

Ab Initio Study of Dipole-induced Threshold Voltage Shift in HfO₂/Al₂O₃/(100)Si

E. Chen*, Y.T. Tung, Z.R. Xiao, T.M. Shen, J. Wu, C.H. Diaz
TCAD Division, Taiwan Semiconductor Manufacturing Company (TSMC)
No. 168, Park Ave. 2, Hsinchu Science Park, Hsinchu County, Taiwan
*e-mail: chenjhm@tsmc.com

INTRODUCTION

Metal-oxide-semiconductor (MOS) devices have been aggressively scaled down to sub-20nm technologies nowadays. HfO₂/Al₂O₃ (HA) bi-layer high- κ dielectric is promising to keep EOT scaling while limiting gate leakage current due to Al₂O₃ larger bandgap (~8.8 eV), band offsets, and relatively higher dielectric constant ($\kappa \approx 10$) than that of SiO₂. Threshold voltage (V_{th}) control and reliability are key challenges for CMOS with such high- κ stack. The dipole formed at high- κ dielectrics has been proposed to explain the V_{th} shift observed in the experimental results [1-2]. Lin and Robertson have also shown the qualitative mechanism using *ab initio* methods [3]. However, the quantitative study compared to experimental results has not been done yet. In this paper, the HA atomic model has been established on (100) Si. The dominant dipole moment in HfO₂/Al₂O₃/Si which affects the V_{th} shift has been identified. From our gate stack model, the dipole strength has been found being correlated to the thickness of Al₂O₃ (3~13 Å). On account of the effect, the CMOS ΔV_{th} with different Al₂O₃ thicknesses is calculated using *ab initio* methods and the calculation quantitatively explains the experimental results.

METHODOLOGY

The gate stack model of HfO₂/Al₂O₃/(100)Si with ammonia (NH₃) pretreatment is shown in Fig. 1. The θ phase alumina has been chosen for better lattice matching of the (100) HfO₂ and (100) Si substrate [4]. To obtain the dipole moment, Mulliken charge [5] and dipole correction [6] methods, built in CASTEP and VASP (Vienna *Ab initio* Simulation Package), respectively, have been used to evaluate the accuracy of the dipole moment calculation for the selected diatomic molecules. As shown in Fig. 2, the dipole correction method accurately answers the experimental dipole moment for the diatomic molecules with the covalent bond characteristics, which is exactly in the domain of our interest.

RESULT AND DISCUSSION

To identify the most important dipole moment in HA gate stack, the dipole densities of four bi-layer

models have been calculated in Fig. 3, which suggests the dominant one in the gate stack is formed at the interface of HfO₂/Al₂O₃. The dipole densities for both water vapor (H₂O) and ammonia pretreatments at Al₂O₃/Si are one order smaller than that at HfO₂/Al₂O₃. Since the thickness of Al₂O₃ is controlled within a few angstroms in the gate stack, the thickness dependence of the dipole density at the interface of HfO₂/Al₂O₃ is investigated (Fig. 4). The dipole density decreases almost linearly as the thickness of Al₂O₃ decreases from four monolayers (13 Å) to one monolayer (3 Å).

$$\Delta\Phi_{ms} = \Phi_{dipole} = \frac{\bar{q} \cdot \bar{d}}{A\kappa_{hk}} = \frac{\bar{p}}{A\kappa_{hk}} \quad (1)$$

Using Gauss's law to calculate the voltage drop at the parallel dipole "plate" (Eq. 1), ΔV_{thn} and ΔV_{thp} for the CMOS with the different Al₂O₃ thickness are shown in Fig. 5 and Fig. 6, respectively. On account of the V_{th} shift effects from ΔEOT and dipole moment, our *ab initio* calculation quantitatively explains the experimental data.

CONCLUSION

The gate stack model of HfO₂/Al₂O₃/(100)Si is established in the paper. Using the dipole correction method, the dominant dipole moment is found at the interface of HfO₂/Al₂O₃. The dipole moment decreases as the thickness of Al₂O₃ decreases from four monolayers (13 Å) to one monolayer (3 Å). Our *ab initio* calculation quantitatively explains the threshold voltage shift of the CMOS experimental results.

ACKNOWLEDGMENT

We would like to express our sincere thanks to the management support from Dr. Jack Y.C. Sun and Dr. C.C. Wu.

REFERENCES

- [1] T. Nabatame *et al.*, ECE Trans. **11**, 543 (2007).
- [2] P.D. Kirsch *et al.*, Appl. Phys. Lett. **92**, 092901 (2008).
- [3] L. Lin and J. Robertson, J. of Appl. Phys. **109**, 094502 (2011).
- [4] C-K Lee *et al.*, Phys. Rev. B **76**, 245110 (2007).
- [5] R.S. Mulliken, J. Chem. Phys. **23**, 1833 (1955).

[6] J. Neugebauer and M. Scheffler, Phys. Rev. B **46**, 16067 (1992)

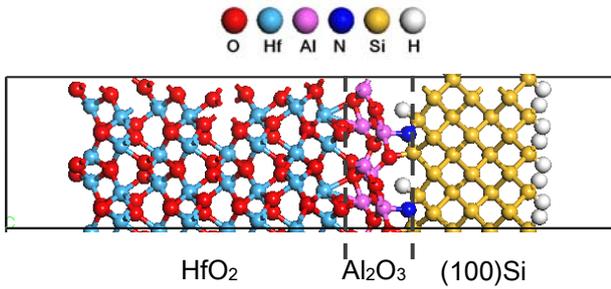


Fig. 1. The gate stack model of $\text{HfO}_2/\text{Al}_2\text{O}_3/(100)\text{Si}$ with ammonia (NH_3) pretreatment.

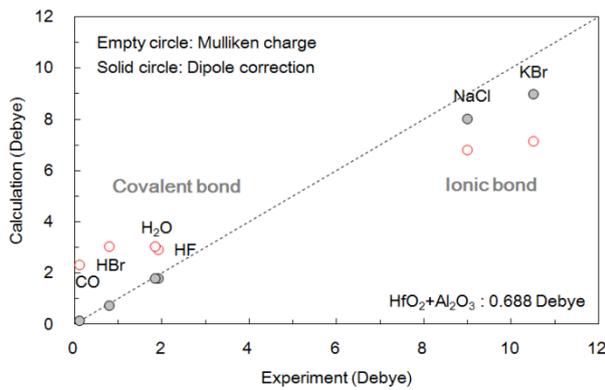


Fig. 2. The Mulliken charge and dipole correction methods, built in CASTEP and VASP (Vienna *Ab initio* Simulation Package), respectively, have been used to evaluate the accuracy of the dipole moment calculation for the selected diatomic molecules. The dash line means *ab initio* calculation and experimental results agree each other. The dipole correction method accurately answers the experimental dipole moment for the diatomic molecules with the covalent bond characteristics, which is the in domain of our interest ($\text{HfO}_2/\text{Al}_2\text{O}_3$).

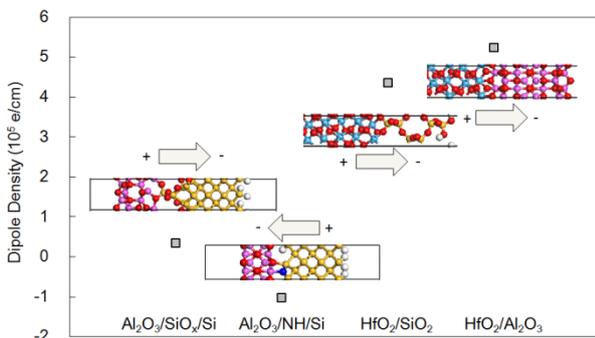


Fig. 3. The dipole densities of four bi-layer models have been calculated using the dipole correction method, which suggests the dominant one in the stack of $\text{HfO}_2/\text{Al}_2\text{O}_3/(100)\text{Si}$ is formed at the interface of $\text{HfO}_2/\text{Al}_2\text{O}_3$.

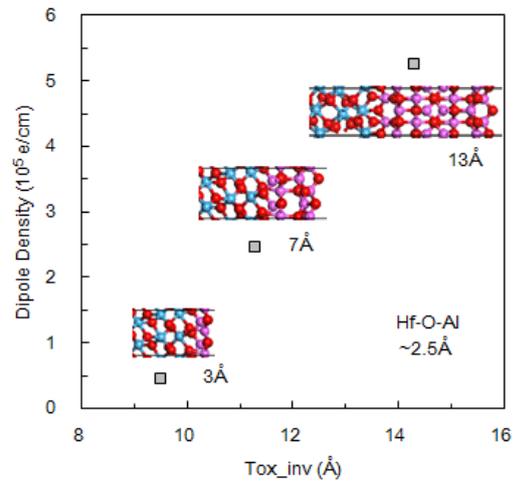


Fig. 4. The dipole density of the bi-layer $\text{HfO}_2/\text{Al}_2\text{O}_3$ decreases almost linearly as the thickness of Al_2O_3 decreases from four monolayers (13 Å) to one monolayer (3 Å).

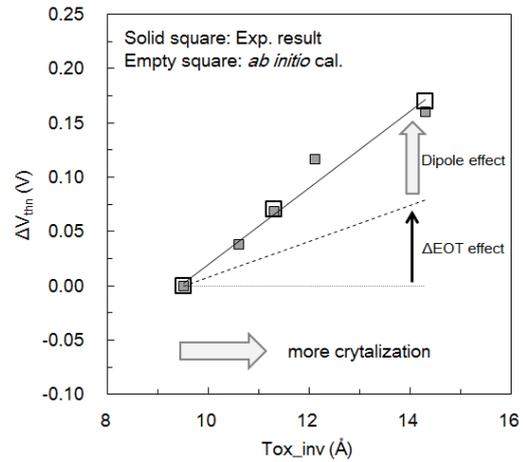


Fig. 5. The solid square shows NMOS ΔV_{th} experimental results with the different monolayer thickness of Al_2O_3 , and the empty square show the *ab initio* calculation with the Al_2O_3 physical thickness of 3 Å, 7 Å, and 13 Å.

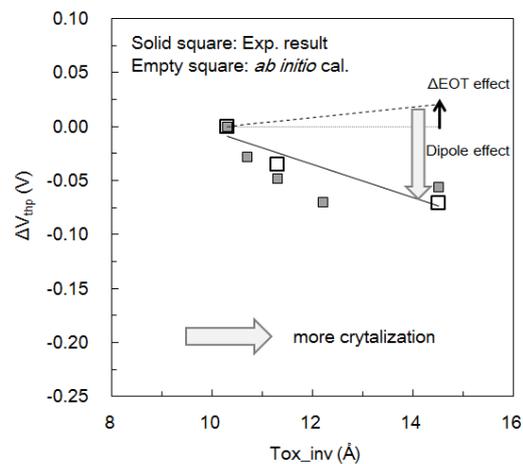


Fig. 6. PMOS threshold voltage shift (ΔV_{thp}) with the different Al_2O_3 thickness.