Integrated Modeling of High-Temperature Gate-Bias (HTGB) Reliability Degradation in 4H-SiC Power MOSFETs

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Overview

- Introduction
- Reliability issues in 4H-SiC MOSFETs (Problem statements).
- Integrated Modeling Approach
  - Density Functional Theory plus related modeling tools.
- High-temperature reliability modeling.
- NO passivation and device reliability.
- Summary
Problem statements

Critical reliability concern – High-temperature $V_{th}$ instability*

Development of Passivation processes

- After identifying the root-causes of reliability degradation, how can we alter device processing to mitigate them???
  - Effect of commonly used NO passivation.

* Measurements by our collaborators at U.S. Army Research Lab, Adelphi, MD.
Integrated Modeling Approach

- Ground state energy
- Electron density
- Density of States
- Interatomic Forces
- Trap levels and Activation energies
- Molecular dynamics
- Defect reactions
- Passivation processes

TCAD / Rate equations

Integrated Modeling
Bridging the gap between fundamental physics and MOSFET engineering

Reliability / performance-limiting mechanisms and models
Density Functional Theory

- Schrödinger wave equation that accounts for all the electrons and nuclei in the system and their interactions.

\[ \hat{H} = -\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 + \sum_{i,j} -\frac{Z_I e^2}{|\vec{r}_i - \vec{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_I \frac{\hbar^2}{2M_I} \nabla_I^2 + \frac{1}{2} \sum_{I \neq J} \frac{Z_I Z_J e^2}{|\vec{R}_I - \vec{R}_J|} \]

- The kinetic and potential energies are altered by quantum effects like Pauli’s exclusion – not quantifiable.
- DFT provides a tractable accurate solution for the ground state eigenvalues (energy) and electron density.
  - Replaces the complicated interacting system Hamiltonian by a sum of non-interacting Hamiltonians.
  - Uses electron density (one function in space) as the fundamental property instead of \( \psi_{\text{tot}} \).
Energy Levels of Defects from DFT

- The defect formation reaction for different charge states
  \[ \{\text{bulk}\} + \{D\} + qe^- \rightarrow \{[D + \text{bulk}]^q\} \]

- The feasibility of defect formation is given by its formation energy
  \[ E_{form,q} = E_{[D + \text{bulk}]^q} - E_{\text{bulk}} - \mu_D - q(E_F + E_v) \]

- Stability of the defect in its charged state $q$, and its trap level obtained from formation energy vs Fermi level plot.

- Charge Transition Level (CTL), representing the thermodynamic trap level, is the intersection between two formation energy curves.
High-temperature reliability modeling of 4H-SiC MOSFETs

• Amorphous SiO$_2$ model generation
• Role of oxide defects in reliability degradation.
• Transient modeling of high-temperature $V_{th}$ instability.


Reliability issues in 4H-SiC MOSFETs

Critical reliability concern – High-temperature threshold voltage instability ($\Delta V_{th}$)

- $\Delta V_{th}$ vs log-stress time is linear.
- Typically attributed to oxygen vacancies (direct two-way tunneling model [1, 2]).
  - Also, ESR evidence.3,4

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**Room-Temperature $\Delta V_{th}$ [1]*

**High-Temperature $\Delta V_{th}$ [5]*

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* Measurements by our collaborators at U.S. Army Research Lab, Adelphi, MD.
Amorphous SiO$_2$ model generation

Method 1 – Sequential Back-bond Break (SBB Method)
• New method – Exploits the periodicity of supercell models, inherent in DFT.
• Represents bond-switched regions of oxide (high-amorphousness).

Method 2 – Quantum molecular dynamics
• Represents non-bond-switched regions of oxide (low-amorphousness).
Amorphous SiO2 model – structural properties

- Bond angle and bond length distributions agree well with other models generated using molecular dynamics [1].
- Pair correlation functions agree well with experimental reports [2]. Further work with larger models will be helpful to confirm the results.

Oxygen vacancy (OV) defects in SBB models

- The structural and electronic properties of OV defects in ‘bond-switched’ oxide regions (SBB model) was studied.

**Structures of OV in ‘bond-switched’ oxide regions:**

1. Basic Low-energy Dimer,
2. High-energy forward-projected (fp),
3. High-energy back-projected (bp)

- Upon hole capture, basic dimer spontaneously forms positive fp.
- fp thermally transforms to bp.
- Also, fp and bp are stable when neutral.
Electrical activity of OVs in high disorder regions:

- All configurations are electrically active permanently.
- The +1/0 CTL moves to right consistently, as the OV assumes higher energy configurations – predicts formation of ‘fixed’ positive charges.
- These OVs in bond-switched regions contribute to room temperature $V_{th}$ instability.
  
  - Supports previous models [1,2].

Oxygen vacancies (OV) in MD models

- Studied structural and electronic properties of OVs in ‘non-bond-switched’ oxide regions (low amorphousness).

Configurations of OV in silicon dioxide:

Neutral:
(1) Basic Low-energy Dimer,

Positive (upon hole capture)
(1) Low energy dimer
(2) High-energy forward-projected (fp-bb1),
(3) High-energy back-projected (bp-bb1),
(4) High-energy forward-projected (fp-bb2),
(5) High-energy back-projected (bp-bb2),

- Thermal barriers for transformation calculated using DFT-based Nudged Elastic Band (NEB) method.

How do these structures behave electrically??

Electrical properties of Oxygen vacancies

Electrical activity of Oxygen Vacancy:

- Basic neutral dimers are electrically *inactive*.
- Higher energy configurations are active.

![Diagram of energy levels and structures](image)

*Under NBTS, neutral dimers are ‘activated’ to form active forward-projected and back-projected structures.*

Transient modeling of OV hole trap activation

- What is the time dependence of activation process???
- Solve Arrhenius rate equations bases on DFT-calculated activation barriers!

- Activation barriers from DFT
- $k_{12}$ and $k_{21}$ from SRH model

$$k_{12} = \sigma v_{th} p T(z, F)$$
Transient modeling of OV hole trap activation

- The time-dependent total concentration of activated hole traps (positive charges) is translated to voltage shift.

$$|\Delta V(t)| = \frac{q N \left( \sum_{i=2}^{6} x_i(t) \right)}{C}$$

RT Vth instability post HTGB stress

The model explains:

– Short-term reliability degradation [1].
– Long-term reliability degradation [1].
– ESR observations [2].

NO Passivation of E’ centers

Oxygen vacancy – NO treatment

- NO molecule could be ‘trapped’ by oxygen vacancy to form ‘nitroxyl’ configuration.
- ‘Nitroxyl’ can also be formed by incorporation of atomic Nitrogen into oxide lattice near the interface.

Overall effects of NO:
- Carboxyl hole trap removal under dilute NO - Mitigates $\Delta V_{th}$ [1].
- NO can be counter productive – switching oxide traps.
- NO mitigates interface traps [2].
- Thus, optimized NO passivation mitigates $V_{th}$ instability.

Other effects on NO treatment – Counter-doping

- NO can incorporate at the interface.
  - Nitrogen substitution of C or counter-doping.
    - Improved channel mobility [1].
  - It could re-oxidize 4H-SiC surface.
  - Create additional oxygen vacancy defects due to ‘scarcity’ of oxygen.

- Optimization of NO passivation is extremely important for improved MOSFETs !!!!

Overall summary

- Unified Density functional theory with device modeling techniques.
  - Can solve practical problems encountered by semiconductor device physicists and process engineers.
  - Reliability and mobility models in semiconductor devices.
- High Temperature $\Delta V_{th}$ in 4H-SiC MOSFETs.
  - Due to the activation of electrically ‘inactive’ oxygen vacancies to form switching oxide hole traps over time.
  - Long term reliability degradation is due to residual activated hole trap centers.
- Passivation effects using molecular dynamics
  - Nitric Oxide
    - Controlled NO could be effective, Excess NO can have adverse effects.
    - Counter-doping during NO passivation is energetically feasible.
Thank you,
Questions?
Additional defects involved in hole trapping

• Role of carbon-related defects
• Stability-providing bonding mechanisms
Single carbon interstitial in SiO2 – DFT Based Molecular Dynamics simulation

- Atomic carbon has been suggested to be emitted into the oxide during 4H-SiC oxidation \([1]\).
- Our DFT based molecular dynamics simulation of atomic carbon in SiO2 resulted in the rapid formation of Si-O-C-Si bridges.

![Diagram of C interstitial in SiO2](image)

- The existence of carbon-containing interlayers has been observed in TEM measurements \([2]\).

Formation of carboxyl defect from Si-O-C-Si bridges in SiO₂

- \( SiO₂ + C \rightarrow Si - O - C - Si \rightarrow Si - [C = O] - Si \)
- Carboxyl defect, Si-[C=O]-Si, are more stable than Si-O-C-Si defect – based on simple octet rule.
- Simple bond energy based calculations indicated \( \sim 3.2 \) eV energy release.
- The kinetics of conversion of Si-O-C-Si bridge to carboxyl configuration was studied using nudged-elastic band method.

- Exothermic reaction, energy released = \( \sim 2 \) eV
- Activation barrier = 0.5 eV
Electrical activity of carboxyl defects in 4H-SiC MOSFETs

- Based on bandgap alignment, a +2 to neutral charge transition level is observed for carboxyl defect within the 4H-SiC bandgap (at $E_{v,4H-SiC} + 1.4$ eV) – implies that the charge is electrically active.

- The defect is predicted to be a border trap.
- For 4H-SiC Fermi level $> 1.4$ eV, defect is neutral.
- For 4H-SiC Fermi level $< 1.4$ eV, defect is in +2 state (hole trap).
- Thus, the defect is a border hole trap causing $V_{th}$ instability.
Structural transformations in the carboxyl defect

- In the neutral state, Si-C band length corresponds to that in 4H-SiC.
- Weak bond due to the electronegative carboxyl oxygen imparting partial positive charge to carbon – Coulomb repulsion between partially positive Si and C.
- The bond can be broken by radiation or high applied bias and temperature making it positively charged (h⁺ trapping) – similar to Si-Si precursor bond in E’ centers.

- In the stable +2 state, significant puckering and back-bonding of positive Si with oxygen was observed – similar to O vacancy hole traps.
- This structural change imparts stability in +2 state.
- Significant resemblance with well-established E’ center hole traps.
Bonding in the carboxyl defect - ELF

- In the neutral state, at high ELF of 0.89, two lone pairs on Oxygen are distinctly visible.
- By comparing with Lewis perspective of bonding, this indicates a carbon-oxygen double bond (C=O).
- In the stable +2 state, at a high ELF of 0.89, a single lone pair was observed on carboxyl oxygen.
- This indicates a triple bond between C and O.
- Apart from puckering, the increase in C-O bond order from 2 to 3 imparts stability to the defect in +2 state. **ESR invisible in 0 and +2.**
• Mobility degradation in 4H-SiC MOSFETs
  • Drift Diffusion simulation of 4H-SiC MOSFET.
  • Algorithm for trap characterization.
Performance issues in 4H-SiC MOSFETs

Critical performance concern – Very low channel electron mobility

- Very poor Hall mobility.
- Even poorer effective mobility.
- Very high density of interface traps near the conduction band edge.
  - Poor quality of interface.

Identify the number of distinct defects, their atomic make-up, their energy levels and individual concentrations.

2D-Device Simulation of a SiC power MOSFET

Poisson’s equation
\[ \nabla^2 \Phi = -\frac{q(p-n + N_D - N_A)}{\varepsilon} \]

Current equations
\[ J_n = -q\mu_n n \nabla \Phi + qD_n \nabla n \]
\[ J_p = -q\mu_p p \nabla \Phi - qD_p \nabla p \]

Continuity equations
\[ \frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot J_n + G_n - R_n \]
\[ \frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot J_p + G_p - R_p \]

Einstein’s relation
\[ \frac{D}{\mu} = \frac{kT}{q} \]

- Solve equations simultaneously.
- Allows us to calculate I-V characteristics based on the internal structural detail of the device and probe inside the device where experiments cannot reach.

Experimentally Verified Mobility Models

**Bulk Mobility**

Bulk Phonons and Impurity Scattering

\[
\mu_B(T) = \mu_{\text{max}} \left( \frac{300}{T} \right)^{\eta_B} - \mu_{\text{min}} + \mu_{\text{min}} + \left( \frac{D}{N_{\text{ref}}} \right)^{\gamma_B} \]

\[1+\left( \frac{D}{N_{\text{ref}}} \right)^{\gamma_B} \rightarrow \text{Doping} \]

**Coulomb Scattering Mobility**

\[
\mu_C(T) = \frac{16 \pi \epsilon^2 \hbar k_B T}{m^* e^3 (N_{it} + N_{OT})} \cdot \frac{1}{F(z, z_i, T)} \]

\[\rightarrow \text{Trapped Charge} \]

**Surface Phonon Mobility**

\[
\mu_{SP}(T) = \frac{A}{E_\perp} + \frac{B}{T E_\perp^{1/3}} \]

**Surface Roughness Mobility**

\[
\mu_{SR}(T) = \frac{1}{E_\perp^2} \cdot \frac{\hbar^3}{2 m^* m_d^* e \Delta L^2} \cdot \frac{1}{F_{SR}(T)} \]

\[\rightarrow \text{Step Height} \quad \text{Correlation Length} \]

**High Field Mobility**

\[
\mu_{HF}(T) = \frac{v_{\text{sat}}(T)}{E_{||}} \rightarrow \text{Saturation Velocity} \]
Methodology: Trap characterization

Part 1 - Drift-Diffusion Simulation

- Interface trap density modeled as exponential – represents experiments [1,2]

\[ E_F = E_C - k_b T \ln\left(\frac{N_c}{n}\right) \]
\[ f = \frac{1}{1 + \frac{1}{2} \exp\left(\frac{E_t - E_F}{k_b T}\right)} \]

\[ N_{tot,DS}(V_{GS}, T) = \int_{E_{mid}}^{E_c} D_{it,DS}(E_t) f(E_t, E_F(V_{GS}), T) \, dE_t \]

Energy gap is discretized into $N$ parts.

Assume $m$ traps, sample space is $N^C_m$.

Pick a set $\{E_j\}$, ($j = 1$ to $m$) from the sample space.

$$DOS = \sum_{j=1}^{m} h_j \delta(E_t - E_j)$$

For a given gate bias and temperature, find fermi level and $f(E)$ from DD simulation.

Find total occupied trap density.

$$N_{tot\_alg}(V_{GS}, T) = \sum_{j=1}^{m} h_j f(E_j, E_F(V_{GS}), T)$$

Methodology: Trap characterization (contd..)
Methodology: Trap characterization (contd..)

- To form a system of equations, the process is repeated for \(n\) voltages, \(n > m\)

Temp 1

\[
\begin{bmatrix}
  f(E_1, V_1, T_1) & f(E_2, V_1, T_1) & \cdots & f(E_m, V_1, T_1) \\
  f(E_1, V_2, T_1) & f(E_2, V_2, T_1) & \cdots & f(E_m, V_2, T_1) \\
  \vdots & \vdots & \ddots & \vdots \\
  f(E_1, V_n, T_1) & f(E_2, V_n, T_1) & \cdots & f(E_m, V_n, T_1) \\
  1 & 1 & \cdots & 1
\end{bmatrix}
\begin{bmatrix}
  h_1 \\
  h_2 \\
  \vdots \\
  h_m
\end{bmatrix}
= \begin{bmatrix}
  N_{i1}(V_1, T_1) \\
  N_{i2}(V_2, T_1) \\
  \vdots \\
  N_{in}(V_n, T_1)
\end{bmatrix}
\]

Temp \(p\)

\[
\begin{bmatrix}
  f(E_1, V_1, T_p) & f(E_2, V_1, T_p) & \cdots & f(E_m, V_1, T_p) \\
  f(E_1, V_2, T_p) & f(E_2, V_2, T_p) & \cdots & f(E_m, V_2, T_p) \\
  \vdots & \vdots & \ddots & \vdots \\
  f(E_1, V_n, T_p) & f(E_2, V_n, T_p) & \cdots & f(E_m, V_n, T_p) \\
  1 & 1 & \cdots & 1
\end{bmatrix}
\begin{bmatrix}
  h_1 \\
  h_2 \\
  \vdots \\
  h_m
\end{bmatrix}
= \begin{bmatrix}
  N_{i1}(V_1, T_p) \\
  N_{i2}(V_2, T_p) \\
  \vdots \\
  N_{in}(V_n, T_p)
\end{bmatrix}
\]

Defects are at \([E_1, E_2, \ldots, E_m]\)

Is \([h_1, h_2, \ldots, h_m]\) same for all \(T\)?

Missing some defects. Repeat with new \(m\)!
Results: Major mobility-limiting traps

- Based on the methodology, three trap types are predicted.
- Temperature invariance < 20%
  - E1: 2.8-2.85 eV  (2.3 \times 10^{11} / \text{cm}^2)
  - E2: 3.05 eV  (5.4 \times 10^{11} / \text{cm}^2)
  - E3: 3.1-3.2 eV  (1 \times 10^{12} / \text{cm}^2)

- Trap energies match with traps determined by experiments
  - DLTS [1] and
  - C-V measurements [2]

Next step: Use DFT to find atomic nature of defect

Trap identification from DFT

- Considered trap levels of two possible SiC defects.
  - Si vacancy [1,2].
  - Carbon dimer defect [3,4].

- No trap level seen near the conduction band edge from Si vacancy.
  - Unlikely to be a major cause of poor mobility.
- C dimer defect gave trap levels close to conduction band edge.
  - Similar to the energy extracted by our methodology.
- By comparison, the nature of defect at 3.1-3.2 eV could be Carbon dimer.

Overall summary

• Unified Density functional theory with device modeling techniques.
  – Can solve practical problems encountered by semiconductor device physicists and process engineers.

• Reliability and mobility models in semiconductor devices.

• Proposed a methodology that combines drift-diffusion simulation and density functional theory to predict:
  – The existence of three types of mobility reducing defect in SiC/SiO2 interface.
  – High density of interface trapping likely from Carbon dimer defects in SiC side of the interface.
Thank you, Questions?
Backup slides
Bonding in the H2-passivated carboxyl defect

- In the neutral state, at high ELF of 0.9, two lone pairs on Oxygen are distinctly visible.
- By comparing with Lewis perspective of bonding, this shows C-O single bond.
- In the stable +2 state, a single lone pair was seen on carboxyl oxygen - indicates a C=O double bond.
- Apart from puckering, increase in C-O bond order from 1 to 2 imparts stability to the defect in +2 state.

Resembles carboxyl defect and continues to act as hole trap – H2 has no/minimal effect. ESR invisible defect in 0 and +2 states.
Room Temperature $\Delta V_{th}$ - background

Switching oxide hole trap model

- Holes tunnel into and out of near-interfacial border hole traps, causing $V_{th}$ instability.
  - Two-way tunneling model
  - Explains room temperature $V_{th}$ instability [1].
  - Depth of oxide traps into which holes tunnel change at a rate of $\sim 2\text{Å}$ per decade of stress time.
- Predicts $\Delta V_{th}$ vs log-stress time to be linear, as seen experimentally.

- Well-known switching oxide hole trap = E’ centers (Oxygen vacancy) [2].
  - Traditionally held responsible for $V_{th}$ instability in 4H-SiC and Si MOSFETs.
  - Observed using electron spin resonance spectroscopy [3, 4].

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Problem statements

Critical reliability concern – High-temperature $V_{th}$ instability*

Room-Temperature $\Delta V_{th}$ [1]

High-Temperature $\Delta V_{th}$ [2]

Critical performance concern – Very low channel electron mobility

Poor Hall and effective mobility [3]

Typical $D_{it}$ spectrum [4]

* Measurements by our collaborators at U.S. Army Research Lab, MD.

Nitric Oxide Diffusion
Bandgap alignment
Thermal transitions between OV configurations

- Activation barriers for thermal transitions between various OV configurations (in low disorder oxide regions).
  - Calculated from DFT (Nudged Elastic Band method).
  - Barriers are generally lower for positively charged states → *negative bias is critical for trap activation.*
Switching oxide hole trap model

- Holes tunnel into and out of near-interfacial border hole traps, causing $V_{th}$ instability.
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Transient modeling of OV hole trap activation - 1

- Under NBTS, inactive neutral dimers are ‘activated’ to form electrically active structures.

- What is the time dependence of activation process??? - Very critical to $V_{th}$ stability

\[
\frac{dx_1}{dt} = -k_{12} e^{-\frac{E_{12}}{kT}} x_1 + k_{21} e^{-\frac{E_{21}}{kT}} x_2
\]

\[
\frac{dx_2}{dt} = -\left( k_{21} e^{-\frac{E_{21}}{kT}} + v_0 e^{-\frac{E_{23}}{kT}} + v_0 e^{-\frac{E_{25}}{kT}} \right) x_2 + k_{12} e^{-\frac{E_{12}}{kT}} x_1
\]

\[
\frac{dx_3}{dt} = -v_0 e^{-\frac{E_{32}}{kT}} x_3 + v_0 e^{-\frac{E_{34}}{kT}} x_4 + v_0 e^{-\frac{E_{35}}{kT}} x_5
\]

\[
\frac{dx_4}{dt} = -\left( v_0 e^{-\frac{E_{43}}{kT}} + v_0 e^{-\frac{E_{46}}{kT}} + v_0 e^{-\frac{E_{43}}{kT}} \right) x_4 + v_0 e^{-\frac{E_{34}}{kT}} x_3 + v_0 e^{-\frac{E_{35}}{kT}} x_5
\]

\[
\frac{dx_5}{dt} = -\left( v_0 e^{-\frac{E_{52}}{kT}} + v_0 e^{-\frac{E_{56}}{kT}} + v_0 e^{-\frac{E_{53}}{kT}} \right) x_5 + v_0 e^{-\frac{E_{52}}{kT}} x_2
\]

\[
\sum_{i=1}^{6} x_i e^{-\frac{E_{65}}{kT}} x_6 + v_0 e^{-\frac{E_{35}}{kT}} x_3
\]

- Activation barriers from DFT
- $k_{12}$ and $k_{21}$ from SRH

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Density Functional Theory (2)

• Bonn-Oppenheimer approximation
  – Nuclei are much more massive than electrons. So, they are considered still.
  – Thus, the electronic Hamiltonian becomes

\[
\hat{H} = -\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 + \sum_{i,I} \frac{-Ze^2}{|\vec{r}_i - \vec{R}_I|} + \frac{1}{2} \sum_{i\neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}
\]

  – The nuclei-nuclei potential can be separately calculated.

• Hohenberg-Kohn theorem 1
  – The ground state energy, \( E[n(r)] \), of a multi-body system is a unique functional of electron density, \( n(r) \).

• Hohenberg-Kohn theorem 2
  – The \( n(r) \) which minimizes \( E[n(r)] \) is the true ground state \( n(r) \) corresponding to the solution of SWE.

• While the energy functional is the sum of all kinetic and potential energies, the effect of QM interactions are not explicitly known. In short, the mathematical form of the functional is unknown.
Molecular dynamics from DFT

- Can determine the time evolution of atoms in a system.
- From DFT, force on individual atom is calculated.
- Force on atom $i$ due to $j$’s= - (gradient of energy in ground state, $E$) → From DFT

$$F_i(R_j) = - \frac{\partial E}{\partial R_i}$$

- Verlet Algorithm for tracking the position of atoms in time:

From Newton’s law:

$$\frac{d^2}{dt^2} R_i = \frac{F_i}{M_i}$$

Discretization in time to solve the differential equation.

$$R_i(t + \Delta t) = 2R_i(t) + R_i(t - \Delta t) + \frac{(\Delta t)^2}{M_i} F_i(R_j)$$

Effect of temperature included externally (velocity rescaling)
- By tracking $R_i$, the trajectories of atoms are calculated.
- Can study
  - diffusion,
  - chemical reactions (passivation), etc
Electrical activity of defects in 4H-SiC MOSFETs

Which defects matter in 4H-SiC MOSFETs?

- The Fermi Level is restricted to move within 4H-SiC bandgap.
- Bandgap lineup between 4H-SiC and SiO2 is very critical.
  - Calculated from DFT or internal photoemission [1].

Bandgap lineup procedure using DFT [2]

Density Functional Theory

- The Kohn-Sham formalism of DFT replaces the system of interacting system by non-interacting system of same density, \( n(r) \).
  - This allows the energy functional to be written as
    \[
    E[n(r)] = T_{\text{non\_int}}[n(r)] + \int V_{\text{ion}} n(r) dr + E_H[n(r)] + E_{xc}
    \]
  - \( E_H \) is the Hartree mean field potential – potential energy of an electron in a mean electrostatic potential of other electrons.
    \[
    E_H[n(r)] = \frac{1}{2} \int \int \frac{n(r')n(r)}{r - r'} dr \, dr'
    \]
  - Here, \( E_{xc} \) represents the exchange-correlation functional – includes all the quantum mechanical effects
  - \( E_{xc} \) is an approximation – a challenge in DFT.
    \[
    E_{xc} = T_{\text{real}} - T_{\text{non\_int}} + E_{ee_{\text{real}}} - E_H
    \]
- By using HK theorem 2, we can variationally minimize \( E[n(r)] \) with respect to \( n(r) \).
  - This reduces the complicated SWE into a Schrodiger-like single particle equation with a Kohn-Sham potential – solved using Bloch theorem.
    \[
    - \left( \frac{1}{2} \nabla^2 + V_{KS} \right) \psi_i = \epsilon_i \psi_i \quad \text{where} \quad V_{KS} = V_{\text{ion}} + V_H + \frac{\delta E_{xc}}{\delta n(r)}
    \]
Density Functional Theory - Flow

Flow

The many-body system to be solved is replaced by system of non-interacting particles with same charge density

Initial guess for charge density, \( n(r) \)

Calculate the Kohn-Sham (KS) Potential, \( V_{KS} \)

Solve single particle KS equation

New \( n(r) \)

Calculate \( n(r) \) from single particle KS wavefunctions

Is calculated \( n(r) \) same as initial \( n(r) \)?

Ground state \( n(r) \) and energies
The by-product of NO passivation reaction with the carboxyl defect is the NCO molecule – important to know if this creates new defects.

NCO molecules are large – seen to be trapped inside SiO2 void.

Reacts with NO molecule to give N₂ and CO₂.

**Observations:**

- Intermediate product include nitrosil isocyanate – activation barrier of 0.2 eV.
- This is followed by a cyclic intermediate.
- N₂ and CO₂ are formed with energy release of ~ 3 eV.
- N₂ and CO₂ diffuses out relatively easily, completing the defect passivation reaction.
- NCO is unlikely to create new defects in SiO₂.
3. Overall results on Passivation

- **NO passivation**
  - Studied the mechanism of NO treatment of carboxyl defect.
  - NO was seen to remove the defect.
  - Excess NO seen to result in positive charge build-up.
  - Controlled NO passivation to improve $V_{th}$ instability.
  - By-products of the reaction do not create additional defects.

- **H$_2$ passivation**
  - Was seen to create hole traps similar to the original carboxyl defects.
  - Unlikely to be effective in improving $V_{th}$ instability.

- **F passivation**
  - Passivates E’ and carboxyl – related hole traps completely. Effect of dielectric constant reduction requires further study.

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Bonding in the H2-passivated carboxyl defect

- In the neutral state, at high ELF of 0.9, two lone pairs on Oxygen are distinctly visible.

- By comparing with Lewis perspective of bonding, this shows C-O single bond.

- In the stable +2 state, a single lone pair was seen on carboxyl oxygen - indicates a C=O double bond.

- Apart from puckering, increase in C-O bond order from 1 to 2 imparts stability to the defect in +2 state.

Resembles carboxyl defect and continues to act as hole trap – H2 has no/minimal effect. **ESR invisible defect in 0 and +2 states.**
Amorphous SiO2 model generation

Method 1
- New method – Exploits the periodicity of supercell models, inherent in DFT.
  - An Si-O-Si linkage is randomly broken.
  - The disconnected Si is puckered by 166 pm to back-bond with rear oxygen, making the Oxygen triply coordinated.
  - One of the original Si attached to the triply coordinated O is broken and puckered to generate a new triply coordinated O.
  - Process is repeated until the puckered Si meets the original dangling O, repairing the damage.
- Represents regions of oxide with high-amorphousness.

Method 2
- Melt-and –quench Molecular dynamics.
- Represents regions of oxide with low-amorphousness.
Important considerations

• In theory, one could form infinite number of equations in the over-determined system – but works only for carefully chosen low voltages.
• To minimize errors, the algorithm is applied at low voltages.
  ➢ Voltages at which the equations are formed are chosen in such a way that change in Fermi level is large (or large $f(E)$).
  ➢ Also, Trap-filling happens at low voltages.
• It should be made sure that the Fermi level is such that it falls in the “region of interest” for traps (in case of SiC, near conduction band).

Limitation:
• Cannot resolve mid-gap trap energies.
  ➢ All the mid-gap traps are fully occupied even at low gate bias due to large SiC/SiO2 work-function difference.
Electron Localization Function \([1]\) from DFT

- Chemical bonding can be studied using Electron Localization Function (ELF).
- ELF is the conditional probability of finding an electron in the vicinity of another electron with the same spin – gives a measure of Pauli’s exclusion.
- Defined such that high ELF implies high electron localization – indicates lone pairs, bonding pairs and dangling bonds.
- These different electron localizations occur at local maxima in ELF.
- Plotted as isosurfaces at different values to distinctly “see” chemical bonding.
- ELF used to study bonding transformations in defects during hole capture – help to identify defect stabilizing mechanisms.

BTS measurements