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Theoretical insights into the impact of border and interface traps on hysteresis in monolayer MoS₂ FETs

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<i>Keywords:</i> 2D FET Hysteresis CMOS Reliability Physics-based models	Threshold voltage hysteresis (ΔV_h) in two-dimensional transistor transfer characteristics poses a bottleneck in achieving stable 2D CMOS integrated circuits. Hysteresis is primarily attributed to traps at the channel/oxide interface as well as in the oxide. In this study, we present a physics-based self-consistent modeling framework to investigate the impact of border and interface traps on ΔV_h and apply it to monolayer (1-L) MoS ₂ field-effect transistors (FETs). The transient trapping and detrapping of charges during gate voltage sweeps across a wide range of frequencies and temperatures is analyzed using a two-state non-radiative multi-phonon (NMP) model. Our results reveal distinct dynamic responses for slow border and fast interface traps, with border traps exhibiting slower time constants due to larger relaxation energies and interface traps showing fast nuclear tunneling-dominated dynamics resulting from the smaller relaxation energies. These simulations highlights the critical role of the spatial and energetic distributions of the traps in determining ΔV_h , providing insights into the stability of 2D EETs and paving the way for improved device engineering

1. Introduction

For the continuation of Moore's law into the sub-decananometer regime, the use of two-dimensional (2D) materials has been suggested [1–3]. Among them, two-dimensional molybdenum disulfide (2D MoS₂) is widely studied as a promising channel material for atomically scaled transistors [4,5]. In contrast to conventional silicon technology, mono-layer (1-L) MoS₂ offers a sizeable mobility at atomic thinness, ideally a clean surface, as well as direct electronic band gap. This was first demonstrated by Radisavljevic et al. in 2011 by integrating a 1-L MoS₂ with a double gated FET architecture [6]. These devices exhibited ON-OFF current ratios of about 10^8 and a sub-threshold swing (SS) of 74 mV/dec.

While 2D FETs show promising electrical and mechanical properties, their stability and reliability has not yet met the rigorous standards set by silicon technologies [7]. Most importantly, due to material quality issues and unfavorable electronic band alignments, 2D FETs exhibit threshold voltage ($V_{\rm th}$) drifts in the $I_{\rm D}(V_{\rm G})$ transfer characteristics as a result of charge trapping from pre-existing oxide traps [8–10]. Such instabilities pose a challenge for achieving stable 2D complementary metal-oxide semiconductor (CMOS) technology. The resulting

electrostatic degradation highlights the sub-par quality of current 2D channel/oxide interfaces and the significant trap density in gate insulators deposited on the 2D materials as a result of the weak out-ofplane van der Waals interactions [8]. It is well-known that one of the primary reasons for the observed threshold voltage hysteresis ($\Delta V_{\rm h}$) in the $I_D(V_G)$ up/down gate voltage sweep originates from charge carriers being trapped at localized trap states. However, ΔV_h is sensitive to the spatial and energetic position of these traps within the oxide. In this context, traps can be classified into slow border and fast interface traps. Oxide traps located within a few nanometers from the channel are referred to as border traps. Their energy levels, relaxation energy and spatial distribution results in broad time constant (τ) distributions. Particularly in amorphous insulators such as HfO₂ and Al₂O₃, these distributions can be exceptionally wide. On the other hand, traps in the channel have a narrow τ distribution due to the more crystalline environment. In addition, the time constants are typically much smaller since the charge carriers are in very close vicinty to the traps. Extensive studies on these border and interface traps were conducted by Fleetwood et al. on the conventional Si/SiO₂ system [11]. Similarly, a comprehensive physics-based framework is needed to understand the impact of border and interface traps on the stability of 2D channel/oxide

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systems.

In our recent study [12], we have reported a physics-based modeling technique for border and interface traps and their impact on $\Delta V_{\rm h}$ in 1-L MoS₂ FETs. Although the study used suitable trap relaxation energies $(E_{\rm R})$ and trap level $(E_{\rm t})$ for modeling the traps, an in-depth investigation of the factors affecting ΔV_h is required. In this study, we employ a selfconsistent modeling approach using our 1-D TCAD simulator Comphy [13,14]. Slow border and fast interface traps are modeled using available trap parameters from literature [15,16]. We employ a two-state non-radiative multi-phonon (NMP) model in the simulation framework to describe transient trapping/detrapping of charges. We analyzed $\Delta V_{\rm h}$ dynamics over a wide range of sweep frequencies $(1/t_{\rm sweep})$ to develop a closer understanding of the intricate trapping/detrapping dynamics. While it is commonly suggested that interface traps are too fast for observable $\Delta V_{\rm h}$ [17], our dynamic simulations show that degradation from some interface traps could be measured at lower temperatures.

2. Device under test and simulation framework

In this study, an example 1-L MoS₂ FET is analyzed within the simulation framework. The device schematic is illustrated in Fig. 1(a). The device architecture employs an atomically thin 1-L MoS₂ with an electronic band gap of 2.06 eV [18-20], deposited on 12 nm thick hafnium dioxide (HfO₂) along with a 4.3 nm thick HfO₂ layer on top of the 1-L MoS₂ acting as a top gate (TG) insulator. The work function (E_w) of the palladium TG is assumed to be 5.2 eV [21]. The device dimensions are identical with our previous work [12] with $W=1 \mu m$ and $L=5 \mu m$. The electronic band gap of HfO₂ is 5.7 eV [22]. Furthermore, the electron affinity (χ_s) of 1-L MoS₂ and HfO₂ is set to 4.2 eV [23] and 2.7 eV [24] respectively. The carrier mobility is assumed to be 80 cm²/Vs along with an electron mass (m_e^*) of 0.56 and a hole mass (m_h^*) of 0.55 [25]. The device $I_D(V_{TG})$ is evaluated with $V_{TG} \in [-1.5 \text{ V}, 2 \text{ V}]$ for increasing drain voltage $V_D \in [0.01 \text{ V}, 0.5 \text{ V}]$ in Fig. 1(b) and (c) at room temperature. In this 1D compact model, the $I_{\rm D}(V_{\rm TG})$ characteristics are obtained by using an analytic drift-diffusion based approach described in [26].

3. Physics based modeling

The time-dependent threshold voltage drift (ΔV_{th}) in the $I_{\text{D}}(V_{\text{TG}})$ is modeled using the NMP model. In our 1D model, the ΔV_{th} that results from the capture of a single electron is evaluated using the charge sheet approximation (CSA) that assumes a uniform distribution of the net oxide charge (Q_{t}) parallel to the channel/oxide interface at a distance (x_{T}):

$$\Delta V_{\rm th}(t) = -Q_t \left(1 - \frac{x_T}{t_{\rm ox}} \right) \frac{t_{\rm ox}}{\epsilon_0 \epsilon_r WL} \tag{1}$$

Here, the net oxide charge (Q_t) is determined by the elementary charge multiplied by the trap occupation probability, t_{ox} represents the oxide thickness, ϵ_0 is the vacuum permittivity and ϵ_r is the relative permittivity of the oxide. The NMP model approximates the two different trap charge states as parabolic energy curves (PECs) shown in Fig. 2, where a trap is characterized by E_R , E_T , x_T and the PEC minima offset (ΔQ) [13,27,28]. In the classical limit, the charge transfer between the trap and the reservoir occurs by overcoming a thermal barrier (ϵ_{12}) given by the intersection points of the PECs. This thermal barrier is governed by the parameters introduced above. The charge transition rates (k_{12}) depend exponentially on the thermal barriers and are given by [13,14,28]:

$$k_{12} = n v_{\rm th} \sigma \vartheta e^{-(\epsilon_{12} - E_{\rm F} + E_{\rm CB})/k_{\rm B}T}$$
⁽²⁾

where *n* represents the channel electron density, $v_{\rm th}$ is the thermal velocity, σ denotes the capture cross section, $E_{\rm F}$ is the Fermi level in the channel, $E_{\rm CB}$ is the channel conduction band energy and ϑ is the Wentzel-Kramers–Brillouin (WKB) tunneling coefficient. It is important to note that the trap occupation probability is a function of k_{12} which then influences $\Delta V_{\rm th}$. To model the border traps in HfO₂, the previously extracted trap parameters $E_{\rm T}=1.9$ eV above MoS₂ valence band maxima (VBM), $E_{\rm R}=1.2$ eV and $\Delta Q=3$ amu^{1/2}Å were used [15,16,28] along with $\sigma_{\rm E_{\rm T}}$ and $\sigma_{\rm E_{\rm R}}$ of 0.1 eV and 0.3 respectively [29]. Typically, traps located within the first few nanometers of the oxide contribute to an observable $\Delta V_{\rm h}$. Fig. 2(a) shows the PECs of both states (1 and 2) with an



Fig. 1. (a) 3-D schematic of the 1-L MoS₂ FET. Simulated I_D(V_{TG}) characteristics for increasing drain voltages (V_D): (b) linear scale, (c) logarithmic scale.



Fig. 2. Configuration coordinate diagram and the associated parameters (E_R , E_T , x_T , ΔQ) defining charge exchange within the harmonic approximation for (a) a border trap (b) an interface trap used in the NMP model. C_1 , C_2 are the curvatures, R is the ratio of curvatures and ΔE is the energetic difference of the two PECs.

intersection between the two minima, indicating the strong electronphonon coupling regime which is well described by Eq. (2). The comparatively large $E_{\rm R}$ of traps in the oxide together with the tunneling distance $x_{\rm T}$ leads to slower trap dynamics.

However, interface traps are right at the channel/oxide interface, meaning that $x_T=0$. In addition, since the channel is crystalline, E_R is small [30]. This typically results in weak electron-phonon coupling. To model interface traps, we use parameters typically for sulfur vacancies in MoS₂, $E_T=1.5$ eV above MoS₂ VBM and $E_R=0.1$ eV [12,30]. Compared to border traps, a much smaller value of σ_{E_T} , 0.05 eV is used. Hereby ΔQ is the crucial parameter as its value determines the nuclear tunneling

probability which can (in many cases) be larger than the low probability to go over the thermally activated intersection point [13,28] as shown in Fig. 2 (b). Here, we use $\Delta Q = 1 \text{ amu}^{1/2} \text{ Å}$ [28,31]. In this regime, Eq. (2) cannot be used. Instead, full quantum mechanical (QM) charge transition rates $\left(k_{12}^{\text{QM}}\right)$ based on Fermi's golden rule have to be used [32]:

$$k_{12}^{\rm QM}(T) = \frac{2\pi}{\hbar} |\theta_{12}|^2 \frac{1}{Z} \sum_{a\beta} \left| \left\langle \eta_{1a} | \eta_{2\beta} \right\rangle \right|^2 \delta \left(E_{1a} - E_{2\beta} \right) e^{-E_{1a}/k_B T}$$
(3)

where θ_{12} represents the electronic matrix element, $E_{1\alpha}$ and $E_{2\beta}$ are the vibrational eigenenergies of each charge states. Here, the eigenenergy indices are denoted as α and β , $\eta_{1\alpha}$ and $\eta_{2\beta}$ are the vibrational wave functions and Z is the canonical partition function. The parameters used are consistent with the crystalline nature of the semiconductor (here 1-L MoS₂), which means that smaller $E_{\rm R}$ increases overlapping of the vibrational wave functions, allowing nuclear tunneling-mediated charge state transitions.

The impact of the gate bias on the trap occupation is shown in the energetic band diagrams in Fig. 3. Note that the border trap band is located within the MoS₂ electronic band gap. In Fig. 3(a), as V_{TG} becomes more positive, the border trap band bends downward, resulting in an increased number of trapping events within the oxide. On the contrary, since there is no spatial distribution of the interface traps as shown in Fig. 3(b), the trapping events are mostly independent of the oxide electric field ($F_{\rm ox}$). A border trap density ($N_{\rm bt}$) of 10^{19} cm⁻³ based on earlier studies [29] and an interface trap density $(N_{\rm it})$ of 10^{12} cm⁻² [25] is used in our simulations. The density of the occupied traps increases when the Fermi level $(E_{\rm F})$ is swept across the band gap, shifting $V_{\rm th}$ during the corresponding up/down sweep. $\Delta V_{\rm h}$ is extracted at $1/t_{\rm Sweep}$ = 10^3 Hz, shown in Fig. 4. Here, t_{Sweep} represents the sweep time for a complete up (V_{up}) and down sweep (V_{down}) . To establish a consistent extraction method, a current criterion of $10^{-5} \,\mathrm{mA}/\mu\mathrm{m}$ is used. ΔV_{h} is extracted using this criterion by interpolating V_{up} and V_{down} near V_{th} . Fig. 4 (a) shows an observable $\Delta V_h \approx 18.6 \text{ mV}$ for the slow border traps while a significantly smaller $\Delta V_h \approx 0.01 \text{ mV}$ is obtained from the fast interface traps in Fig. 4 (b). The capture (τ_c) and emission (τ_e) time



Fig. 3. Energy band diagram representing electron trapping in 1-L MoS_2/HfO_2 with suitable E_T for (a) border traps (b) interface traps.



Fig. 4. ΔV_h extraction from the $I_D(V_{TG})$ profiles for (a) border traps and (b) interface traps. The capture and emission time constants for a single trap as a function of V_{TG} for (c) a selected border and (d) interface trap at room temperature.

constants as a function of V_{TG} are investigated for a selected border and interface trap in Fig. 4 (c) and (d), respectively. Traps can only actively contribute to ΔV_{h} if they can capture an electron during the up sweep but are too slow to emit it during the down sweep. In other words, this requires $\tau_{\text{c}} < \tau_{\text{e}}$ at the highest V_{TG} and $\tau_{\text{c}} > \tau_{\text{e}}$ at the lowest V_{TG} [25]. As discussed above, the slow border traps are associated with larger τ distributions which is consistent with Fig. 4 (c). Unlike slow border traps, fast interface traps can exchange carriers instantly with the semiconductor bands via nuclear tunneling, meaning that τ_{e} is independent of F_{ox} as shown in Fig. 4(d).

To study the complete ΔV_h dynamics, it has been suggested to consider a wide range of $1/t_{Sweep}$ [10,12,33,34]. In this work, we used $1/t_{Sweep} \in [10^{-6} \,\mathrm{Hz}, 10^{9} \,\mathrm{Hz}]$ for the theoretical analysis with an assumed measurement window of $1/t_{\text{Sweep}} \in [10^{-4} \text{Hz}, 10^{4} \text{Hz}]$ [10,33,34]. ΔV_h , when evaluated across a wide range of $1/t_{Sweep}$ values typically yields a bell-shaped curve. At slow $1/t_{Sweep}$, the traps remain close to their equilibrium state at every bias condition, which results in a small $\Delta V_{\rm h}$. A small $\Delta V_{\rm h}$ is also observed at fast enough $1/t_{\rm Sweep}$ since there is insufficient time for charge trapping/detrapping. Hence, $\Delta V_{\rm h}$ at the peak $1/t_{\text{Sweep}}$ is the combination of suitably fast and slow sweeps. Fig. 5 (a)-(c) focuses on the dynamic response of $\Delta V_{\rm h}$ as a function of $1/t_{\rm Sweep}$ across different temperatures. Contrary to the slow border traps (blue line), the $\Delta V_{\rm h}$ from fast interface traps (red line) lies mostly outside the measurement window for the studied temperatures. Notably, the validity of the NMP model at $1/t_{Sweep} > 1$ MHz remains uncertain due to factors such as the failure of the drift-diffusion model [35] and the frequency dependence of the permittivity [36]. Based on [37], the $\Delta V_{\rm h}$ shift across $1/t_{Sweep}$ with temperature can be explained from the temperature



Fig. 5. Extracted ΔV_h vs. $1/t_{\text{Sweep}}$ for slower border (blue) and fast interface (red) traps at (a) 200 K (b) 300 K and (c) 400 K. Shaded regions show the $1/t_{\text{Sweep}}$ space outside the measurement window. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

dependence of the time constants. Therefore, an increase in the temperature reduces τ , making the traps faster thereby shifting ΔV_h towards faster $1/t_{\text{Sweep}}$. A key takeaway is that the Gaussian tail for the interface traps ΔV_h can shift inside the measurement window at lower temperatures, meaning that device degradation due to fast interface traps could be measurable at lower temperatures.

4. Conclusions

In this work, we have employed a physics-based self-consistent modeling framework to investigate the impact of border and interface traps on ΔV_h in 1-L MoS₂ FETs. Our simulations reveal that the spatial and energetic position critically influence their dynamic behavior. Border traps exhibit slower time constants due to large thermal barriers resulting from the large E_R , while the small E_R of interface traps results in the dominance of nuclear tunneling and shorter time constants. These findings provide a detailed understanding of the mechanisms governing ΔV_h , offering clarity on why border traps dominate within the typical measurement window, while interface traps can only contribute under specific conditions, such as lower temperatures or high sweep frequencies. Overall, the modeling approach presented lays the foundation for future studies exploring hysteresis phenomena in other 2D material systems or more complex device architectures.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Rittik Ghosh reports financial support was provided by TU Wien University. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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