

Consideration on the effective dipole length in Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interface dipole layers via temperature dependences of their dipole strength

Siri Nittayakasetwat and Koji Kita

Department of Materials Engineering, The University of Tokyo,
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
Phone: +81-3-5841-7164 E-mail: siri.n@scio.t.u-tokyo.ac.jp

Abstract

The temperature dependences of the dipole layer strengths at Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interfaces were investigated. It was found that both interface dipole layer strengths increased but in the opposite direction at the rates of ~2.8 mV·K⁻¹ and ~0.7 mV·K⁻¹ for Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interfaces, respectively. Both temperature dependences were possibly explainable by the increase in the width of a space-charge region near the interface by temperature.

1. Introduction

Multiple studies have been developed to explain the physical origin of the dipole layer formation at high-*k*/SiO₂ interface [1–4]. However, no report had yet considered the effect of temperature on the interface dipole layer. For a wider range of field effect devices operating at various temperatures, it is crucial to comprehend its behavior with the change in temperatures. In this study, we investigate the temperature dependences of the dipole layer strengths in Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interfaces from 100–400 K. Note that the Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interfaces were chosen for this study because their dipole layer strengths and directions have already been well addressed at room temperature [4].

2. Experimental Method

Two types of MOS capacitors (MOS-cap) with different high-*k* dielectrics were used in this experiment: sample (i) – Au/Al₂O₃/SiO₂/Si and sample (ii) – Au/Y₂O₃/SiO₂/Si. ~10 nm thick SiO₂ was thermally grown on a *p*-type Si wafer. Next, wedge-shaped Al₂O₃ or Y₂O₃ was deposited on SiO₂/Si stacks using rf-sputtering. Then, post-deposition annealing was performed in 0.1% O₂ ambient for 5 min – at 800°C and 400°C for Al₂O₃/SiO₂/Si and Y₂O₃/SiO₂/Si stacks, respectively. Finally, Au top gates were deposited by vacuum evaporation. To study the interface dipole layer strength, each sample was made together with a reference MOS-cap, which is a MOS cap without the top high-*k* dielectric layer. The flat-band (*V*_{fb}) were extracted from CV curves measured at the frequency of 1 MHz.

In general, *V*_{fb} of a typical Si MOS-cap with a bilayer dielectric is described by the following equation:

$$V_{fb} = \varphi_{ms} - Q_{fix} \frac{CET_{high-k}}{\epsilon_{SiO_2}} \pm \varphi_{dipole} \quad (1)$$

where φ_{ms} , Q_{fix} , CET_{high-k} , ϵ_{SiO_2} , and φ_{dipole} are the work function miss-match, interface fixed charge density at the high-*k*/SiO₂ interface, capacitance equivalent thickness of the high-*k* oxide, the permittivity of SiO₂ and the high-*k*/SiO₂ interface dipole layer strength, respectively. The fixed charges at the SiO₂/Si interface can also contribute to the *V*_{fb} shift. Nonetheless, it was omitted in eq. (1) for simplification. In this study,

the direction of a dipole layer strength is defined as positive when the *V*_{fb} shifts positively. By excluding the first two terms in eq. (1), the dipole layer strength at each temperature can be extracted.

3. Result and Discussion

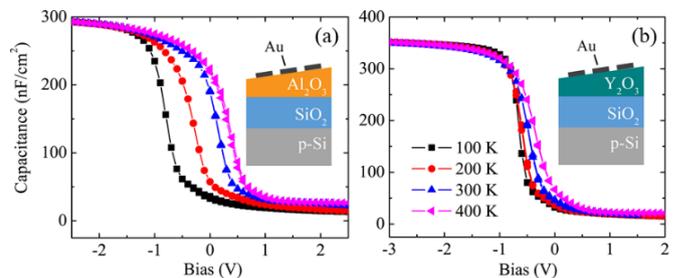


Fig. 1 CV curves of (a) sample (i) and (b) sample (ii) measured at 1 MHz at various temperatures. The top Al₂O₃ and Y₂O₃ thicknesses were ~5 nm and ~10 nm, respectively.

The CV curves of sample (i) and (ii) at different temperatures are shown in Fig. 1 (a) and (b), respectively. The temperature-induced *V*_{fb} shifts both in samples (i) and (ii) were comprised of the temperature effects of the ‘intrinsic’ component (*i.e.* φ_{ms}), the fixed charges at high-*k*/SiO₂ interface, and the interface dipole layer at the same interface. The temperature-induced *V*_{fb} shift in sample (ii) seemed much less pronounced than the one in sample (i), due to the relatively small dipole layer strength of the Y₂O₃/SiO₂ interface when comparing to the Al₂O₃/SiO₂ interface. By excluding the effect of interface fixed charges and the ‘intrinsic’ component, then the dipole layer strength at each temperature can be extracted [5].

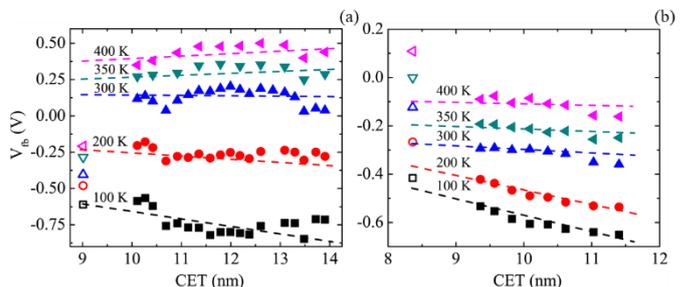


Fig. 2 *V*_{fb} vs *CET* at different temperature for (a) sample (i) and (b) sample (ii). Th solid and open symbols represent *V*_{fb} of the samples and their references (*i.e.* without the high-*k* layer), respectively.

Series of *V*_{fb} in Fig. 2 (a) and (b) were obtained from various top high-*k* thicknesses in sample (i) and sample (ii), along with their references at several temperatures. The thickness of the top high-*k* oxide was extrapolated to zero (*i.e.* $CET_{high-k} \rightarrow 0$) to eliminate the second term in eq. (1). Then, the extrapolated *V*_{fb} of the samples were compared with their

references. From the difference, the dipole layer strength at the high- k /SiO₂ interfaces were finally quantified by eliminating the first term in eq. (1).

Fig. 3 shows the temperature dependences of the Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interface dipole layers. From the graph, almost no dipole layers were observed at both Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interfaces at 100 K. Nevertheless, the Al₂O₃/SiO₂ interface dipole layer strengths increased at the rate of ~ 2.8 mV·K⁻¹ when the temperature was raised from 100 K to 300 K. At higher temperature region, the increasing rate of the Al₂O₃/SiO₂ interface dipole layer strength reduced. Whereas, the dipole layer strength at the Y₂O₃/SiO₂ interface increase at a steady rate, but in the opposite direction to the Al₂O₃/SiO₂ interface, ~ 0.7 mV·K⁻¹ from 100 K to 400 K.

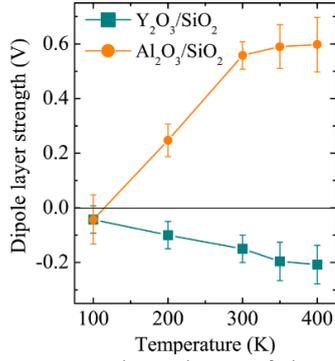


Fig. 3 The temperature dependence of the extracted dipole layer strength at Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interfaces.

Despite the fact that the strength and direction of both interfaces have already been studied in the oxygen density model [4], such temperature dependence of the dipole layer strengths have never been discussed. Generally, a dipole layer strength is proportional to the dipole length and the amount of charges.

$$\varphi_{\text{dipole}} \cong \frac{qN_{\text{dipole}}d_{\text{eff}}}{\varepsilon_{\text{int}}}, \quad (2)$$

where q , N_{dipole} , d_{eff} , and ε_{int} are the elementary charge, the areal dipole density, the effective dipole length, and the permittivity of the interface, respectively. Note that ε_{int} can be approximated to be the average of bulk $\varepsilon_{\text{high-}k}$ and $\varepsilon_{\text{SiO}_2}$. Assuming the N_{dipole} does not change significantly by temperature. If the thermal expansion is assumed to be the cause of the increase in the dipole layer strength by physically lengthening the d_{eff} , the temperature coefficient of the dipole layer strength should be in a similar order as the thermal expansion coefficients of Al₂O₃, Y₂O₃, and SiO₂. However, the thermal expansion coefficients of Al₂O₃, Y₂O₃, and SiO₂ only ranges in the order of 10^{-6} K⁻¹ [6], 10^{-6} K⁻¹ [7], and 10^{-7} K⁻¹ [8], respectively, while the temperature coefficients [$d\varphi_{\text{dipole}}/(dT \cdot \varphi_{\text{dipole}})$] of Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interfaces in Fig. 3 are in the order of 10^{-2} K⁻¹ and 10^{-3} K⁻¹, respectively. Clearly, the thermal expansions of oxides could only contribute to a small change in the dipole layer strength.

As one of the other possible explanations, we propose a model that the effective dipole length in high- k /SiO₂ interfaces is not limited only by the physical distance between the charge pairs but determined by the width of a space-charge region (SCR) near the interface. In this model, we explain the

increase in the dipole layer strength by the expansion of the SCR with the increase in temperatures.

Due to the relatively low density of charges in dielectric layers compared to a metal, charges are less electrostatically screened, in which the screening length can be approximated by the Debye length $L_D = \sqrt{\varepsilon_{\text{int}}kT/\rho_{\text{charge}}q^2}$, where k , T , and ρ_{charge} are the Boltzman constant, the temperature, and the charge density, respectively. Although ρ_{charge} is normally negligibly small in bulk dielectrics, some charges in the order of fixed charge or dipole densities can be expected near the interface. Conceptually, the relationship between the dipole layer strength and the Debye length can be made by treating d_{eff} , in eq. (2) to be proportional to L_D .

The temperature dependences of the experimental Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interface dipole layer strengths, plotted along with their theoretical Debye length at several charge densities are shown in Fig. 4 (a) and (b), respectively. At the charge density of 10^{18} cm⁻³, the L_D can extend by a few nanometers with the increase in temperatures from 100-400 K. By assuming a reasonable set parameter on N_{dipole} , the proposed model roughly explains the observed temperature dependences of Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interface dipole layer strengths.

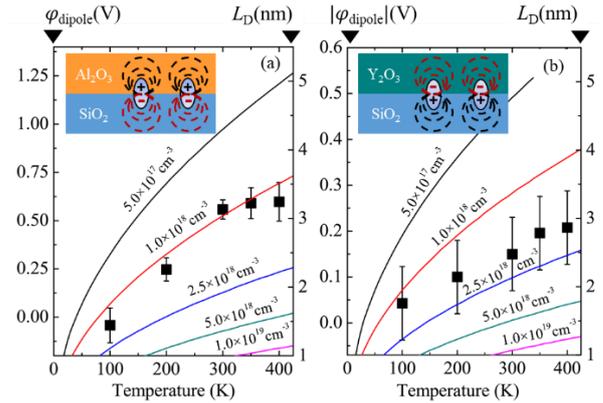


Fig. 4 The temperature dependence of the experimentally observed (a) Al₂O₃/SiO₂ and (b) Y₂O₃/SiO₂ interface dipole layer strengths (black square) and their calculated Debye lengths at different charge densities (solid lines).

4. Conclusion

The temperature dependences of the interface dipole layer strengths at Al₂O₃/SiO₂ and Y₂O₃/SiO₂ interfaces were investigated from 100 K to 400 K. We found that the dipole layer strengths increased at the rate of ~ 2.8 mV·K⁻¹ in the positive direction for the Al₂O₃/SiO₂ interface and at the rate of ~ 0.7 mV·K⁻¹ in the negative direction for the Y₂O₃/SiO₂ interface. Our conceptual model in which the effective dipole length in the interface dipole layers is mainly determined by the width of the space-charge region would explain the experimentally observed temperature dependences.

References

- [1] P.D. Kirsch, *et al.*, Appl. Phys. Lett. 92, 092901 (2008).
- [2] S. Guha, *et al.*, Appl. Phys. Lett. 96, 152907 (2010).
- [3] L. Lin and J. Robertson, J. Appl. Phys. 109, 094502 (2011).
- [4] K. Kita and A. Toriumi, Appl. Phys. Lett. 94, 132902 (2009).
- [5] S. Nittayakasetwat and K. Kita, IWDTF, pp 120-1, (2017)
- [6] S. Skirl, *et al.*, Acta Mater. 46, 2493 (1998).
- [7] P.H. Klein and W.J. Croft, J. Appl. Phys. 38, 1603 (1967).
- [8] H. Tada, *et al.*, J. Appl. Phys. 87, 4189 (2000).