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Study on interface dipole layer strength change by temperature in high-*k*/SiO_2 and high-*k*/high-*k* systems and its possible origin

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Abstract

Temperature dependence of interface dipole layer strength was experimentally investigated for high-*k*/SiO_2 and high-*k*/high-*k* interfaces. A larger temperature dependence was found for high-*k*/SiO_2 interface than high-*k*/high-*k* interface. The possible origin of such temperature dependence is also discussed based on the temperature-effects on interface structures.

1. Introduction

Electric dipole layers are often formed at the hetero-interfaces of two dielectric materials, including high-*k*/SiO_2 interfaces in advanced gate stacks [1], and even at some of high-*k*/high-*k* interfaces like MgO/Al_2O_3 [2]. However, it has not been clarified that how those dipole layer strength change with the measurement temperatures. The temperature-induced change of dipole layer strength should induce serious impact on the reliability in the MOS devices operated at either high- or low-temperatures for harsh environment applications. In this study, temperature dependence of dipole layer strength was investigated for both high-*k*/SiO_2 and high-*k*/high-*k* interfaces, to investigate the relationship between the temperature-effects on the dipole layer strength and the temperature-induced strain at the interface.

2. Experimental methods

The MOS capacitors with four kinds of dielectric layers were fabricated as shown in **Fig. 1**: (i)SiO_2, (ii)MgO/SiO_2, (iii)Al_2O_3/SiO_2, and (iv)MgO/Al_2O_3/SiO_2. These layers were deposited on p-Si substrates, by thermal oxidation for SiO_2 (10 nm) while rf-sputtering for Al_2O_3 and MgO layers (various thickness). Post-deposition annealing in 0.1% O_2 ambient was done at 600°C for (ii), but 800°C for (iii) and (iv). Finally, Au was deposited as the gate electrode. The 1MHz C-V characteristics at several temperatures from 100K to 400K were measured to determine the temperature dependence of flat-band voltage (V_{FB}).

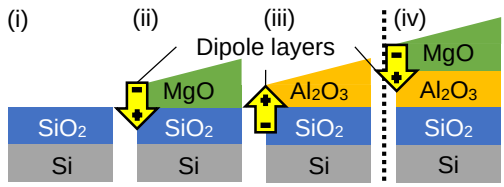

Fig.1. Sample structures for measuring temperature dependence of dipole layer strength. The arrows indicate the direction of interface dipoles, observed at room temperature.

3. Results and Discussions

The temperature dependent C-V characteristics of the capacitor (ii) is shown in **Fig.2**. In addition to the intrinsic change of V_{FB} due to the temperature dependence of Fermi level and intrinsic shape change of the curve by raising measurement temperature, we found an additional parallel shift of the curve by temperature. This is attributable to the change of dipole layer strength, in addition to a certain change of fixed charge density by temperature. When the effects of bulk fixed charges in SiO_2 and high-*k* layers are ignored, the V_{FB} of bi-layer dielectric capacitors whose interface is high-*k*/SiO_2 are given by,

$$V_{FB} = \varphi_{ms} - \frac{Q_1}{\varepsilon_{SiO_2}} d_{SiO_2} - \frac{Q_1 + Q_2}{\varepsilon_{high-k}} d_{high-k} + V_{dipole} \quad (1)$$

where φ_{ms} is the difference between the work function of gate metal and semiconductor, Q_1 and Q_2 are the fixed charge density at SiO_2/Si and high-*k*/SiO_2 interface, respectively, and d_{SiO2} and d_{high-k} are the physical thickness of SiO_2 and high-k layers, respectively, and V_{dipole} is the dipole layer strength at high-*k*/SiO_2 interface. For the capacitors (ii) with different MgO thicknesses, the relationships between capacitance equivalent thickness (CET) and V_{FB} were obtained as shown in **Fig. 3**. The extrapolation of the slope obtained by a linear fitting of the thickness dependence, to the left end of the horizontal axis where the top-oxide thickness equals zero, gives the hypothetical value of V_{FB}' at each temperature, where the effects of the third term of Eq. (1) was eliminated. In the same way, the values of hypothetical V_{FB}' for (iii) Al_2O_3/SiO_2 and (iv) MgO/Al_2O_3/SiO_2 stacks by the extrapolation of slopes of the top-layer thickness dependence of V_{FB} were shown in **Fig. 4** and **Fig. 5**, respectively.

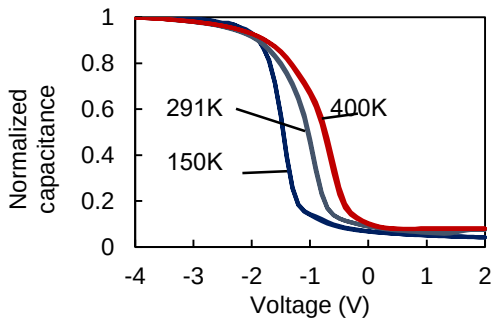

Fig.2. Typical example of temperature dependent C-V characteristics (for capacitor (ii)).

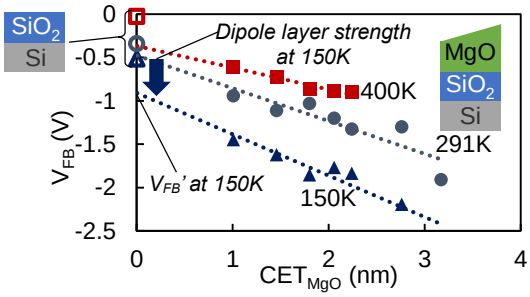

Fig.3. V_{FB} of capacitors (ii) (filled) and (i) as a reference (open) at different temperatures.

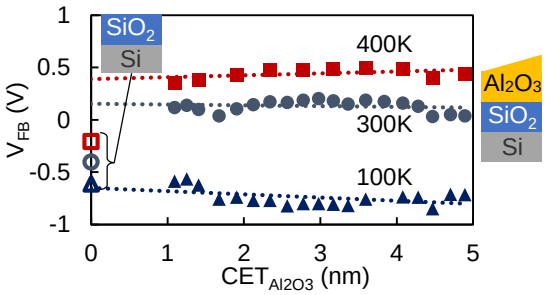

Fig.4. V_{FB} of capacitors (iii) (filled) and (i) as a reference (open) at different temperatures.

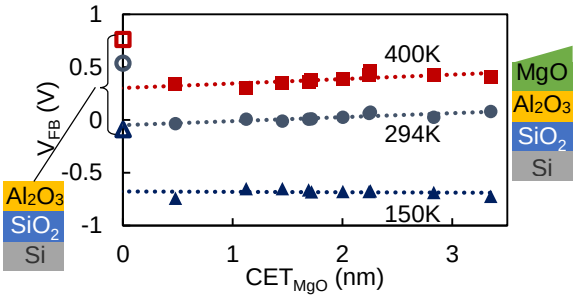

Fig.5. V_{FB} of capacitors (iv) (filled) and (iii) as a reference (open) at different temperatures.

Finally, the difference between the values of V_{FB}' obtained by the above extrapolation and the V_{FB} obtained for the stack of the identical CET without the top layer deposition was determined at each measurement temperature to extract the dipole-layer-induced V_{FB} shift (V_{dipole}) which is the fourth term in Eq. (1). For example, from the difference of V_{FB}' for (ii) MgO/SiO_2 and V_{FB} for (i) SiO_2, a certain temperature dependence of the difference between Au work function and Si Fermi level, as well as the effects of the fixed charges at SiO_2/Si interface (the second term in Eq. (1)) can be eliminated, as long as we can regard the fixed charge density at SiO_2/Si is common for those two samples.

As a result the temperature coefficient of the dipole strength at MgO/SiO_2 interface was ~2 mV/K, and that for Al_2O_3/SiO_2 interface was 2−3 mV/K as shown in **Fig. 6**. On the other hand, dipole layer strength at MgO/Al_2O_3 interface showed significantly less temperature dependence ~0.4mV/K.

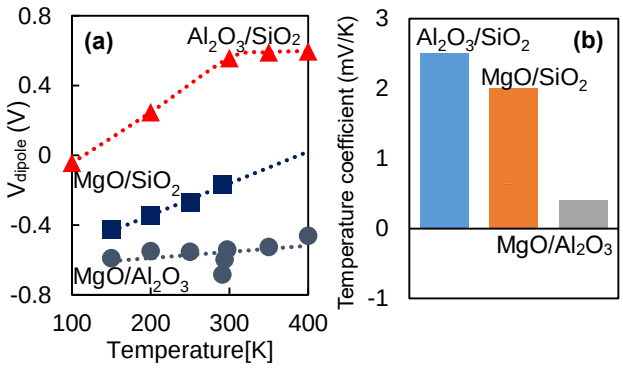

Fig.6. (a) Temperature dependence of dipole layer strength (V_{dipole}) at the three interfaces: MgO/SiO_2, Al_2O_3/SiO_2, and MgO/Al_2O_3. **(b)** Temperature coefficient of dipole layer strength of those three interfaces.

Considering that the thermal expansion coefficient (β) of SiO_2 (3×10^{-7} K^{-1} [5]) is significantly smaller than high-*k* materials like MgO (1×10^{-5} K^{-1} [3]) and Al_2O_3 (7×10^{-6} K^{-1} [4]), the difference of β which determines the thermal strain at the interface is much smaller for high-*k*/high-*k* interface, compared to high-*k*/SiO_2. Considering the proposed mechanism of the interface dipole layer formation [1] that the structural relaxation of oxide hetero-interface is the driving force of the dipole layer formation by the ionic rearrangement at the interface, it would be possible that temperature effect on the strength of interface dipole layer is due to the change of interface strain caused by the difference of thermal expansion coefficient of the two oxides.

4. Conclusions

A larger temperature dependence of interface dipole layer strength was observed for high-*k*/SiO_2 interfaces (Al_2O_3/SiO_2 and MgO/SiO_2) than that for high-*k*/high-*k* interface (MgO/Al_2O_3). A correlation between the temperature coefficient of dipole layer strength and the difference of β between the two dielectrics was indicated. As one of the possible origins of the temperature dependence of dipole layer strength, the thermally-induced change of interface strain can be considered, which is not conflicting with the consideration that structural strain at the interface is the driving force to induce dipole layer.

Acknowledgements

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References

[1] K. Kita and A. Toriumi, Appl. Phys. Lett. **94**, 132902 (2009).
[2] J. Fei and K. Kita., Microelectronic Eng., **178**, 225 (2017).
[3] R. J. Beals *et al.*, J. Amer. Ceram. Soc. **40**, 279 (1957).
[4] S. Skirl *et al.*, Acta Mater., **46**, 2493 (1998).
[5] H. Tada *et al.*, J. Appl. Phys., **87**, 4189 (2000).