

Valency of cation rather than Oxygen Density may govern the Dipole Moment at high-k/SiO₂ interfaces

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1 Introduction

In high-k/metal gate stack, a threshold voltage shift can be observed, which is caused by the formation of a dipole at the high-k/SiO₂ interface [1]. According to the oxygen density difference accommodation model [2], the oxygen atoms migrate from the higher-oxygen-density material to the lower-oxygen-density material, causing a charge redistribution near the interface which creates the dipole.

In previous publications [3], the dipole formation at high-k/SiO₂ interfaces was successfully reproduced by molecular dynamics (MD) simulation. Al₂O₃/SiO₂, MgO/SiO₂ and SrO/SiO₂ interfaces were reproduced to observe the dipole characteristics. A positive dipole was formed at the Al₂O₃/SiO₂ interface, while MgO/SiO₂ and SrO/SiO₂ interfaces showed a negative dipole. When comparing these results to what the oxygen density difference of every high-k/SiO₂ interface would predict, the dipole orientation ties in with the oxygen density accommodation model in the case of Al₂O₃/SiO₂ and SrO/SiO₂, whereas this isn't true for the MgO/SiO₂ interface, suggesting that the dipole moment might be related to cation migration.

In this work, different variations of Al, Mg, Sr and Ti hybrid oxides were simulated, including the pure high-k oxides (Al₂O₃, MgO, SrO and TiO₂, respectively), and we investigated what is the best descriptor to predict the dipole moment at high-k/SiO₂ interface.

2 Simulation Method

The simulation was conducted using the MD simulation platform SCIGRESS, from Fujitsu Ltd. The SiO₂ and high-k were prepared separately by melting their crystalline structure at 4000K. After, these amorphous structures were connected to each other and annealed by the isothermal-isobaric MD calculation at 1000K under atmospheric pressure. Finally, the high-k/SiO₂ block was cooled down to 300K.

Near 1300 Al_xMg_ySr_zTi_tO_{1.5x+y+z+2t} variations were reproduced. The Born-Mayer-Huggins potential was used as the interatomic potential, with a Completely Ionic Model (CIM) parameter set [4].

3 Results and Discussion

Fig. 1 shows the correlation between the dipole moment and the normalized oxygen density (NOD, normalized by that of SiO₂). According to the oxygen density accommodation model, when NOD < 1 the dipole moment should always be positive. However, there are many irregular cases showing negative dipoles do exist, as indicated by the red-circled area in Fig. 1.

Mean valence number of cations in high-k oxide (Fig. 2) shows a stronger correlation coefficient (R = 0.841) than that of NOD (R = 0.680). Furthermore, the dipole moment doesn't show consistency when plotted against the oxygen density. For instance, MgO shows the highest negative dipole value in the present simulation, even though SrO has a much lower oxygen density, and the same is applicable to Al₂O₃ and TiO₂, hence the lower correlation coefficient.

4 Conclusion

Even though the oxygen density difference accommodation model is successfully applicable to many high-k materials, the model shows inconsistencies when applied to multi-component high-k oxides.

As of now, our MD simulation results suggest that the dipole moment is strongly correlated to the valence number of cations.

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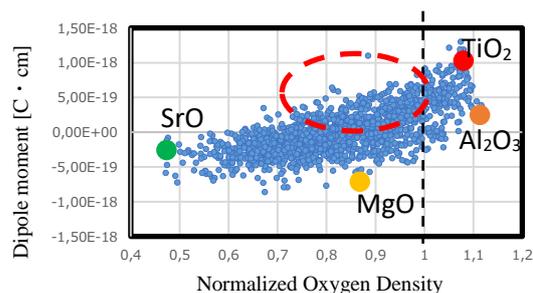


Fig. 1. Dipole moment VS oxygen density, normalized around SiO₂ OD. R = 0.680

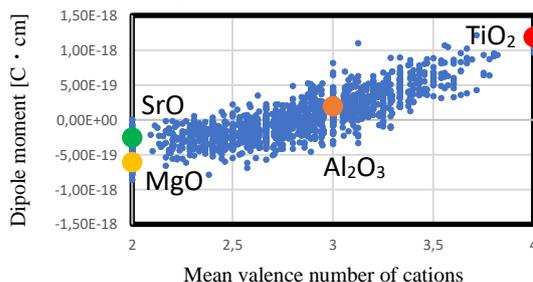


Fig. 2. Dipole moment VS cation charge. R = 0.841