate by MBE using metal Ce and O₂ as source materials [1]. TEM (a cross-sectional image is shown in Fig. 1) and in-situ RHEED observations confirmed that CeO₂ was single crystalline and epitaxially grown on the Si substrate.

We performed in-plane X-ray diffraction (XRD) measurements to evaluate lattice spacings normal to a sample surface in thin films, as shown in Fig. 2. Fig.3 shows the reciprocal space map around the (220) planes. It can be seen that the 2θ angle of CeO₂ is lower than that of the Si substrate, which means that the lattice spacing in CeO₂ (110) (dCeO₂(110)) is larger than that of the Si substrate. The relative change in dCeO₂(110) from the Si substrate (∆dCeO₂(110)) is calculated to be +0.60% (±0.02%).

In order to examine the relative change in the lattice spacing parallel to the sample surface (∆dCeO₂(111)) with dCeO₂(111) electron diffraction patterns (EDP) of CeO₂ were observed by TEM and compared with the standard spot positions of the Si substrate (250 nm depth from the interface) [2]. ∆dCeO₂(111) by EDP is evaluated to be +0.5%, which coincides with the in-plane XRD result, as shown in Table 1. The value of dCeO₂(111) is also larger than that of the Si substrate (∆dCeO₂(111)) = +0.6%. The lattice constant of bulk CeO₂ is reported to be 0.541 nm, which is smaller than that of Si (0.543 nm) by ~0.3%. It is found that the lattice spacings in epitaxial CeO₂ are isotropically expanded (~1%), compared with those in bulk CeO₂.

We focused on the lack of oxygen in epitaxial CeO₂ as a reason for expansion of the lattice spacings. It is reported that the lattice constant of Ce oxide increases (~3%) as a result of the change of the crystal structure from CeO₂ to Ce₂O₅ [3]. Coulomb interaction in ionic crystal would decrease owing to the oxygen reduction, resulting in expansion of the lattice constant. In order to confirm the lack of oxygen in epitaxial CeO₂, we performed X-ray photoelectron spectroscopy (XPS) measurements. An additional in-gap state is observed in the valence band spectrum as shown in Fig. 4, which is determined to be due to the oxygen-defect-induced state [4]. It is considered that expansion of the lattice spacings in epitaxial CeO₂ is due to the oxygen defects.

To clarify the strain in Si, the relative changes of the lattice spacings in Si at 50 nm depth from the CeO₂/Si interface (∆dSi(110) and ∆dSi(111)) were evaluated by EDP, as summarized in Table 1 with the CeO₂ data. The value of ∆dSi(110) is positive (+0.5%), while ∆dSi(111) is a negative value of ~0.1%. It means that Si is tensile strained due to expansion of ∆dCeO₂(111) even at 50 nm depth from the CeO₂/Si interface. As the elastic coefficient of CeO₂ is about sixty times larger than that of Si (CeO₂ crystal is much harder than Si) and strong bonds between CeO₂ and Si are formed, the Si lattices far from the interface may be deformed, compared with the SiO₂ case (only 1-2 monolayer of Si (111) is distorted) [5]. Such tensile strained Si is preferable for enhancement of carrier mobility in CMOS transistors.

In conclusion, we found that the lattice spacings in CeO₂ epitaxially grown on Si were greatly expanded compared with those in bulk CeO₂ due to the oxygen defects, resulting in the tensile strain in Si. Oxygen defects in epitaxial crystalline gate dielectrics must be controlled by taking account of Si channel properties.