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 an 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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SiON gate dielectrics have reached a physical thickness ($T_{phys}$) scaling limit of 1.3 nm, making high permittivity (k) dielectrics such as HfO$_x$ necessary to scale oxide electrical thickness ($T_{ox}$), suppress gate tunneling current, and control short channel effects. Recently, high-k/metal gate devices have improved significantly. For example, electron mobility similar to SiON$^3$, low charge trapping, and scalability to $T_{inv}$=1.3 nm (Ref. 5) have been achieved. An open issue with high-k/metal gate stacks is achievement of acceptably low threshold voltage ($V_t$) after high temperature processing (>1000 °C). Target p-channel field effect transistor (pFET) $V_t$ has been achieved utilizing a SiGe channel.$^6$ Target n-channel FET $V_t$ has been achieved by doping Hf(Si)O(N) with rare earth (RE) oxides such as LaO$_x$ (Refs. 7 and 8) or DyO$_x$. $^9$ 2 nm HfSiO films were deposited on Si (100) by atomic layer deposition.$^{11}$ The interfacial SiO$_x$ formed between Si(100) and HfSiO is estimated to be 1 nm. N was incorporated by postdeposition annealing. RE dopants were introduced as follows: LaO$_x$ and SrO$_x$ caps were formed by molecular beam deposition (MBD). Sc, Er, and Sc+Er caps were formed by physical vapor deposition (PVD) and oxidized. All cap layers were of similar thickness (0.5 nm), according to quartz crystal microbalance (MBD) or x-ray reflectivity calibration. Metal gate (MG) was deposited by PVD followed by 100 nm amorphous Si (a-Si) capping. The remaining process was a standard gate first flow including 1070 °C spike annealing. $V_t$ results and drain current-gate voltage ($I_dV_t$) results were extracted from $10\times1\mu$m nFETs with channel doping $\approx5\times10^{17}$ cm$^{-3}$. $V_t$ was extracted from the linear regime with drain bias of 50 mV using the peak transconductance method. Fourier transform infrared spectroscopy (FTIR) blanket Si/SiO$_x$/HfSiON/REO$_x$/MG/a-Si samples were formed similarly to the device samples. MG and a-Si were wet etched from FTIR samples after 1070 °C annealing. Capacitance equivalent thickness in inversion (CETinv) was 1.5 ± 0.1 nm for the doped samples and 1.7 nm for undoped HfSiON.

$I_dV_t$ results in Fig. 1(a) show that each dopant affects the $n$FET transfer characteristics differently. Device threshold and threshold regions depend on the dopant type with Sr shifting the $I_dV_t$ the most and Sc shifting the least versus the control. This difference is expected and, as shown below, trends with dopant size and EN. These data support the hypothesis that a high-k/low-k interface dipole controls the $V_t$. Figure 1(b) shows $V_t$ distributions for doped HfSiON gate dielectrics. $V_t$ for SiON/n-poly-Si control is near 0.30 V. Compared to HfSiON, Sc doping results in the smallest $V_t$ tuning (250 mV) while SrO$_x$ doping results in the largest $V_t$ tuning (600 mV). A $V_t$ trend for

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HfSiON/REOx/MG stacks indicates the following order: Sr<Er<Sc<La<Sc<none.

To understand if REOx Vt tuning is a bulk or interfacial phenomena, FTIR was done to probe the chemical bonds associated with the REOx. Figure 2 shows FTIR results from the Si/SiO2/HfSiON/REOx/MG stacks. The feature at ~1225 cm⁻¹ is assigned to the O–Si–O longitudinal optic phonon mode in the interfacial SiO2. 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. Therefore, the peak at 1025 cm⁻¹ is attributed to RE–Si–O. Data in Fig. 2 suggest that RE diffuses to the high-k/low-k interface forming RE–Si–O at the expense of SiO2 volume. A reaction between RE and SiO2 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 SiO2 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 Vt 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 model causing local charge transfer may explain the Vt results. Since RE forms RE–Si–O13 while HfO2 separates from SiO23, 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 Δ depending on dopant EN and r (Fig. 3). It is this 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. Because Sc, Er, and La are all +3, they would be expected to form the same number of positively charged V0 in HfO2, 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 SiO2 is a key part of the mechanism. If the RE were exclusively creating positive charge in the SiO2 interlayer (rather than a dipole),
we would expect mobility loss, but 92% SiO₂ mobility has been achieved with La doping.\(^8\)

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/SiO₂ interface.

\(\Delta \propto \sum \vec{\mu}\)

\(\sum \vec{\mu} \propto \Delta\)

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.