Dipole model explaining high-k/metal gate field effect transistor threshold voltage tuning

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An interface dipole model explaining threshold voltage \((V_t)\) tuning in HfSiON gated \(n\)-channel field effect transistors (nFETs) is proposed. \(V_t\) tuning depends on rare earth (RE) type and diffusion in Si/SiO\(_x\)/HfSiON/REO\(_x\)/metal gated nFETs as follows: Sr<Er<Sc+Er<La<Sc<none. This \(V_t\) ordering is very similar to the trends in dopant electronegativity (EN) (dipole charge transfer) and ionic radius \((r)\) (dipole separation) expected for a interfacial dipole mechanism. The resulting \(V_t\) dependence on RE dopant allows distinction between a dipole model (dependent on EN and \(r\)) and an oxygen vacancy model (dependent on valence). © 2008 American Institute of Physics.

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HfSiON/REO/MG stacks indicates the following order: Sr<Er<Sc+Er<La<Sc<none. To understand if REO Vt tuning is a bulk or interfacial phenomena, FTIR was done to probe the chemical bonds associated with the REO. Figure 2 shows FTIR results from the Si/SlOx/HfSiON/REO/MG stacks. The feature at ~1225 cm^{-1} is assigned to the O–Si–O longitudinal optic phonon mode in the interfacial SiOx. RE–Si–O is expected to show a peak ~200 cm^{-1} lower than O–Si–O due to the lower vibrational frequency of the heavier RE.13 Therefore, the peak at 1025 cm^{-1} is attributed to RE–O–Si. Data in Fig. 2 suggest that RE diffuses to the high-k/low-k interface forming RE–Si–O at the expense of SiOx volume. A reaction between RE and SiOx is expected based on results in Refs. 13 and 14. The extent of this reaction correlates with the size of the RE, with larger RE forming more RE–Si–O. This prior observation is consistent with our Vt and FTIR results. For example, Er (r=100 pm) forms more interfacial RE–O–Si than Sc (r=86 pm) (Fig. 2), yielding a greater density of dipoles shifting Vt more versus Sc. The 1070 °C thermal budget is key to diffuse RE to the interfacial SiOx forming RE–O–Si as demonstrated in Fig. 2 (inset) for the case of LaOx. Backside SIMS for SrOx and LaOx doping indicate no penetration into Si (not shown). Because FTIR shows interfacial RE–Si–O formation, we focus on a high-k/low-k interfacial model rather than a bulk VOx model to explain the Vt data.

As mentioned earlier, nFET Vt correlates with dopant EN and ionic radii. Figure 3 shows the experimentally observed Vt correlation to EN and r (inset). This Vt dependence on dopant EN and r suggests that an interface dipole model15 causing local charge transfer16 may explain the Vt results. Since RE forms RE–Si–O,13 while HfOx separates from SiOx,17 RE likely diffuses to the high-k/low-k interface (Fig. 2). Once at this interface, RE may form a Hf–O–RE configuration resulting in a charge transfer and the observation of Vt tuning. The amount of charge transfer determines the magnitude of the dipole μ. μ is determined by +Q (charge on + pole) and −Q (charge on − pole), separated by a distance d; μ=Q·d. +Q is expected to be inversely proportional to dopant EN and d is expected to be proportional to dopant r. Figure 4 shows the interfacial Hf–O–RE and the resulting dipole. This dipole vector shifts the effective metal work function (EWF) a variable amount ∆ depending on dopant EN and r (Fig. 3). This is its dopant induced shift in EWF that results in the observed Vt tuning in Fig. 1.

A model attributing Vt tuning to aliovalent substitution of La for Hf forming positively charged V0 does not explain our data for +3 dopants.1 Because Sc, Er, and La are all +3, they would be expected to form the same number of positively charged V0 in HfOx, and, therefore, shift Vt similarly. However, as shown in Fig. 1, Sc, Er, and La shift Vt differently, in accordance with EN and r rather than valence. Furthermore, pure La2O3 films on Si, where La3+ cannot substitute for Hf4+, also show large negative Vth/Vt tuning supporting the notion that RE interaction with SiOx is a key part of the mechanism.18 If the RE were exclusively creating positive charge in the SiOx interlayer (rather than a dipole),
we would expect mobility loss, but 92% SiO\_2 mobility has been achieved with La doping.\textsuperscript{8}

We have investigated the effect of HfSiON doping (Sr, Sc, Er, and La) on nFET \( V_t \) tuning. The \( V_t \) tuning correlates with dopant EN and dopant ionic radii. A proposed model explaining this \( V_t \) tuning is the dipole moment of the Hf–O and RE–O bonds at the high-\( k/\)SiO\_2 interface.

FIG. 4. Interface dipole moment model. EWF shift (\( \Delta \)) is proportional to dipole moment due to the charge transfer in the Hf–O–RE configuration. The dipole moment magnitude varies with dopant type explaining the \( V_t \) dependence on dopant type in Fig. 1.


