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## Direct Growth of Single Crystalline CeO<sub>2</sub> High-k Gate Dielectrics

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### 1. Introduction

Epitaxial single crystalline high-k dielectrics directly grown on Si, which enable further reduction of equivalent oxide thickness (EOT), would be a potential candidate for a gate oxide in the 40nm CMOS technology. As it is well known that elimination of an amorphous interfacial layer is difficult, there are quite few reports on direct growth of high-k oxides on Si. Although McKee et al. reported direct growth of SrTiO<sub>3</sub> on Si and FET operation using SrTiO<sub>3</sub>/Si as gate oxide [1], ability of single crystalline oxide directly grown on Si is still unclear.

CeO<sub>2</sub> is considered to be a good alternative dielectric for the Si-based devices due its good lattice matching with Si ( $\Delta d = -0.35\%$ ) and stable chemical properties. Previous studies indicate that Si (111) substrates are necessary for growth of single crystalline CeO<sub>2</sub> [2]. In this paper, we have successfully grown epitaxial CeO<sub>2</sub> directly on Si (111) and demonstrated a 5nm-thick CeO<sub>2</sub> MIS capacitor with EOT=0.38nm. We believe single crystalline CeO<sub>2</sub> has high potential as an alternative gate oxide.

### 2. Experiment

CeO<sub>2</sub> was grown on p-Si(111) substrates by molecular beam epitaxy (MBE) using metal Ce and O<sub>3</sub> as source materials. To avoid the formation of an amorphous interfacial layer, 0.6 monolayer of Ce was deposited on Si prior to O<sub>3</sub> supply. Physical thickness ( $T_{\text{phys}}$ ) of CeO<sub>2</sub> were 5nm and 10nm. MIS capacitors were fabricated by evaporating Au using metal masks.

### 3. Results and discussions

Figure 1 shows the Rheed pattern of CeO<sub>2</sub> grown at 700°C. Sharp streak patterns indicate a flat surface of epitaxial CeO<sub>2</sub>. A cross-sectional TEM image of the CeO<sub>2</sub>/Si(111) interface is shown in Fig.2. It can be seen that CeO<sub>2</sub> was directly grown on Si without any interfacial layer. An atomic step is also clearly observed.

We have proposed a new method to construct "ideal" CV curves for ultra-thin gate dielectrics taking account of quantum mechanical effects in a Si substrate [3]. As shown in Fig.3, "ideal" CV curves (re-constructed from the experimental CV data of a SiO<sub>2</sub>(3.5nm)/Si(111) capacitor) show good agreements with CV data of CeO<sub>2</sub>/Si(111) capacitors, which were obtained by the two frequency CV method ( $f=200\text{kHz}$  and  $1\text{MHz}$ ) [4]. No hysteresis was observed in the CV measurements. EOT of CeO<sub>2</sub> epitaxial layers ( $T_{\text{phys}} = 5\text{nm}$  and  $10\text{nm}$ ) were estimated to be 0.38nm and 0.75nm, respectively. EOT has a good linear relation with  $T_{\text{phys}}$  as shown in Fig.4.

The dielectric constant ( $\epsilon$ ) is  $\sim 52$ , calculated from the slope. This value is twice as large as the reported value of bulk (polycrystalline) CeO<sub>2</sub> ( $\epsilon \sim 26$ ). This large value would be due to anisotropy of  $\epsilon$  in single crystalline and/or lattice distortion of CeO<sub>2</sub> on Si.

We have performed the conductance method [5] to determine  $D_{\text{it}}$ . Figure.5 shows the equivalent parallel conductance ( $G_p$ ) of the CeO<sub>2</sub> MIS capacitor ( $T_{\text{phys}} = 10\text{nm}$ ) as a function of measurement frequency ( $f$ ). No post annealing process was performed to the capacitor.  $D_{\text{it}}$  is obtained to be  $1.2 \times 10^{13} \text{cm}^{-2} \text{eV}^{-1}$  from the maximum  $G_p/\omega$  at  $f=200\text{kHz}$  ( $D_{\text{it}} = 2(G_p/\omega)_{\text{max}}/q$ ). This  $D_{\text{it}}$  value is the same order as that of a Zr-silicate MIS capacitor without post annealing [3]. Further reduction of  $D_{\text{it}}$  will be investigated.

Figure 6 shows the relationship between EOT and leakage current density ( $J$ ) at an equivalent electrical field of 5 MV/cm for a CeO<sub>2</sub> MIS capacitor ( $T_{\text{phys}}=5\text{nm}$ ), compared with SiO<sub>2</sub> MIS capacitors [6].  $J$  ( $0.9\text{A}/\text{cm}^2$ ) for the CeO<sub>2</sub> capacitor (EOT=0.38nm) is six orders of magnitude lower than the expected  $J$  for SiO<sub>2</sub> capacitors with the same EOT.

### 4. Conclusions

We have grown CeO<sub>2</sub> directly on Si (111) by MBE. EOT as low as 0.38nm and high  $\epsilon$  ( $\sim 52$ ) were obtained by elimination of an interfacial layer and single crystalline properties of CeO<sub>2</sub>. We revealed that single crystalline CeO<sub>2</sub> directly grown on Si really works as gate dielectrics.

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### References

- [1] R. A. McKee, F. J. Walker and M. F. Chisholm, *Science* **293**, 468 (2001).
- [2] M. Yoshimoto, K. Shimozono, T. Maeda, T. Ohnishi, M. Kumagai, T. Chikyow, O. Ishiyama, M. Shinohara and H. Koinuma, *Jpn. J. Appl. Phys.* **34**, L686 (1995).
- [3] N. Yasuda and H. Satake, to be published in *Extended Abstracts of the 2001 International Conference on Solid State Devices and Materials, 2001*.
- [4] A. Nara, N. Yasuda, H. Satake and A. Toriumi, *Extended Abstracts of the 2000 International Conference on Solid State Devices and Materials, 2000* (2000) p. 452.
- [5] D. K. Schroder, "Semiconductor Material and Device Characterization", John Wiley & Sons, Inc. (1990).
- [6] M. Hirose, M. Koh, W. Misubayashi, H. Murakami, K. Shibahara and S. Miyazaki, *Semicond. Sci. Technol.* **15**, 485 (2000).

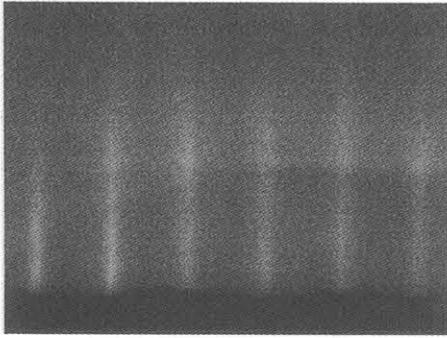


Fig.1 Rheed pattern along the  $\langle 211 \rangle$  azimuth after growth of 10nm  $\text{CeO}_2$  on Si (111) at  $700^\circ\text{C}$ .

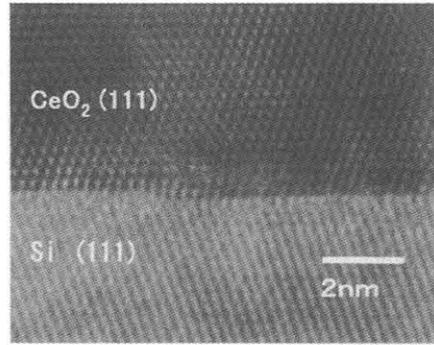


Fig.2 A cross-sectional TEM image of  $\text{CeO}_2$  / Si (111) interface without any amorphous layer.

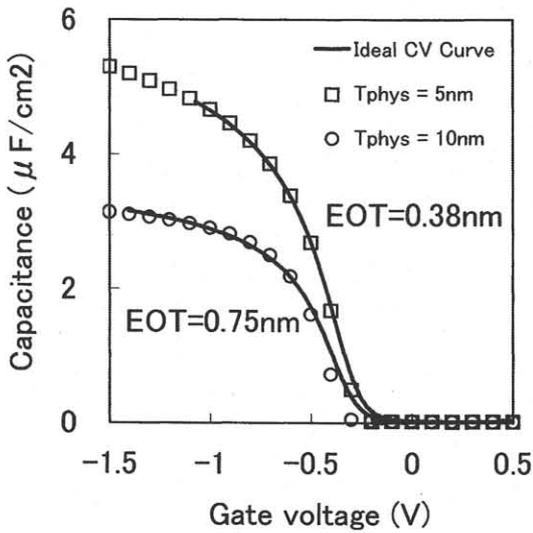


Fig.3 CV data of  $\text{CeO}_2$  MIS capacitors ( $T_{\text{phys}}=5, 10$  nm) and the "ideal" CV curves for  $\text{EOT}=0.38$  and  $0.75$  nm constructed by a new method.

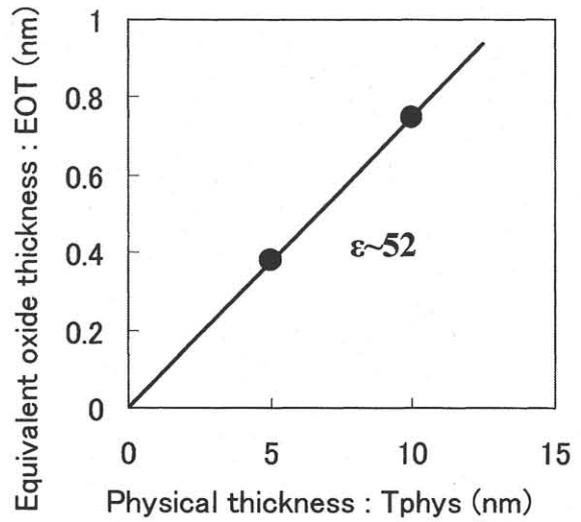


Fig.4  $T_{\text{phys}}$  vs. EOT for  $\text{CeO}_2$  MIS capacitors. The dielectric constant ( $\epsilon$ ) is calculated to be  $\sim 52$  from the linear slope.

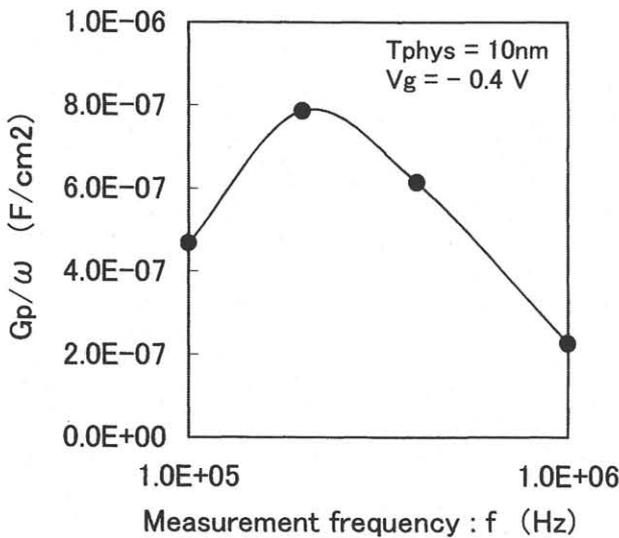


Fig.5 The equivalent parallel conductance ( $G_p$ ) as a function of measurement frequency ( $f$ ).  $D_{\text{it}}$  is estimated to be  $1.2 \times 10^{13} \text{cm}^{-2} \text{eV}^{-1}$ .

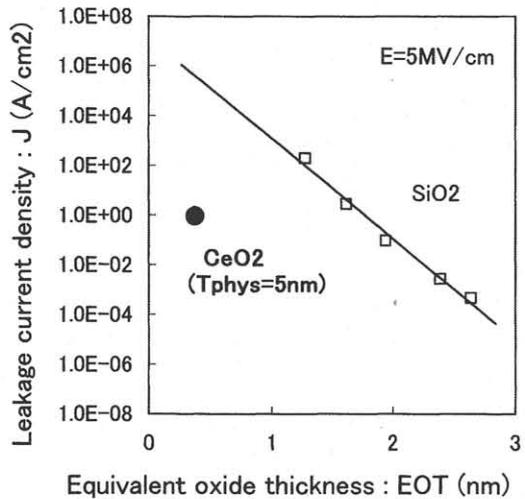


Fig.6 Relationship between EOT and  $J$  at  $E=5\text{MV/cm}$  for a  $\text{CeO}_2$  ( $T_{\text{phys}}=5\text{nm}$ ) and  $\text{SiO}_2$  MIS capacitors [6].