Charging Phenomena at the Interface Between High-\(k\) Dielectrics and \(\text{SiO}_x\) Interlayers


Abstract—The transition regions of GdSiO/\(\text{SiO}_x\) and HfO\(_2/\)\(\text{SiO}_x\) interfaces have been studied with the high-\(k\) layers deposited on silicon substrates. The existence of transition regions was verified by medium energy ion scattering (MEIS) data and transmission electron microscopy (TEM). From measurements of thermally stimulated current (TSC), electron states were found in the transition region of the HfO\(_2/\text{SiO}_x\) structures, exhibiting instability attributed to the flexible structural molecular network expected to surround the trap states. We found that flat-band voltage shifts of MOS structures, that reach constant values for increasing oxide thickness, cannot be taken as unique evidence for the existence of dipole layers.

Keywords—defects, dielectrics, high-\(k\), metal oxide semiconductor.

1. Introduction

The gate function of future metal oxide semiconductor (MOS) transistors has attracted a large scientific community to an expedition into the periodic system for tracking the Dielectric Grail. Wanted is a material with acceptable energy offset values, \(\Delta E\), between the energy bands of the dielectric and the silicon crystal, while, in addition, having a high enough dielectric constant, \(k\). Yet, to fulfill the demands of low current leakage and high capacitive coupling between gate metal and transistor channel, the crucial property is the product \(k \times \Delta E\) of these two quantities [1]. So far, for CMOS applications most of these efforts have been limited to metal oxides. The change from the extremely well mastered thermal SiO\(_2\) material, to an oxide based on metals among the transition or rare earth series, has disclosed obstacles that were unnoticeable for traditional technology. Beside the problems of chemical stability between these new “high-\(k\)” oxides and the silicon substrate, crystallization, sensitivity to humid environment, higher concentrations of oxide traps and interface states are properties, not uncommon among these materials. Driven by technology, this has given rise to needs for understanding their microscopic properties from chemical, physical and electrical point of view.

A common attribute of high-\(k\) oxide films deposited on silicon is the occurrence of an \(\text{SiO}_x\) interlayer between the high-\(k\) material and the silicon crystal. This evokes interface electron state properties similar to those at thermal SiO\(_2/\text{Si}\) interfaces [2], [3]. Even if the interlayer lowers the effective \(k\) value of the film, it often gives better conditions for a transistor channel than those offered by a direct interface due to lower charge carrier scattering by the former. However, it must be paid for by an extra interface occurring between SiO\(_2\) and the high-\(k\) material [4]. As the total physical thickness of the film is in the range of 5 nm or smaller, on this length scale the transition from SiO\(_2\) to the high-\(k\) material can hardly be considered abrupt. It is found to include a transition region with undefined stoichiometry and thus with possible structural instabilities [5]–[11]. Recently, the occurrence of traps either singular or in dipole configurations have been noticed as the potential origin of charge sources decreasing the quality of presumptive gate insulators [11]–[16]. In the present paper, we will describe the physical and electrical properties of transition regions at GdSiO/\(\text{SiO}_x\) and HfO\(_2/\text{SiO}_x\) interfaces and demonstrate how charge carrier traffic at such positions can be interpreted in order to characterize the trap properties. Based on this reasoning, the possible existence of a dipole layer in the transition region will be addressed.

2. Properties of Transition Regions

The dominating defect causing charge carrier traps in the bulk of transition and rare-earth metal oxides is commonly considered to be the oxygen vacancy. It has similar properties as the E’ center in SiO\(_2\) and has been the object of a rich theoretical [15], [16] and experimental [10], [11] literature. In HfO\(_2\) it has been predicted to be an amphoteric center with four [15] or five [16] charge states ranging from double donor to double acceptor behavior with the latter states positioned in the range 1–2 eV from the HfO\(_2\) conduction band edge. Furthermore, the double acceptor level is argued to be connected with large lattice relaxation [16]. It has even been proposed that the double negatively charged energy level falls below the single negatively charged level, thus exhibiting negative-U property [17]. These trap properties will be further discussed below in relation to the results from electrical measurements.

As one example of the complex high-\(k\) oxide/\(\text{SiO}_x\) interface, we will discuss data from GdSiO. This dielectric was...
MEIS data for samples with GdSiO evaporated on top of a 4 nm thermal oxide: (a) as deposited and (b) after RTA at 900°C for 1 s.

prepared by evaporating Gd₂O₃ on a 4 nm thick thermal SiO₂ layer on silicon [18]–[21]. The double layer was partly transformed into GdSiO by rapid thermal anneal (RTA) for 1 s at 900°C. The depth distribution of elements before and after the thermal anneal is shown by medium energy ion scattering (MEIS) data in Fig. 1. A steeply decreasing silicon concentration from the silicon side into the oxide directly after deposition (Fig. 1(a)), reflects a complicated diffusion process taking place already at this stage. At the 10 nm mark, the concentration of oxygen is a factor of 2 higher than the concentration of silicon. This indicates a reminiscence of SiO₂ which quickly becomes a suboxide at larger distances from this interface, where a nearly stoichiometric Gd₂O₃ takes over. The extremely high gradient of Si at the 10 nm point would be expected to stage structural instability. After the RTA at 900°C, silicon has penetrated the whole oxide layer (Fig. 1(b)) creating a GdSiO with varying concentration of Si. This structure has been demonstrated to fulfill the industrial target for low standby power, 22 nm double gate SOI transistors [18].

A second example is given by a transmission electron microscopy (TEM) picture showing the interface between HfO₂ and SiOₓ in Fig. 2. This sample was prepared by reactive sputtering of Hf and O₂ followed by an anneal at 800°C for 10 min [12]. Between the white string showing the SiOₓ layer and HfO₂, appearing as a black area, a milky band is shown with a width of about 2 nm. Here, one may expect the same type of diffusion taking place as in the case of GdSiO above. As will be shown below, traps formed in this region consequently have an unusual electric behavior.

3. Charge Carrier Traffic at Transition Regions

3.1. Energy Relations and Charge Exchange

We consider an interface between a high-k oxide and an SiOₓ interlayer on silicon as schematically shown in Fig. 3. The transition region is marked by a wide patterned band and includes a trap level at an energy distance ΔE below the silicon conduction band edge. A negative net charge is present in the interlayer, such that an electric field \( F \) is directed from the silicon crystal towards the high-k oxide. Assuming that the thickness of the interlayer is about 1 nm, tunneling through this layer is non-negligible and can be described as assisted by a decay of the effective density of states, \( N_C \), from the silicon conduction band determined by \( N_C \exp\left[\frac{-x_0}{\lambda}\right] \), where \( x_0 \) is the distance from the SiOₓ/Si interface to the trap and \( \lambda \) is a damping factor. A captured electron can be transferred into the Si bulk by a two step process, starting with a thermally driven mechanism to the tunneling states at the energy level of the silicon conduction band edge. As long as the electric field is high enough, this process is followed by tunneling into the silicon conduction band as depicted in Fig. 3. Emitting electrons from the trap position will lower the electric field. The system
may, therefore, reach a situation where the electric field becomes too low for the second transfer step to occur, which means that the emission process stops. As the tunneling probability is very sensitive to the magnitude of the electric field, this termination may be very abrupt as we will see in the experimental data following.

As long as the tunneling rate dominates, the bottleneck of this process is the thermal electron emission rate, $e_n$, from the trap to an effective density of states decreased by the tunneling probability

$$e_n = \sigma_n v_{th} N_c \exp \left( -\frac{\lambda_0}{\lambda} \right) \exp \left( -\frac{\Delta E}{k_B T} \right),$$  

(1)

where $\sigma_n$ is the capture cross section representing a local transition from the tunneling state to the trap state, $v_{th}$ is the average thermal velocity of electrons in the silicon conduction band, $k_B$ is Boltzmann’s constant and $T$ is absolute temperature. As will be described in detail below, using thermally stimulated current (TSC) technique to determine the emission rate, the temperature is linearly increased with time during the measurement cycle. As the electric field, $F$, decreases due to the decrease of negative charge in the SiO$_x$ layer, the energy distance $\Delta E$ will increase. In addition, the temperature increase will move the Fermi level in the silicon bulk to deeper energy in the band gap. For a given applied voltage across the structure, this will lower the position of the silicon conduction band edge at the SiO$_x$/Si interface which will increase the voltage drop across the interlayer and tend to decrease $\Delta E$. Assuming, as a first order approximation, that both these processes are linear with temperature, we write

$$\Delta E = \Delta E_0 - \alpha T,$$

(2)

where $\Delta E_0$ is the energy distance between the silicon conduction band edge and the trap level extrapolated to $T = 0$ K and $\alpha$ is a constant determined by the two competing processes described above. Using Eq. (2) in (1), we get

$$e_n = \sigma_n v_{th} N_c \exp \left( -\frac{\Delta E_0}{k_B T} \right),$$

(3)

where

$$\sigma_n = \sigma_0 \exp \left( \frac{\alpha}{k_B} \right) \exp \left( -\frac{\lambda_0}{\lambda} \right),$$

(4)

can be considered as an effective capture cross section, influenced by the changing energy level position and the tunneling probability. We notice that, measuring the emission rate as a function of temperature and plotting this quantity in an Arrhenius graph would give an activation energy corresponding to an extrapolation of $\Delta E$ to $T = 0$ K under the assumption of linear conditions. However, this reasoning does not take into account the properties related to local molecular dynamics of the trap volume.

For a case like the oxygen vacancy, where the transition is argued to be connected with a strong lattice relaxation [16], the emission process would be influenced also by the vibronic properties of the trap [21] and characterized by “hysteretic tunneling”, adding a simultaneous trap relaxation and tunneling into the picture [22]. This would lead to two additional pre-exponential factors in the expressions for the thermal emission rate one originating from a possible thermally activated $\sigma_n$;

$$\sigma_n = \sigma_0 \exp \left( -\frac{\Delta U}{k_B T} \right),$$

(5)

where $\sigma_0$ depends on a combination of matrix elements including electronic and atomic wave functions involved in the process while $\Delta U$ is an activation energy originating from the vibronic properties of the trap system [21], [23]. The second effect comes from the entropy factor [21], [23], [24]:

$$x_n = \exp \left( \frac{\Delta S}{k_B} \right),$$

(6)

where $\Delta S$ is the change in entropy due to the change in vibrational frequency of the ionic part of the trap when the electron is released. Hence, combining the effects of the change in $\Delta E$ due to de-charging and those of a vibrating electron-ion trap system, we find from Eqs. (1)–(6):

$$e_n = \sigma_0 \exp \left( -\frac{\Delta U}{k_B T} \right) \exp \left( \frac{\Delta S}{k_B} \right) \exp \left( \frac{\alpha}{k_B} \right) \times \exp \left( -\frac{\lambda_0}{\lambda} \right) v_{th} N_c \exp \left( -\frac{\Delta E_0}{k_B T} \right),$$

(7)

where the activation energy now is represented by an enthalpy, $\Delta H_0 = \Delta E_0 + \Delta S T$, including the heat, $\Delta S T$, stored by the local vibrational modes [21], [23], [24].
For this case the first factors in Eq. (7) make up an "effective" capture cross section, \( \sigma_c \), which would be obtained from an Arrhenius plot of the thermal emission rate, \( e_n \):

\[
\sigma_c = \sigma_0 \exp\left( -\frac{\Delta U}{k_B T} \right) \exp\left( \frac{\Delta S}{k_B} \right) \exp\left( -\frac{\alpha}{k_B} \right) \exp\left( -\frac{x_0}{\lambda_0} \right). \tag{8}
\]

As will be shown below, TSC results demonstrate instabilities among the traps investigated in the HfO_2/SiO_x transition region. This is most probably originating from restructuring of the molecular arrangement around the trap volume, thus changing the matrix elements for charge carrier transition involved in \( \sigma_c \) as well as quantities of the vibrational properties reflected by \( \Delta U \), \( \Delta S \), and \( \Delta H_0 \) in Eqs. (7) and (8).

### 3.2. Thermally Stimulated Current

When measuring TSC from traps in a MOS system [12], the sample is first brought into accumulation at room temperature followed by a temperature decrease to about 50 K. During this procedure, traps at the interface and in the oxide are filled by charge carriers. At the low temperature point, the system is biased into deep depletion and a temperature increase, linear as a function of time, is applied. For an n-type semiconductor this gate bias is negative. As long as the temperature is lower than about 200 K and the total scanning time up to that temperature is shorter than about 10 min, it should be noticed that, due to the low temperature, an extremely low concentration of holes is expected in the valence band of the silicon crystal. Therefore, all de-charging processes observed as a TSC can be expected to originate from electron exchange at the insulator/silicon interface. The current created by emitted electrons is expressed by [12]

\[
i(T) = \frac{C_{ox}}{C_S + C_{ox}} q N_T e_n \exp\left[ \frac{T - T_1}{T_0} \right] \int_{T_0}^{T_1} \beta e_n(u)dU, \tag{9}
\]

where \( C_{ox} \) and \( C_x \) are the capacitances of the oxide and the depleted semiconductor, respectively, \( N_T \) is the surface concentration of captured carriers and \( \beta \) is the scanning rate of the temperature, linear in time, \( t \), such that \( T = \beta t \). The function given by Eq. (9) is plotted in Fig. 4(a) for an activation energy of 0.13 eV and an effective capture cross section of \( 10^{-22} \text{ cm}^2 \). Using the rather complicated expression in Eq. (8) for parameter extraction from experimental data is not practical. However, calculating the integral factor in this equation as a function of temperature, for the same input data as used above, one finds the graph shown in Fig. 4(b). It is noticed that the integral takes a value close to 1 for the initial part of the TSC curve in Fig. 4(a). Furthermore, as \( C_{ox} \gg C_s \) for the deep depletion conditions used in the experiment, this part of the experimental data is proportional to the thermal emission rate \( e_n \). Estimating the total concentration, \( N_T \), of trap levels from the area under the TSC peak, therefore, gives a possibility to find effective capture cross sections from Arrhenius plots of \( e_n \) [12].

### 3.3. Experimental TSC Results on the HfO_2/SiO_x Interface

Figure 5 shows experimental TSC data from electron emission at the transition region of an MOS capacitor with an Al/HfO_2/SiO_x/Si structure like the one shown by TEM in Fig. 2. Two important features can be observed in Fig. 5:

1) repeated measurement gives a different TSC peak position on the temperature scale;

2) the TSC curves are terminated before they reach the maximum point of the theoretical curves (solid curves) fitted to the experimental data.

These results are typical and occur for a large majority of the present samples with HfO_2 prepared by reactive sputtering as well as for samples prepared by atomic layer deposition (ALD) [25]. The observation (1), reveals an instability of the traps as mentioned above in relation to Eq. (9). Such instability after voltage stress under similar conditions as in the present experiment, was observed also by Bersuker et al. in [10]. The observation (2), can be interpreted as a result of the tunneling process involved in the electron emission. During the emission process, the negative charge in the transition region, born by the captured...
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Waiting time: 5 min, 1
Waiting time: 5 min, 2
Theory

Charging at 2 V
Discharging at -3 V
Temp. ramp of 20 K/min

Temperature [K]

\(50 \quad 75 \quad 100 \quad 125 \quad 150 \quad 175\)

\(0 \times 10^{-11} \quad 1 \times 10^{-11} \quad 2 \times 10^{-11} \quad 3 \times 10^{-11} \quad 4 \times 10^{-11}\)

Fig. 5. Experimental TSC data (points) for MOS structures with HfO\(_2\) prepared by reactive sputtering compared with theoretical calculations (solid curves) calculated from Eq. (9). Repeated measurement gave rise to a shift of the TSC peak along the temperature axis, reflecting structural changes of the emitting electron traps. The activation energy for the curves A and B is 0.13 eV and 0.16 eV, respectively, and the corresponding capture cross sections are \(6 \times 10^{-22} \text{ cm}^2\) and \(9 \times 10^{-21} \text{ cm}^2\), respectively.

electrons, will decrease. This will decrease the electric field driving the tunneling until the field strength is too weak for continued emission. As the tunneling probability is very sensitive to a change in electric field, the TSC will get an abrupt termination as shown for the two curves in Fig. 5.

4. Single Charge Versus Dipole Charge

The recent increasing interest in the properties of high-\(k\)/SiO\(_x\) transition layers includes novel ideas about a possible occurrence of closely separated charge planes with different polarities within this region [13]. It has been described as dipole planes occurring as a result of oxygen transfer across the interface between the high-\(k\) and the SiO\(_x\) material [14]. According to an idea proposed in [14], such transition would take place from the material with the highest surface density of oxygen atoms to that with lower density. For transition metal oxides, like HfO\(_2\), this would imply that oxygen is transferred from this material into SiO\(_x\), creating interstitials and leaving oxygen vacancies behind. As the relation between oxygen surface densities of rare-earth metal oxides, like Gd\(_2\)O\(_3\) and SiO\(_x\), is the opposite, such transfer would instead go from the SiO\(_x\) to the high-\(k\) side.

The influence of a single negative charge and a dipole surface on the conduction band relations for the metal/HfO\(_2\)/SiO\(_x\)/n-type Si structure is depicted in Fig. 6. The geometries are shown in Fig. 6(a), while Fig. 6(b) and Fig. 6(c) show the charge relations and the conduction band relations for an open circuit case and a short circuit case, respectively. In order to demonstrate the specific influences of these charge planes, we assume that no other charges are present in the structure. Considering first the single charge case in the left column of Fig. 6 for an open circuit case in Fig. 6(b), where the opposite positive charge is assumed to exist at a long distance, the electron energy of the whole structure is lifted in parallel in relation to an earth plane. Short circuiting, as shown in Fig. 6(c), will cause positive charge to appear at the metal gate and in the depletion region occurring in the n-type semiconductor. Compared with an ideal structure without charge, an increased positive voltage, \(V_{FB}\), on the gate would be needed to obtain flat-band condition for this case. Furthermore, \(V_{FB}\) would increase linearly with increasing thickness of the HfO\(_2\) layer.

Fig. 6. Illustration of (a) charge configuration, and conduction band relations for (b) open circuit and (c) short circuit conditions of a metal/high-\(k\)/SiO\(_x\)/Si structure. The columns demonstrate the conditions for a single charge plane (left) and a dipole plane (right), respectively.

For a dipole layer at the HfO\(_2\)/SiO\(_x\) interface, as shown in the right column of Fig. 6, under open-circuit conditions, one would expect an electric field between the two charge planes only (Fig. 6(b)). This would create a potential drop in that domain, while constant potentials would occur outside the two planes separated by a voltage created inside the dipole. Short-circuiting this structure gives rise to a positive charge on the gate and a negative charge in
the semiconductor, forcing the latter into accumulation condition. These two charges are exactly equal and vary depending on the HfO₂ thickness in such a way that the sum of the energy drops in HfO₂ and in the semiconductor is constant and equal to $qV_{FB}$. In this case a negative $V_{FB}$ equal to the potential drop inside the dipole, is needed to obtain flat-band conditions. However, contrary to the situation with a single negative charge, the dipole combination would give a $V_{FB}$ which is independent of the thickness of HfO₂. Such a behavior was indicated in [14] for HfOₓ/Siₓ interfaces.

The single charge case demonstrated by Fig. 6(a) offers a model for straightforward explanation of the anomalous TSC data as discussed in Section 3. The dipole case in Fig. 6(b) likewise gives rise to an energy relation of the conduction bands supporting electron injection into the silicon and thus a TSC with similar behavior as that from a single negative charge plane. Therefore, TSC does not give direct information on which of these two charge constellations is the source of current.

5. Discussion

In order to explain the saturating flat-band voltage and its positive sign as observed in [12] when increasing the thickness of HfO₂, the idea put forward in [13] requires injection of negatively charged traps from the high-k side into SiOₓ. This would give rise to a dipole directed in the opposite way to that discussed in relation to Fig. 6. Such a model is not completely unproblematic. First, injecting an oxygen ion from the HfO₂ into the SiOₓ layer might be expected to give rise to an interstitial, leaving behind a vacancy in the HfO₂. According to recent theoretical results [15], [16], vacancies are amphoteric and act as acceptors with energy levels at about 1.5 eV from the HfO₂ conduction band. They may therefore tend to be filled by electrons from the silicon conduction band and thus become negatively charged. On the other hand, the donor levels connected with oxygen vacancies are expected close to the middle of the bandgap of HfO₂ and are most probably occupied by electrons and neutral at voltages of the flat-band values at about 0.5 V in [13]. The origin of positive charge required on the HfO₂ side, therefore, is questionable.

A second problem with a dipole model may be the quantity of charge needed to obtain $V_{FB}$ shifts in the range of 0.3 – 0.5 V as observed in [13]. As the thickness of the SiOₓ layer normally is about 1 nm, the maximum value for the distance between the two charge sheets of an assumed dipole would be about that value. In order to achieve a shift of 0.3 V, this requires a charge density of more than $5 \times 10^{15}$ As cm⁻². It can be compared with the charge contained in the TSC curves of Fig. 5, which is in the range of $10^{13}$ As cm⁻². Finally, the strongest argument for a dipole model might be the saturating flat-band voltage. However, this result does not uniquely lead to a dipole configuration as shown in the following. Taking into account the continuous character of the transition region, a saturating $V_{FB}$ may result also from single charge condition. Contrary to the assumption made in [13], the transition from HfO₂ to SiO₂ cannot be considered abrupt on length scales in the range of a few nm. As noticed in Fig. 1, the oxygen concentration increases with distance from the silicon side due to diffusion into the silicon crystal. Similar behavior of oxygen concentration has been observed by elastic recoil detection analysis (ERDA) studies on HfPrO samples [26]. Therefore, it is reasonable to assume that the concentration of oxygen vacancies decreases with distance from the silicon side. Furthermore, assuming that thinner HfO₂ layers, due to the out-diffusion of oxygen to the surface, also as observed in Fig. 1, have a lower decay of vacancies, it is probable that they have a smaller decay in concentration.

![Fig. 7.](image)

A theoretical example is shown in Fig. 7(a), where the concentration of traps is plotted for different thicknesses as a function of normalized distance from a defined reference point in the transition region. Such a point could be the one, where SiO₂ transfers to suboxides. (b) The flat-band voltage as a function of HfO₂ thickness for acceptor concentrations as shown in (a) with the decay constant, $\alpha$, varying as a function of $x_h$ as shown in the inset of (b).
shown in the inset of Fig. 7(b). Solving Poisson’s equation for the functions in Fig. 7(a):

$$d^2V \over dx^2 = -\frac{\rho_0}{k\varepsilon_0} \exp\left(-\frac{x_h-x}{\alpha}\right),$$  \hspace{1cm} (10)

where $V$ is electrical potential, $\rho_0$ is the volume charge density at the reference point, $x_h$, $\varepsilon_0$ is the dielectric permittivity of vacuum and $x$ is distance from the HfO$_2$ surface, we find $V_{FB}$ from the potential at $x = 0$ as

$$k\varepsilon_0 V_{FB} = -\alpha \left\{ x_h + \alpha \left[ 1 - \exp\left(-\frac{x_h-x}{\alpha}\right) \right] \right\}. \hspace{1cm} (11)$$

The $V_{FB}$ normalized by the pre-factor in Eq. (11) is plotted in Fig. 7(b) as a function of HfO$_2$ thickness, $x_h$. The shape of this curve, with a tendency to saturate for increasing $x_h$, was interpreted in [12] as a result of a dipole layer. Figure 7(b) demonstrates that under assumptions based on MEIS data, it is possible to obtain similar behavior from a singly charged layer.

6. Conclusions

The theoretical TSC curves shown in Fig. 5 were calculated assuming an ensemble of electron states with one common discrete energy level. The agreement between the initial curvature of these graphs and the experimental data indicates that the majority of traps observed by TSC have similar properties of their charge carrier statistics and are positioned with limited spread in distance from the silicon/SiO$_2$ interface. This excludes bulk traps in the HfO$_2$ as candidates and suggests a trap distribution concentrated at the HfO$_2$/SiO$_2$ interface as depicted in Fig. 7(a) for delivering electrons to the TSC. Also, TSC peaks from states at the Si/SiO$_2$ interface are ruled out by earlier experiments as they have been demonstrated to occur at temperatures above 200 K, outside the scale of Fig. 5 [12]. The extremely low values of capture cross sections in the range $10^{-26}$ to $10^{-19}$ cm$^2$, normally found by TSC for this kind of experiments [11], [27], are explained by the tunneling process needed for carrier injection into the silicon substrate and the thermally activated process expected for carrier capture into oxygen vacancies [16]. Also, taking into account the flexible structural network anticipated in the transition region, the shift of the TSC peaks as shown in Fig. 5 may be assigned to the restructuring of oxygen vacancy defects as discussed in Section 2. The argument in [13], for the existence of a dipole plane at the interface between HfO$_2$ and SiO$_2$ layers, was based on the observation of flat-band voltage as a function of the thickness of HfO$_2$. It was shown that $V_{FB}$ saturated to a near constant value when this thickness increases as expected for a dipole charge and discussed above in connection with Fig. 6. However, such a result is not unique for a dipole. By assuming an oxygen vacancy distribution in the high-$k$ layer as estimated from MEIS data, we have demonstrated in the present work that similar $V_{FB}$ dependence may be the result of a single charge distribution. We conclude, therefore, that more evidence is necessary before the existence of a dipole layer occurring in high-$k$/SiO$_2$ transition regions is confirmed.

Acknowledgment

The authors collaborate under the banner of the “High-$k$-Gang” (http://www.high-k-gang.eu/). The work has benefited from funding provided by the European Network of Excellence NANOSIL within FP7 (ICT-216171).

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Note: this text is reprinted from JTIT 1/2010

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