Integration of DFT, Process and Device Modeling: 
The Virtual Fab

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Outline

1. Neil Goldsman
   a) Summary of Virtual Fab Simulation Platform
   b) Conclusions on The Mobility
   c) Key Density Functional Theory Results on Atomic Defects: Reliability and Mobility

2. Dev Ettisserry
   a) Integrated DFT Modeling
   b) Hole Traps and E’ Centers
   c) Process Development
SiC World Today

**SiC:**

**Benefit:** SiC is the Super Semiconductor that will Revolutionize the Power Electronics World.

**Problem:** It has not happened yet because processing and understanding is sooo... difficult:

**Hope:** Devices have been made and are being used commercially.
SiC Device Virtual Fab, Design and Analysis Platform

Process & Fabrication Modeling
(Device Structure & Defect Generation)

Device Modeling
(I-V & Performance)

Monte Carlo:
(Transport)

Density Functional Theory
(Defects)

Σ

Device Meet Specs?

NO

YES

CoolSPICE Circuit Design
Summary of Key Results:
Identified Coupling Virtual Fab & Experiment

1. Low Vgs: Mobility dominated by interface states.
2. Higher Vgs: Mobility dominated by surface roughness and Transition Region
4. Interface states trap channel electrons reducing mobile electron concentration and current.
5. Near Interface transition region of reduced mobility due to non-stoichiometric defects: (Identified by Monte Carlo and DFT)
6. MOSFET Channel ~5nm
7. Transition Region of 2nm Significant (Josh & Lourdes)
Summary of Key Results: Transition Region & Atomic Origin of Defects

• Reliability: Threshold Instabilities
  – Due to Oxide Vacancies and Carboxyl Substitutions in SiO$_2$ side of Trans. Region (TR)

• Interface States: Mobility Degradation at Low V$_{gs}$.
  – Due to atomic defects in SiC side TR.
  – Thee specific State Energy Levels fit DFT & Dev. Modeling & Exp.
  – One state identified specifically from Carbon Dimer Defect.

• Transition Region: Mobility Degradation due to Disruptions in Bloch Functions and Increased Density of States.
  – Non-Stoichiometric Substitutions and Interstitials in SiC side of Interface
  – Oxygen substituting for Carbon and Carbon Interstitials identified and key Non-Stoichiometric Structures in TR.
Interpretation of the Interface from Device and DFT Simulations and Experiment
Summary of Key Results: Passivation

• Nitrogen:
  – Passivates Carboxyl Defects in Oxide
  – Passivates carbon interstitials
  – But too much N generates more (+) charge & more states near CB.
  – Gives rise to counter doping layer at interface
    • Improves field effect mobility mainly due to counter doping.
Next, Dev Ettissery will explain new reliability work on atomic origin of E’ centers in SiO$_2$

Virtually all results have been published in JAP an IEEE with details provided.