Overview of Modeling and Simulation
TCAD - FLOOPS / FLOODS
A 21st Century Approach to Reliability

Outline

• Modeling Overview
  – Strain Effects
  – Thermal Modeling

• TCAD Modeling
  – FLOOPS / FLOODS Introduction
  – Progress on GaN Devices
  – Prospects for Reliability Simulation
Self-consistent Procedure

- $k\cdot p$ self-consistent solution to Poisson and Schrödinger’s equation

$$- \frac{d^2}{dz^2} V(z) = q / \varepsilon_S [N(z) + N_D(z)]$$

$$\left[ \frac{P^2}{2m} + V(z) \right] \Psi_n(z) = E \Psi_n(z)$$

$$N(z) = 2 \sum_n | \Psi_n(z) |^2 f_{2D}(E)$$
In and Out-of-Plane Masses (Ge)

Biaxial Stress

Uniaxial Stress

Using $k \cdot p$ methods to compute bands

A 21st Century Approach to Reliability
Confinement and Strain Sub-band Shifts

Low Vertical Field

High Vertical Field

SiO₂

Splitting (increases) / (decreases)
under confinement

Band splitting due to strain

Uniaxial

Biaxial

E_v

E_{top}

E_{second}
Same Physics for IV, III-V Materials

Si

Ge

GaAs

Unstressed  1GPa Biaxial Tension  1GPa Uniaxial Compression
Thermal Simulations

- Use finite element modeling to optimize package design
- Most important factors in thermal management: heat transfer at the system boundaries and substrate thickness
- Couple w/ FLOOPS / FLOODS simulations as well
Thermal Simulations and IR Imaging

- $T(\text{Junc})$ of power devices is often significantly hotter than $T(\text{stage})$
- Accurate extraction of activation energy requires knowledge of the true channel temperature.
- We have extensive experience in estimating heat transfer even in complex structures.
- Purchasing a high-resolution IR camera for direct imaging of the device operating temperature. We have collaborated with Nitronex on thermal imaging—a typical example is shown at right for a multi-finger power HEMT.

- Possible Collaborations w/ Samuel Graham, Georgia Tech
Outline

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  – Thermal Modeling
  – TCAD Based Approaches

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FLOOPS / FLOODS

- Object-oriented codes
- Multi-dimensional
- $P = \text{Process} / D = \text{Device}$ 90% code shared
- Scripting capability for PDE’s - Alagator

- Commercialized - ISE / Synopsis
  - Sentaurus - Process is based on FLOOPS
- Licensed at over 300 sites world-wide
  - 2008 release
  - Manual is online (but needs updating)
What is Alagator?

- Scripting language for PDE’s
- Parsed into an expression tree
- Assembled using FV / FE techniques
- Stored in hierarchical parameter data base

- Models are accessible, easily modified
What is Alagator?

<table>
<thead>
<tr>
<th>Operator</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>“ddt”</td>
<td>Time derivative</td>
</tr>
<tr>
<td>“grad”</td>
<td>Spatial derivative</td>
</tr>
<tr>
<td>“sgrad”</td>
<td>Scharfetter / Gummel Discretization Operator</td>
</tr>
<tr>
<td>“dot”</td>
<td>Returns the dot product of the gradient of two field – electric field in direction of current floq</td>
</tr>
<tr>
<td>“elastic”</td>
<td>Compute elastic forces - FEM balance</td>
</tr>
</tbody>
</table>

- Example use of operators for diffusion equation
- Fick’s Second Law of Diffusion
  - $ddt(Boron) - 9.0e-16 \times grad(Boron) - K \times (Boron - Trap)$
  - $\partial C(x,t) / \partial t = D \partial^2 C(x,t) / \partial x^2$
Strained PMOS

- To enhance channel mobility, PMOS strain processing includes embedded SiGe in the source/drain regions and compressive capping layers.
- FLOOXS predicts strain/stress profiles where the channel stress is ~1 GPa.

Cheng, et al. IEDM 2007
Horstmann, et al. IEDM 2005

FLOOXS predicted stress profile [dyne/cm²]
(YY component - channel direction)
Complex Mobility Models Construction

Unifies the description of majority and minority carrier bulk mobilities
• temperature dependence
• electron–hole scattering
• screening of ionized impurities by carriers
• clustering of impurities

Surface scattering terms (Vertical Field)
Velocity Saturation
EffMass changes w/ strain (more later)
**Piezoresistance**

- Piezoresistivity is the change in electrical resistivity with mechanical stress and involves the relationships between electric field $E_i$, current density $J_j$, and mechanical stress $\sigma_{kl}$.

$E_i = (\rho_{ij} + \Pi_{ijkl} \sigma_{kl}) J_j$

(Small Change Limit)

$$
\begin{bmatrix}
- \Delta \mu_{xx} / \mu_{xx} \\
- \Delta \mu_{yy} / \mu_{yy} \\
- \Delta \mu_{zz} / \mu_{zz} \\
- \Delta \mu_{yz} / \mu_{yz} \\
- \Delta \mu_{zx} / \mu_{zx} \\
- \Delta \mu_{xy} / \mu_{xy}
\end{bmatrix}
= 
\begin{bmatrix}
\Delta \rho_{xx} / \rho_{xx} \\
\Delta \rho_{yy} / \rho_{yy} \\
\Delta \rho_{zz} / \rho_{zz} \\
\Delta \rho_{yz} / \rho_{yz} \\
\Delta \rho_{zx} / \rho_{zx} \\
\Delta \rho_{xy} / \rho_{xy}
\end{bmatrix}
= 
\begin{bmatrix}
\pi_{11} & \pi_{12} & 0 & 0 & 0 \\
\pi_{12} & \pi_{11} & \pi_{12} & 0 & 0 \\
\pi_{12} & \pi_{12} & \pi_{11} & 0 & 0 \\
0 & 0 & 0 & \pi_{44} & 0 \\
0 & 0 & 0 & 0 & \pi_{44} \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\sigma_{yz} \\
\sigma_{zx} \\
\sigma_{xy}
\end{bmatrix}
$$

Mobility Change \quad Resistivity Change \quad Piezoresistance coefficients \quad Stress components

$$
J_{n,p} = - q n \mu_{n,p} \nabla \phi_{n,p}
$$

$$
\begin{bmatrix}
J_X (\sigma) \\
J_Y (\sigma) \\
J_Z (\sigma)
\end{bmatrix}
= 
\begin{bmatrix}
1 - \Delta \mu_{xx} / \mu_{xx} & - \Delta \mu_{xy} / \mu_{xy} & - \Delta \mu_{xz} / \mu_{xz} \\
- \Delta \mu_{yx} / \mu_{yx} & 1 - \Delta \mu_{yy} / \mu_{yy} & - \Delta \mu_{yz} / \mu_{yz} \\
- \Delta \mu_{zx} / \mu_{zx} & - \Delta \mu_{zy} / \mu_{zy} & 1 - \Delta \mu_{zz} / \mu_{zz}
\end{bmatrix}
\begin{bmatrix}
J_X (0) \\
J_Y (0) \\
J_Z (0)
\end{bmatrix}
$$
Piezoresistance example

- Silicon beam with an n-type surface
- Bending induces tensile stress at the surface resulting in an increase in mobility and current.

\[
J_X(\sigma) \equiv \left(1 + \frac{-\Delta \mu_{xx}}{\mu_{xx}}\right)J_X(0) = (1 + \pi_{11} \sigma_{xx})J_X(0)
\]
**Piezoresistance**

- The gradient of the quasi-fermi level gives $J_{n,p}$ vector values for each element

\[
J_{n,p} = -q\eta \mu_{n,p} \nabla \phi_{n,p}
\]

\[
\begin{bmatrix}
J_X(0) \\
J_Y(0)
\end{bmatrix} =
\begin{bmatrix}
1 - \Delta \mu_{xx} / \mu_{xx} & -\Delta \mu_{xy} / \mu_{xy} \\
-\Delta \mu_{xy} / \mu_{xy} & 1 - \Delta \mu_{yy} / \mu_{yy}
\end{bmatrix}
\begin{bmatrix}
J_X(0) \\
J_Y(0)
\end{bmatrix}
\]

- Piezoresistance coefficient matrix can be defined for any orientation using directional cosines

\[
\pi_{ijkl}' = \sum_m \sum_n \sum_o \sum_p a_{mi} a_{nj} a_{ok} a_{pl} \pi_{mnop}
\]

\[
\begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{bmatrix} =
\begin{bmatrix}
cos\phi cos\theta & -sin\phi & cos\phi sin\theta \\
sin\phi cos\theta & cos\phi & sin\phi sin\theta \\
-sin\theta & 0 & cos\theta
\end{bmatrix}
\]
Piezoresistance

- Piezoresistance coefficients can be set to spatially vary in FLOODS
  - Extracted channel and bulk coefficients different (to do)
- Piezoresistance coefficients are function of impurity concentration and temperature $P(N,T)$

$$P_{n,p}(N,T) = \frac{300 F_{s+(1/2)}(E_{F_{n,p}}/(k_B T))}{T F_{s+(1/2)}(E_{F_{n,p}}/(k_B T))}$$


FLOODS simulated piezoresistance factor for $T=300$ K
Strained PMOS Simulations

- PMOS with $L_{\text{gate}} = 30$ nm
- $<110>$ channel orientation
- 2007 ITRS dimensions
- Charge strike dist. in drain

PMOS Current Transient ($V_{gs} = -1.0$ V, $V_{ds} = -1.0$ V)

PMOS Current Transient ($V_{gs} = 0$ V, $V_{ds} = -1.0$ V)
Double-Gate FinFET

- $L_{\text{gate}} = 18 \text{ nm}$, $w_{\text{si}} = 11 \text{ nm}$
- Midgap metal gate (typically TiN)
- Gate-S/D doping underlap to control $V_t$ and short channel effects
- Undoped body

FinFET top cross-sectional view

nFinFET I-V characteristic
AlGaN/GaN HEMT Device

- Can handle heterostructure bands
- Gate offsets
- Field Dependence

Energy Band Diagram

Sample IV curve
Edge Termination

- Edge termination is critical for obtaining high breakdown voltage and reduced on-state resistance.
- Severe electric field crowding around metal contact periphery.
- High leakage current and breakdown at the highest electric field
V_B values are highly sensitive to the charge in the JTE layer.

- Multiple JTE termination technique (JTE1 + JTE2).
Reliability Simulation

- Simulate Device in Quasi-Steady State
  - Electrons and Holes equilibrate quickly
  - Similar to assumption in process simulation
- Generation Events Triggered by
  - Mechanical Stress
  - Current Flow / Electric Field
- Simultaneous solutions
  - Point Defects / Defect Cluster / Interface Capture
  - Hydrogen

TNS, TBP
Vanderbilt + UF
Example: 3.2μm x 90nm bulk nMOSFET

Low frequency measured and simulated noise data

Graphical depiction of Noise Producing oxide trap locations on mesh for simulating the low frequency noise features. Location 1 has 4 traps, locations 2 and 3 0.5 traps each.
Conclusions

• Modeling Integrated
  – Fundamental Physics k•p feeds TCAD
  – Thermal coupled to TCAD

• Experimentally Integrated
  – Failure Mechanism Identification feeds M&S
  – Electrical Measurement feeds