

Modeling of Charge Trapping Induced Threshold-Voltage Instability in High- κ Gate Dielectric FETs

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Abstract—The authors have developed a distributed tunneling model to investigate the threshold-voltage instability induced by charge trapping in field-effect transistors (FETs) using high- κ gate dielectric materials. The charge trapping dynamics in the high- κ layer are modeled based on a rate equation, which is self-consistently incorporated into device-level simulations. The model is used to simulate pulsed operation of HfO₂ based n-type FETs; good agreement is obtained with pulsed measurements including the dependence of the threshold-voltage shift on pulse heights and durations. The trap-energy-level shift due to the polaron effect is found to be critical to model the pulse-height dependence of the threshold-voltage shift.

Index Terms—Charge trapping, field-effect transistors (FETs), hafnium dioxide (HfO₂), high- κ dielectric, tunneling.

I. INTRODUCTION

ELECTRICAL instability is one of the major concerns regarding high- κ -based field-effect transistors (FETs); threshold-voltage (V_T) shifts observed in pulsed measurements is considered to originate from the tunneling of channel electrons into traps in the gate dielectrics [1]–[3]. Of particular interest is the experimentally observed dependence of V_T shifts on the pulse-height and logarithmic stress time. The former effect has been suggested to be due to the relative shift of trap energy level with respect to the channel quasi-Fermi level as gate bias varies [1], and the latter effect has been attributed to the distributed bulk electron traps [2] based on the tunneling front model [4]. A distributed charge trapping/de-trapping model based on tunneling has also been presented by Leroux *et al.* [5]. Some other possible explanations may involve variable range hopping [6] or a continuous time random walk [7]. Although these theoretical models are useful for providing qualitative explanations, a device-level numerical model is nonetheless necessary to quantitatively analyze the origin and impact of the electrical instability in such multistack systems. In this letter, we present a self-consistent model that is capable of simulating pulsed operations of hafnium-based nFETs. A rate equation for the trap occupation factor is incorporated to simulate the

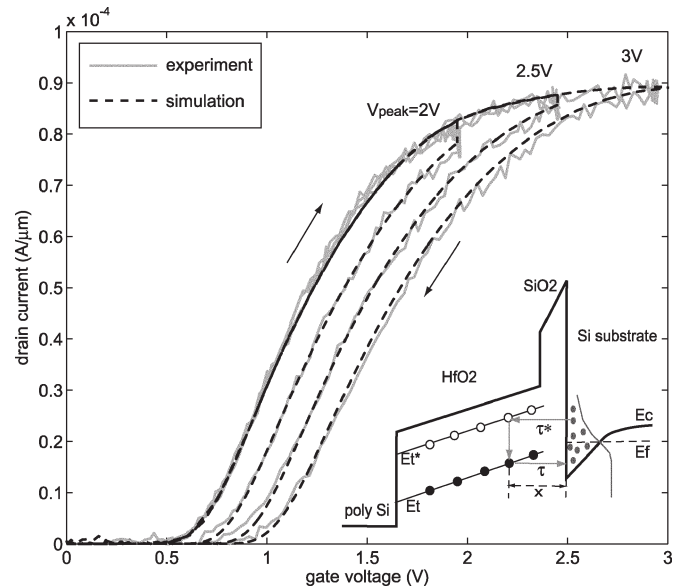


Fig. 1. Measured [2] (sample A) and simulated pulsed I_D - V_G curves for gate pulses with different pulse heights. The channel length of the HfO₂/poly-Si nFET is 1 μm and the drain voltage is 0.3 V. The base voltage of the gate pulses is 0 V. The inset is a schematic conduction band diagram perpendicular to the channel under inversion condition, where different empty and charged trap energy levels are considered.

dynamics of the charge exchange between the channel and the distributed bulk trap centers. The model accounts for the defect energy-level shift caused by the charge trapping (polaron effect), which has been studied based on first principle calculations [8]. Our treatment of the nonlocal tunneling process derives from a general approach originally proposed for Schottky barrier tunneling [9]. Simulation results are compared with measured data of the V_T shift and its dependence on pulse height and duration.

II. MODEL AND SIMULATION RESULTS

The band diagram of a multistack (Si/SiO₂/HfO₂/poly-Si) nFET under inversion conditions is illustrated in the inset of Fig. 1. In this letter, we only consider preexisting electron traps, which are regarded as the major cause of the V_T instability [3]. The electron-trap centers are distributed in the HfO₂ bulk region as well as in the HfO₂/SiO₂ interface [10]. The bulk traps result in a distribution of trapping time constants, which plays a key role in explaining the logarithmic stress-time dependence

Manuscript received February 9, 2006. The review of this letter was arranged by Editor K. De Meyer.

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Digital Object Identifier 10.1109/LED.2006.874760

of V_T shift [2]. Another fact of high- κ metal oxides is their large polarizability [11], indicating the presence of significant polaron effects in such materials. In the work of Torii *et al.* [8], the empty oxygen vacancies ($V_{O_{2+}}$) in HfO_2 were suggested to be responsible for the electron trapping; the polaron-induced defect level shift for V_{O+} and V_O were calculated by first principle method. A review on *ab initio* calculations of high- κ trap energy levels has been given in [10]. Based on those considerations, we developed a rate equation for distributed trapped electrons given by

$$\frac{dn_t}{dt} = \frac{n}{N_0} \cdot \frac{N_t - n_t}{\tau^*} \cdot \frac{1}{1 + \exp(E_t^* - E_f/kT)} - \frac{n}{N_0} \cdot \frac{n_t}{\tau} \cdot \left[1 - \frac{1}{1 + \exp(E_t - E_f/kT)} \right] \quad (1)$$

where n_t is the trapped electron density, N_t the density of the uniform bulk traps in HfO_2 , n the electron concentration in the channel, N_0 a unit normalization factor, E_t^* the empty defect level, E_t the occupied defect level, E_f the channel electron quasi-Fermi level. Here, we made a simplification to neglect the tunneling of trapped electrons to the gate, which is suppressed due to lowering of the charged trap levels. In this model, the electrons tunnel from the channel to the empty defect state and also from the occupied defect state back to the channel. The presence of the Fermi–Dirac distribution function is essential to correctly model the alignment between the trap energy levels and E_f at various gate biases. The two tunneling time constants, τ^* and τ , are obtained using the Wentzel–Kramer–Brillouin (WKB) approximation as follows [4]; for the forward tunneling process from channel to traps, it is given by

$$\tau^* = \tau_0 \cdot \exp \left[\frac{4\sqrt{2m_t^*m_0}}{3\hbar qE} \times \left((E_c^{\text{ox}} - E_t^* + qEx)^{3/2} - (E_c^{\text{ox}} - E_t^*)^{3/2} \right) \right] \quad (2)$$

where m_t^* is the tunneling effective mass, m_0 the free-electron mass, E the electric field, E_c^{ox} the oxide conduction band edge, x the depth of the trap into the oxide, and τ_0 a characteristic tunneling time that has only a weak dependence on x and E . A similar expression for the backward tunneling constant τ is obtained with E_t^* replaced by E_t .

The distributed tunneling model is essentially nonlocal from the device simulation viewpoint [9]. The simulation grid points in the channel are connected to those deep into the gate oxide by (1). This model is incorporated self-consistently with the carrier continuity and Poisson equations in a device simulator PROPHET [12]. Mobility degradation mechanisms of HfO_2 FETs have been discussed in [11] and [13], but a universal mobility model is not yet available; we have adopted the Darwish mobility model [14] with a constant 43% reduction applied. The implemented model is then used for two-dimensional simulations of nFETs with $\text{SiO}_2/\text{HfO}_2/\text{poly-Si}$ gate stacks. An EOT of 1.6 nm is used according to the experiments [2] and the SiO_2 interfacial layer thickness is set to be 0.5 nm. Default values for some simulation parameters include: 25 for the relative dielec-

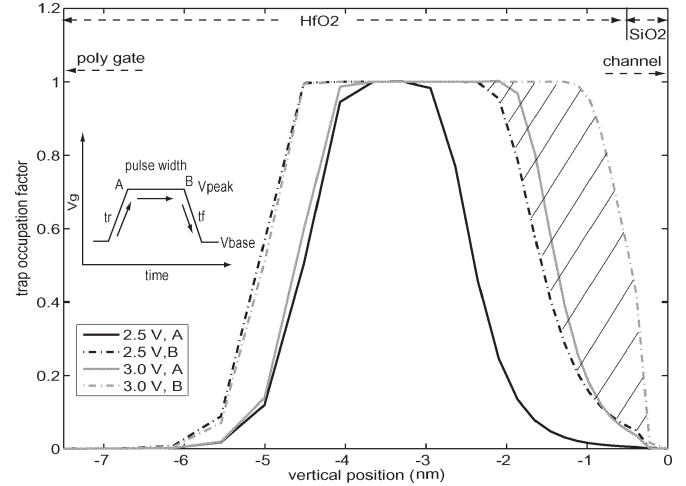


Fig. 2. Simulated profiles of trap occupation factor (n_t/N_t) inside the dielectric for two different pulse heights, each at points A and B of the pulse (labeled in the inset where a gate pulse is shown), respectively.

tric constant of HfO_2 [10]; 0.2 for m_t^* ; 10 ps for τ_0 ; $10^{19}/\text{cm}^3$ for N_0 ; and 1.4 eV HfO_2/Si conduction band offset. A fixed interface charge density $\sim 3 \times 10^{12}/\text{cm}^2$ is also considered. Unless otherwise noted, E_t^* and E_t are set to 0.4 and 1.4 eV below the HfO_2 conduction band minimum (CBM), respectively.

We conducted transient simulations with trapezoidal pulses applied at the gate. The pulsewidth is 200 μs and the rise and fall times are both 80 μs . Simulated I_D – V_G curves for different pulse heights (V_{peak}) are shown in Fig. 1, together with experimental data from pulsed measurements [2]. In the simulations, the total surface density of bulk traps is $1.2 \times 10^{13}/\text{cm}^2$. Quantitative agreement between simulations and data are obtained. The V_T shift reduces drastically with decreasing pulse heights. Fig. 2 shows the simulated spatial profile of trapped electrons for two pulses with different pulse heights, both at the beginning and the end of the pulse, respectively. The difference between the profiles at the end of the two pulses, as marked by the shaded region, corresponds to the difference in V_T shifts. This portion of the traps is only accessible to the channel electrons at $V_G = 3$ V but not to those at $V_G = 2.5$ V within the given pulse duration. As illustrated in the inset of Fig. 1, this is mainly due to the relative alignment between the trap energy level and the channel electron quasi-Fermi level.

The correlation between trap energetics and V_T shift has also been studied. Fig. 3 shows simulated peak voltage dependence of the V_T shift for different values of E_t^* and E_t . Simulation results agree with measured data for $E_t^* = -0.4$ eV and $E_t = -1.4$ eV with respect to HfO_2 CBM. These values are close to those of the oxygen vacancy-related defects from first principle calculations (0.3, 1.3, 1.6 eV below CBM for $V_{O_{2+}}$, V_{O+} , and V_O , respectively [8]), corroborating their assumed role in electron trapping. More severe V_T shifts are found for lower E_t^* levels because of larger trap occupation factors. The necessity of modeling the polaron effect is evidenced by setting $E_t^* = E_t$ in the simulation. Here, the simulated V_T shift is significantly reduced and it has a much weaker dependence on V_{peak} . This is because, without considering the defect energy-level shift, the reversible tunneling process would cause significant tunneling of trapped electrons back into the channel during

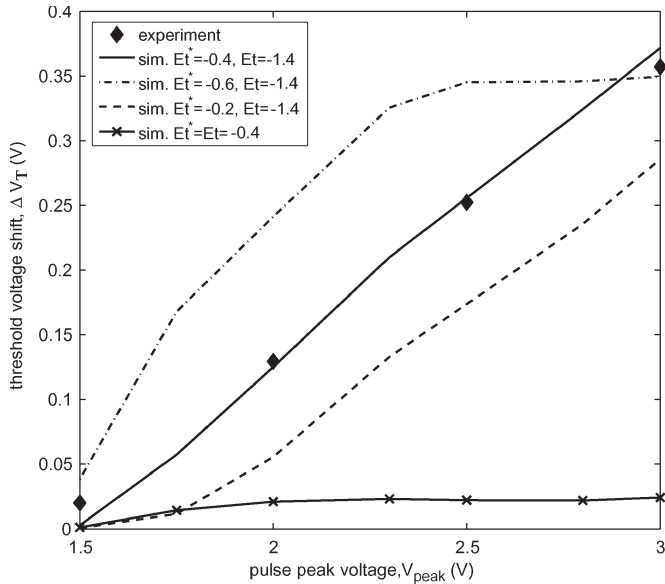


Fig. 3. Measured [2] (sample A) and simulated threshold-voltage shift as a function of the pulse height. Different empty and charged trap energy levels are used in the simulations. The energy reference is the HfO_2 CBM and the energy unit is eV.

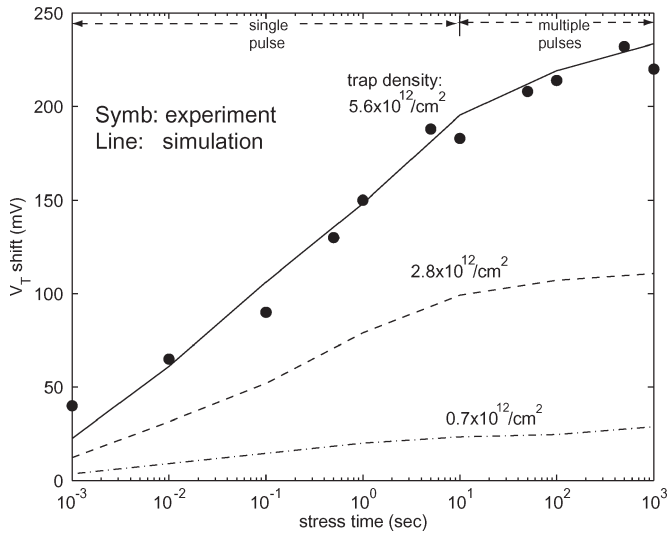


Fig. 4. V_T shift versus stress time for a HfO_2 /poly-Si gate nFET under constant voltage stress from both experimental measurement [2] (sample B) and transient simulations. The stress voltage is 2.5 V.

the pulse falling edge. Such an effect is prominent when the duration of the falling edge is comparable to that of the pulse peak. Therefore, we need to account for the polaron effect to explain the observed V_{peak} dependence of V_T shift.

We also investigated the dependence of the V_T shift on stress time under constant voltage stress. Both the experimental data [2] and simulated results are plotted in Fig. 4. In the measurements, the single-pulse technique was used for stress times up to 10 s and the multiple-pulse technique was used above that. Lower trap densities lead to reduced V_T shifts, as shown by the simulations. A logarithmic stress-time dependence of the V_T shift can be seen for several decades with only moderate saturation at the very long stress times. This trend agrees well with the experimental data, strongly suggesting the

presence of distributed trapping time constants as proposed in the “tunneling front” theory [4].

III. CONCLUSION

We have developed a numerical model to self-consistently simulate the charge trapping dynamics in hafnium-based FETs and their impact on threshold-voltage instability. Simulation results based on this model quantitatively agree with data from pulsed measurements, including dependence of threshold-voltage shifts on pulse height and duration. Accounting for the defect energy-level shift due to charge trapping is found to be critical in modeling these effects. Simulations support theoretical predictions that oxygen vacancy related defects are probably responsible for the electron trapping in such devices.

ACKNOWLEDGMENT

Y. Liu and R. Dutton would like to thank MARCO Materials Structures and Devices (MSD) Focus Center as well as the Stanford Center for Integrated Systems (CIS) customized research program for research support.

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