Characterization of reliability-limiting defects in 4H-SiC MOSFETs using density functional (atomistic) simulations

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1. Silicon Carbide for Electronics - Concerns

- Poor quality of interface - Density of interface traps ($D_{it}$) much greater than Si/SiO2 interface.
- Traps result in very low channel mobility.
- Trapped electrons scatter free channel electrons.
- Poor reliability – threshold voltage instability due to border oxide and interface traps.

Goals:
- Understanding defects causing mobility and reliability degradation.
- How can we process the device to mitigate these defects?
2. Overall results on mobility

• Developed 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.
  – Found interface states located at 2.8-2.85 eV, 3.05 eV and 3.1-3.2 eV.
  – Quantified their individual concentrations.
    • 2.8-2.85 eV trap conc. – 2.3 X 10^{11} / cm^2
    • 3.05 eV trap conc. – 5.4 X 10^{11} / cm^2
    • 3.1-3.2 eV trap conc. – 1 X 10^{12} / cm^2
  – New method indicates the trap at 3.1-3.2 eV originates from Carbon dimers in 4H-SiC side of the interface based on DFT.
  – Si vacancies are unlikely to be the source of mobility-reducing traps.

3. Overall results on reliability

- Proposed single carbon interstitials defect in carboxyl configuration to be a switching oxide hole trap.
  - Studied the behavior of C interstitial in SiO2.
  - Showed that carboxyl configuration is stable.
  - Identified a +2 to neutral charge transition level within 4H-SiC bandgap (1.4 eV).
    - Indicates that carboxyl defect is a switching oxide hole trap.
  - Identified two stability-providing mechanisms for the defect in its +2 state.
    - Back-bonding and puckering of positive Si atom – resembles E’ center hole trap.
    - Chemical bonding studied using electron localization function (ELF).
    - Defect is likely to be ESR invisible in their thermodynamically stable states.

4. Overall results on Passivation\textsuperscript{2}

- Studied the passivation of carboxyl defect in NO and H\textsubscript{2}.

- **NO passivation**
  - Studied the mechanism of NO passivation of carboxyl defect.
    - NO was seen to remove the defect.
    - Will improve threshold voltage instability.
    - By-products of the reaction does not create additional defects.

- **H\textsubscript{2} passivation**
  - Was seen to create hole traps similar to the original carboxyl defects.
    - Studied using formation energy and ELF.
    - Unlikely to be effective in improving $V_{th}$ instability.

Density Functional Theory

- Second order differential equation that accounts for all the electrons and nuclei in the system and their interactions.

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

\[
\hat{H} = \hat{T}_e + \hat{V}_{N-e} + \hat{V}_{e-e} + \hat{T}_N + \hat{V}_{N-N}
\]

\[
\hat{H}\Psi_i(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, \vec{R}_1, \vec{R}_2, ..., \vec{R}_M) = E\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, \vec{R}_1, \vec{R}_2, ..., \vec{R}_M)
\]

- \(T_e\): electron Kinetic energy; \(V_{N-e}\): attractive energy between electrons and nuclei, \(V_{e-e}\): repulsive energy between electrons, \(T_N\): Kinetic energy of nuclei, \(V_{N-N}\): attractive energy between nuclei.

- This SWE is very complicated due to multi-body quantum interactions which are difficult to model.

- DFT provides a tractable accurate solution for the ground state.
Reliability-limiting defects in 4H-SiC MOSFETs
Border hole traps in 4H-SiC MOSFETs and reliability - background

• Oxygen vacancies are traditionally regarded as border hole traps in Silicon devices [1].

• They switch charge state between positive (hole trapped) and neutral states and cause threshold voltage instability.

• Their existence have been verified using electron spin resonance spectroscopy [2, 3].

• E’ centers have been held responsible for $V_{th}$ instability in 4H-SiC MOSFETs as well.

• However, other defects need to be explored for hole trapping, especially due to the presence of carbon.

Single carbon interstitial in SiO2 – Molecular Dynamics simulation

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

![Diagram showing C interstitial and Si-O-C-Si bridge](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 SiO\textsubscript{2}

- \( SiO_2 + C \rightarrow Si - O - C - Si \rightarrow Si - [C = O] - Si \)
- 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 \(~3.2\) 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 = \(~2\) eV
  - Activation barrier = 0.5 eV

**Carboxyl: Likely Defect !!**
Trap Level of Carboxyl Defect: Methodology

- The carboxyl defect formation reaction for different charge states

\[ [SiO_2] + [C] + q \, e^- \rightarrow [Carboxyl]^q \]

- The formation energy of carboxyl defect in charge state \( q \) is

\[ E_{form,q}(E_F) = E_{carboxyl}^q - E_{SiO2} - \mu_C - q(E_F + E_v + \delta V) + E_{corr,q} \]

- Trap levels are defined through charge transition levels (CTL).
- CTL is defined as the Fermi level at which the formation energy of the defect in two charge states is equal.
Stable charge states of carboxyl defect in SiO2

- The formation energies of carboxyl defect in various charge states, with neural as reference, were calculated as a function of Fermi level.

- The defect appears to be stable in +2, 0 and -2 states depending on the Fermi level.

- The electrical activity of this defect in 4H-SiC MOSFET is governed by the position of 4H-SiC bandgap with respect to SiO2 bandgap.

- Thus, the bandgap alignment is critical.
Bandgap alignment

\[ \Delta E_c = 2.59 \quad \Delta E_v = 3.09 \]

Calculated Experimental\(^1\)

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.
Structure of 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.
Passivation of the Carboxyl defect
Modeling NO Passivation with Molecular Dynamics

- NO treatment post oxidation has been shown to improve Vth instability [1] – mechanism not known.
- We studied the reactions between carboxyl defect and NO molecule using molecular dynamics at 1400K.

Observations:
Defect removed through isocyanate formation – low activation barrier.

NO is incorporated if present in excess.

NCO reacts with NO to give N2 and CO2, which diffuse out.

- Defect removal mitigates $V_{th}$ instability.
- NO incorporation observed in XPS measurements.

Passivation in $\text{H}_2$

- Hydrogen was seen to attach to the defect – no defect removal observed.
- Does the H2–passivated carboxyl affect hole trapping? – analysed using formation energy considerations.
- A +2/0 charge transition level was observed at 1.1 eV above 4H-SiC VBM.
- Likely to act as hole trap, similar to the carboxyl defect – backbonding observed upon double hole capture.
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.

(a) neutral, ELF = 0.9
(b) doubly positive, ELF = 0.9
Conclusion

- Carbon interstitial defect existing in carboxyl configuration in the oxide side is a reliability limiting defect.
  - Border hole trap.
  - Introduces hole trap level at 1.4 eV above 4H-SiC bandgap.
  - Structural transformations upon hole capture very similar to conventional oxygen vacancy hole trap (E’ center).
  - Stability-providing mechanisms and bonding studied through electron localization function.

- The carboxyl defect can be passivated by NO treatment.
  - Through the removal of Carbon.

- The carboxyl defect can NOT be passivated by H₂ treatment.
  - Introduces hole trap level similar to the original carboxyl defect.
Thank you,
Questions?
Backup slides
Bandgap alignment (1)

- Line-up of 4H-SiC bandgap with respect to SiO2 bandgap – using Van de Walle’s method [1].

- Procedure:
  1. Using separate hydrid functional calculations, identify three landmarks in bulk SiO2 and bulk 4H-SiC. They include mean electrostatic potential in bulk, conduction and valence band extrema.

2. Construct a 4H-SiC/SiO2 interface and calculate the potential in the interface.
Mobility-limiting defects in 4H-SiC MOSFETs\(^1\) (not presented today)

Proposed methodology

Part 1 - Drift-Diffusion Simulation

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

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

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

Proposed methodology (Contd..)

Part 2 - Algorithm

- Energy gap is discretized into $N$ parts.
- Assume $m$ traps, sample space is $\binom{N}{m}$.
- 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.

$$N_{tot\_alg}(V_{GS}, T) = N_{tot\_DS}(V_{GS}, T)$$

1 equation, $m$ unknowns
Proposed methodology (Contd..)

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

Temp 1

\[
\begin{bmatrix}
  f(E_1, V_1, T_1) & f(E_2, V_1, T_1) & \cdots & f(E_m, V_1, T_1) \\
  f(E_1, V_2, T_1) & f(E_2, V_2, T_1) & \cdots & f(E_m, V_2, T_1) \\
  \vdots & \vdots & \ddots & \vdots \\
  f(E_1, V_n, T_1) & f(E_2, V_n, T_1) & \cdots & f(E_m, V_n, T_1) \\
  1 & 1 & \cdots & 1
\end{bmatrix}
\begin{bmatrix}
  h_1 \\
  h_2 \\
  \vdots \\
  h_m
\end{bmatrix}
= \begin{bmatrix}
  N_{it, 1}(V_1, T_1) \\
  N_{it, 2}(V_2, T_1) \\
  \vdots \\
  N_{it, n}(V_n, T_1) \\
  N_{tot}
\end{bmatrix}
\]

Temp \( p \)

\[
\begin{bmatrix}
  f(E_1, V_1, T_p) & f(E_2, V_1, T_p) & \cdots & f(E_m, V_1, T_p) \\
  f(E_1, V_2, T_p) & f(E_2, V_2, T_p) & \cdots & f(E_m, V_2, T_p) \\
  \vdots & \vdots & \ddots & \vdots \\
  f(E_1, V_n, T_p) & f(E_2, V_n, T_p) & \cdots & f(E_m, V_n, T_p) \\
  1 & 1 & \cdots & 1
\end{bmatrix}
\begin{bmatrix}
  h_1 \\
  h_2 \\
  \vdots \\
  h_m
\end{bmatrix}
= \begin{bmatrix}
  N_{it, 1}(V_1, T_p) \\
  N_{it, 2}(V_2, T_p) \\
  \vdots \\
  N_{it, n}(V_n, T_p) \\
  N_{tot}
\end{bmatrix}
\]

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

Missing some defects. Repeat with new \( m \)!
Results

- Based on the methodology, three trap types are predicted.
- Temperature invariance < 20%
  - E1 : 2.8-2.85 eV
  - E2 : 3.05 eV
  - E3 : 3.1-3.2 eV

<table>
<thead>
<tr>
<th>Distance into channel from source (µm)</th>
<th>Trap 1</th>
<th>Trap 2</th>
<th>Trap 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Energy (eV)</td>
<td>Conc. (10^{11}/ cm^2)</td>
<td>Energy (eV)</td>
</tr>
<tr>
<td>0.34</td>
<td>2.80</td>
<td>2.24</td>
<td>3.05</td>
</tr>
<tr>
<td>0.42</td>
<td>2.85</td>
<td>2.45</td>
<td>3.05</td>
</tr>
</tbody>
</table>

- Predicted trap energies match with traps determined by experiment
  - DLTS [1] and
  - C-V measurements [2]

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.
Density functional simulation of defects

- Considered two possible SiC defects in different charge states.
  - Si vacancy [1,2].
  - Carbon dimer defect [3,4].

- Formation energies are calculated using Hybrid functional DFT.
- Trap levels are estimated through charge transition levels.
- Interface specific polarization is accounted for, as a correction.

Results of DFT

- Trap levels of Si vacancies and C dimer defects were calculated.
- 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 results

• 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.
  – Located at 2.8-2.85 eV, 3.05 eV and 3.1-3.2 eV.
  – Quantified their individual concentrations.
    • 2.8-2.85 eV trap conc. – 2.3 X 10\(^{11}\) / cm\(^{2}\)
    • 3.05 eV trap conc. – 5.4 X 10\(^{11}\) / cm\(^{2}\)
    • 3.1-3.2 eV trap conc. – 1 X 10\(^{12}\) / cm\(^{2}\)
  – The trap at 3.1-3.2 eV could be originating from Carbon dimers in SiC side of the interface based on DFT.
  – Si vacancies are unlikely to be the source of mobility-reducing traps.
Conclusion

- Carbon dimer defect is possibly the major contributor to high density of interface traps at SiC/SiO2 interfaces.
- Two more traps exist – their atomic identification needs more DFT investigation.
- Si vacancies are unlikely to reduce electron mobility.
- Passivation techniques should be directed at removing Carbon dimers to improve mobility.
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

\[ \mu_B(T) = \mu_{\text{max}} \left( \frac{300}{T} \right)^{\eta_B} - \mu_{\text{min}} + \mu_{\text{min}} 1 + \left( \frac{D}{N_{\text{ref}}} \right)^{\gamma_B} \]

\[ \rightarrow \text{Doping} \]

**Coulomb Scattering Mobility**

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

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

**Surface Phonon Mobility**

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

**Surface Roughness Mobility**

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

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

**High Field Mobility**

\[ \mu_{HF}(T) = \frac{v_{\text{sat}}(T)}{E_\parallel} \]

\[ \rightarrow \text{Saturation Velocity} \]
Doping, potential and electron conc. profiles in a power MOSFET

$T = 298\, K$

$V_{GS} = 20\, V$

JFET Channel

source

Drift region

Potential (V)
Density Functional Theory (2)

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

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

  – 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.
Density Functional Theory (3)

- 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.
    \[
    - \left( \frac{1}{2} \nabla^2 + V_{KS} \right) \psi_i = \varepsilon_i \psi_i \quad \text{where} \quad V_{KS} = V_{\text{ion}} + V_H + \frac{\delta E_{xc}}{\delta n(r)}
    \]
Density Functional Theory - Flow

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

Comments

The complex Hamiltonian with summation over all particles (eqn 1.8) is reduced into a single particle SWE-like Kohn-Sham (KS) eqn with a KS potential. Charges are treated classically. All quantum “unknowns” are in the exchange-correlation term.

\[ V_{KS} = V_{ion} + V_{hartree} + V_{xc} \]

\( V_{ion} \) from pseudopotentials;

\( V_{hartree} \) from Poisson’s equation - eqn (1.18)

\( V_{xc} \) based on approximation (LDA or GGA) – eqn (1.17)

\[ -\left(\frac{1}{2} \nabla^2 + V_{KS}\right) \psi_i = \varepsilon_i \psi_i \]

\[ n(r) = 2 \sum_i \psi_i^* \psi_i \]

Gives ground state total energy, band structure, DOS, defect levels etc.
Bonding in the carboxyl defect upon hole capture

- Chemical bonding was 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 bonding regions are represented by distinct local maxima in ELF. Thus they are plotted as isosurfaces at different values to distinctly “see” chemical bonding.

- ELF used to study bonding transformations in the carboxyl defect during hole capture.
Significance of isocyanate molecule (NCO)

- 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.