Modeling of Oxygen-Vacancy Hole Trap Activation in 4H-SiC MOSFETs using Density Functional Theory and Rate Equation Analysis

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***Abstract*—A plausible Density Functional Theory (DFT)-based Oxygen Vacancy (OV) hole trap activation model was recently proposed to explain the High Temperature-Gate Bias (HTGB) stress-induced additional threshold voltage instability in 4H-Silicon Carbide (4H-SiC) power MOSFETs. In this model, certain originally electrically 'inactive' OVs were shown to structurally transform over time to form switching oxide hole traps during HTGB stressing. Here, we use this model to perform transient simulation of the buildup of hole-trapped OVs in HTGB-stressed 4H-SiC power MOSFETs. This is shown to correlate well with the recently observed excessive worsening of threshold voltage instability in HTGB-stressed 4H-SiC power MOSFETs. This helps to validate the role of OVs in the degradation of high-temperature reliability of these devices.**

Keywords—oxygen vacancy; density functional theory; threshold voltage instability; Silicon Carbide; MOSFET reliability

I. Introduction

The state-of-the-art 4H-Silicon Carbide (4H-SiC) power MOSFETs, which are promising for electronic applications at elevated temperatures and power levels, are plagued by poor High Temperature-and-Gate Bias (HTGB) reliability. For example, excessive aggravation in threshold voltage (V_{th}) instability has been recently reported in devices operated at high temperatures (T>125°C) [1]. Here, V_{th} instability was seen to vary super-linearly with the logarithm of applied stress time. This is in clear contrast to the nature of instability observed in room temperature measurements, where ΔV_{th} was observed to vary linearly with the logarithm of applied stress time [2, 3]. The fundamental mechanisms of these differing behaviors are not completely understood.

Near-interfacial Oxygen Vacancies (OV), located in SiO_2, have been traditionally acknowledged to act as switching oxide hole traps, causing room-temperature (RT) V_{th} instability in 4H-SiC power MOSFETs (the HDL model) [2-5]. Here, holes are considered to be exchanged between the OV hole traps and the substrate, through direct tunneling, in response to applied bias stresses. Recently, a two-way direct tunneling model was developed to explain this phenomenon [6]. Additionally, this model explained the experimentally observed linear relationship between the measured room-temperature threshold voltage instability and the logarithm of applied bias stress duration [2]. However, the recently-observed super-linear dependence of high-temperature V_{th} instability on the log of applied stress time merits detailed investigation [1].

In our previous work [7], we had proposed a DFT-based model for plausible OV hole trap activation in 4H-SiC MOSFETs stressed under HTGB conditions. According to this model, certain originally electrically 'inactive' oxygen vacancies could be structurally transformed into electrically 'active' switching oxide hole trap configurations during HTGB stressing of 4H-SiC power MOSFETs.

In this paper, we perform detailed transient modeling of the HTGB-induced V_{th} instability by invoking the oxygen vacancy hole trap activation model. We use Density Functional Theory (DFT)-based minimum energy pathway calculations to calculate the related activation barriers. This model is in agreement with the experimentally measured V_{th} instability behavior observed during HTGB stressing of 4H-SiC power MOSFETs, and helps to validate the role of OVs in high-temperature reliability degradation.

II. Amorphous Silica Model Generation

Our density functional analysis on oxygen vacancies, and related calculations (like minimum energy pathways for structural transformations) are carried out in 72-atom amorphous silica (a-SiO_2) models, which are generated using two types of methods. The first method involves the traditional melt-and-quench quantum molecular dynamics. Here, a 72-atom α-quartz model [8] is rapidly cooled from its molten state at 4000K to 300K through 3000K, 2000K, and 1000K. At each temperature, the trajectories of the atoms were determined for a period of 1ps (in steps of 2fs) by solving their equations of motion based on DFT-calculated forces. The model generated using this method does not have 'bond switches' with respect to α-quartz.

The second method for amorphous silica generation employs a novel approach called the Sequential Back-bond Break (SBB) methodology. A detailed description on this method is provided in Ref. [7]. Here, we briefly summarize it. Firstly, an arbitrarily selected Si-O-Si bridge in α-quartz model

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is broken between O-Si, and the Si atom is artificially puckered backwards to back-bond with an oxygen atom located behind it. This results in a 'dangling' oxygen, and a triply coordinated oxygen in the model. In order to restore the local coordination of the triply coordinated oxygen, one of its original bonds with Si is broken, after which, the Si atom is puckered to form a new triply coordinated Oxygen. This process of propagating the three-fold oxygen is continued till the end of the periodic supercell, where the final Si puckering would result in its bonding with the original 'dangling O' atom. In this work, we apply this process four times to generate an amorphous silica model (72-atom). This is shown in Figure 1(a). Moreover, this model has bonds 'switched' or reorganized with respect to α-quartz.

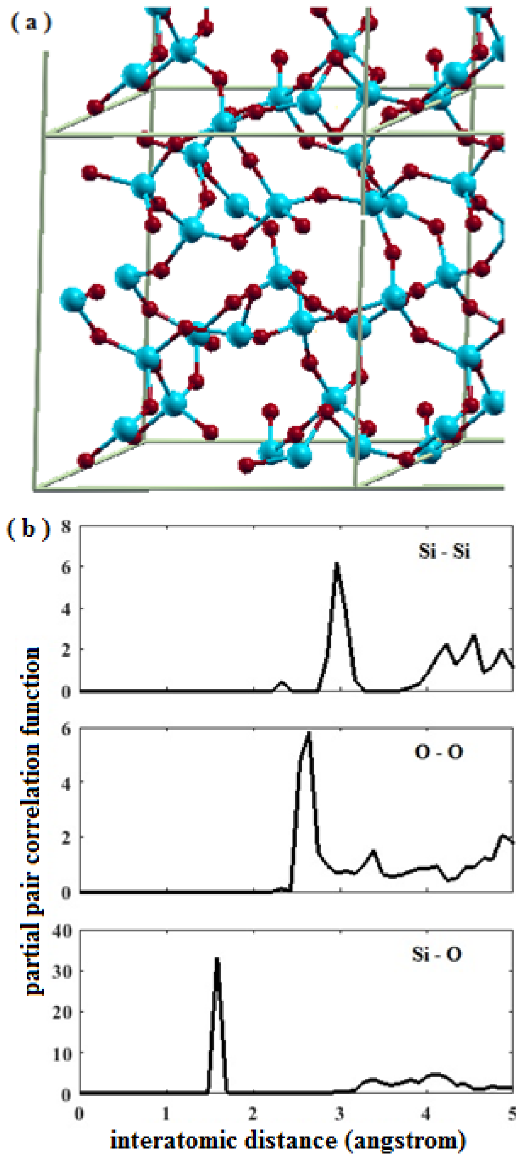

Fig. 1. a) An amorphous silica model generated using the SBB method, representing 'bond-switched' oxide regions. b) partial pair correlation functions for the a-SiO_2 model.

The bond length and bond angle distributions of the SBB-generated a-SiO_2 models were analyzed in Ref. [7]. Here, we study the structural properties of the model using its partial pair correlation functions. Our results are depicted in Figure 1(b). The first major peak in the Si-Si pair correlation function was observed at 2.96Å. The tiny peak at 2.32Å is attributed to a two-membered ring. The O-O and Si-O pair correlation functions indicated first peaks at 2.65 Å and 1.59 Å respectively. These results are in reasonable agreement with previous reports [9], and help to validate the SBB approach. However, owing to the relatively small size of the silica model used in this study, further work would be helpful to confirm the result presented here.

III. Oxygen Vacancy Hole Trap Activation Model-Background

In our previous work [7], the electrical properties of oxygen vacancy defects were studied through their DFT-based Charge Transition Levels (CTL). The defect was interpreted to be electrically active if its CTL occurred within the 4H-SiC bandgap (after 4H-SiC/SiO_2 bandgap alignment [10]). Here, we briefly summarize our results to set a background for the transient modeling of OV hole trap activation model [7], which is discussed in the next section.

OVs were studied in a-SiO_2 models generated using both SBB method (SBB models) and MD method (MD model). This throws light on the effect of bond-switching on their electrical properties. Structurally, the dimer OVs in the SBB model were seen to behave differently from those in MD model during hole capture, as indicated in Figures 2 and 3 respectively. While the former spontaneously converted into a +1 forward-projected back-bonded (fp-bb) state upon hole capture, the latter resulted in a +1 dimer state [4]. However, the +1 dimer in the MD model could be converted into +1 fp-bb state by overcoming a thermal barrier. Alternatively, both the OVs could also be thermally transformed into back-projected back-bonded (bp-bb) configurations during hole capture, as in Figures 2 and 3 [11].

Next, we consider the electrical activity of the two distinct OVs in their different structural configurations (dimer, fp-bb, bp-bb). For all the oxygen vacancy configurations that were generated in the SBB model representing 'bond-switched' oxide regions (Figure 2), the +1/0 CTLs were seen to occur well within the bandgap of 4H-SiC. This indicated that they could behave like electrically 'active' switching oxide hole traps, and potentially contribute to room-temperature V_{th} instability in 4H-SiC power MOSFETs.

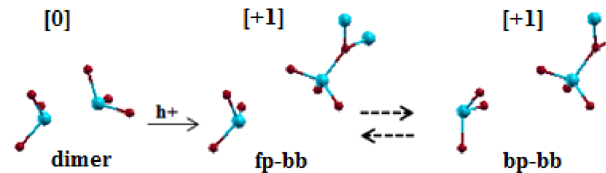

Fig. 2. Structural behavior of 'electrically active' OV during hole trapping. This is seen in the SBB model representing bond-switched oxide regions. fp-bb represents forward-projected back-bonded structure. bp-bb represents back-projected back-bonded configuration. Broken arrow indicates thermal transformations. Blue- Silicon, Red-Oxygen.

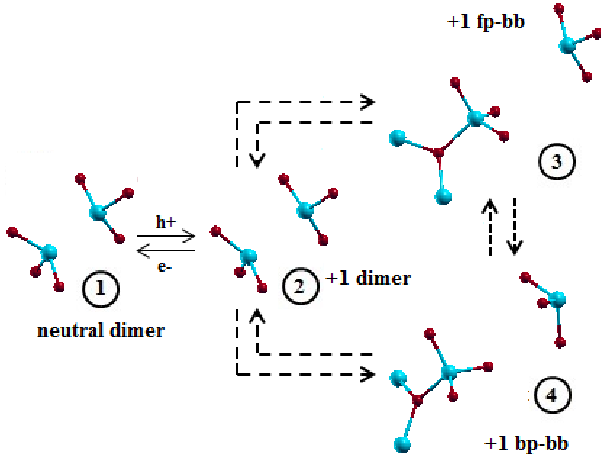

Fig. 3. Structural behavior of 'electrically inactive' OV during hole trapping and HTGB-assisted thermal activation. This is seen in the MD model representing 'non-bond-switched' oxide region. fp-bb represents forward-projected back-bonded structure. bp-bb represents back-projected back-bonded configuration. Broken arrows indicate thermal transformations. Blue- Silicon, Red-Oxygen.

On the other hand, the +1/0 CTL of the OV dimer in the MD model (Figure 3) occurred at ~ 0.8-1.1eV *below* the 4H-SiC Valence Band Edge (VBE). Thus, these OVs in the 'non-bond-switched' oxide regions are unlikely to trap/de-trap holes in 4H-SiC MOSFETs at room temperature, rendering them electrically 'inactive'. However, its higher energy fp-bb and bp-bb configurations (Figure (3)), which could be achieved by overcoming thermal barriers, were found to be electrically 'active' with respective +1/0 CTLs located within the 4H-SiC bandgap. This indicates that these originally electrically 'inactive' OVs could be structurally transformed into electrically 'active' configurations under HTGB stresses.

IV. Transient Modeling of Hole Trap Activation

We modeled the transients of the activation of electrically 'inactive' OV defects to form electrically 'active' hole traps during HTGB stressing of 4H-SiC power MOSFETs. The various configurations involved in the process are indicated in Figure 3. The structural transformations were modeled as Arrhenius processes. The minimum energy pathway and the thermal barriers for the structural transformations were ascertained using the climbing-image Nudged Elastic Band (NEB) method [12]. Furthermore, initial hole capture by the electrically 'inactive' dimers was modeled as Shockley-Reed-Hall tunneling.

The instantaneous fractional population of various positively charged configurations (Figure 3) is determined by simultaneously solving the following differential equations [5].

$$\frac{dx_1}{dt} = -k_{12}e^{\frac{-E_{12}}{kT}}x_1 + k_{21}e^{\frac{-E_{21}}{kT}}x_2 \quad (1)$$

$$\frac{dx_2}{dt} = -\left(k_{21}e^{\frac{-E_{21}}{kT}} + v_0e^{\frac{-E_{23}}{kT}} + v_0e^{\frac{-E_{24}}{kT}}\right)x_2 + k_{12}e^{\frac{-E_{12}}{kT}}x_1 + v_0e^{\frac{-E_{32}}{kT}}x_3 + v_0e^{\frac{-E_{42}}{kT}}x_4 \quad (2)$$

$$\frac{dx_3}{dt} = -\left(v_0e^{\frac{-E_{32}}{kT}} + v_0e^{\frac{-E_{34}}{kT}}\right)x_3 + v_0e^{\frac{-E_{23}}{kT}}x_2 + v_0e^{\frac{-E_{43}}{kT}}x_4 \quad (3)$$

$$x_1 + x_2 + x_3 + x_4 = 1 \quad (4)$$

We then translated the accumulated positive charge ($\sum_i x_i$, i=2,3,4) into V_{th} instability as a function of time, using the following relation.

$$|\Delta V(t)| = \frac{q\, t_{ox}\, N\, (\sum_{i=2}^{4} x_i\,(t))}{\varepsilon_{ox}} \quad (5)$$

The calculated ΔV_{th}, which agreed well with the experimental results as shown in Figure 4, serves to validate the OV hole trap activation model. The barrier energies used in equations (1) to (3) to obtain agreement with experiment are generally supported by our DFT-based NEB calculations. They are indicated in Table 1. The disagreement in barriers suggests that additional stabilization processes are possibly involved in OV hole trapping processes. This requires further investigations.

V. Conclusion

The oxygen vacancy hole trap activation model could provide a plausible explanation for the recently observed excessive aggravation in V_{th} instability in 4H-SiC power MOSFETs under HTGB stresses. According to this model, certain originally electrically 'inactive' vacancies in the 'non-bond-switched' oxide regions could be activated to form switching oxide hole traps. Based on this model, we simulated the time evolution of OV-related switching oxide hole traps using rate equations with inputs from DFT. Our results agreed well with the measurements on threshold voltage instability variation over stress duration. This agreement helps to validate the role of OVs in HTGB instability in 4H-SiC MOSFETs. Moreover, it is likely that two energetically distinct OVs are separately responsible for RT and HT V_{th} instability in 4H-SiC MOSFETs. However, further investigations are required to develop a fully comprehensive model for the role of oxygen vacancies in overall 4H-SiC MOSFET reliability degradation.

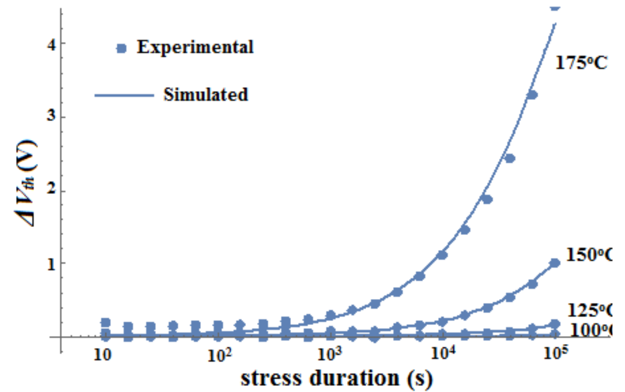

Fig. 4. Transient simulation of HTGB V_{th} instability in 4H-SiC power MOSFET using OV hole trap activation model. The room-temperature contribution is subtracted from the measured threshold voltage instability at the indicated temperatures.

TABLE 1: COMPARISON OF PARAMETERS USED IN THE TRANSIENT MODELING OF HTGB INSTABILITY WITH THOSE CALCULATED FROM DFT.

parameter	DFT	Transient simulation
k_{12} (s^{-1})	-	2.5 X 10^{11}
k_{21} (s^{-1})	-	6 X 10^{11}
E_{12} (eV)	0.8-1.1	0.71
E_{21} (eV)	0	0
E_{23} (eV)	0.5	0.93
E_{32} (eV)	0.5	1.63
E_{24} (eV)	1.4	1.3
E_{42} (eV)	1.0	1.6
E_{34} (eV)	1.5	1.5
E_{43} (eV)	1.1	1.1
N (cm^{-3})	-	10^{19}
v_0 (s^{-1})	-	10^{13}
t_{ox} (nm)	-	50

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