Overview of Modeling and Simulation
Drs. Law, Bosman, Nishida, Thompson
Outline

• Modeling Overview
• Strain Effects
• Noise Modeling
• Device Simulation Development
• Directions
A 21st Century Approach to Reliability

Research Work Plan

Thrust 1
Commercial Parts
Test Structure Fab either in house or partnerships

UF Developed Testing Station - Mech, Elec, Temp

Thrust 3
Failure Analysis - Materials and Electrical, Statistical

Thrust 2, 3, 5
Simulation & Modeling

Insights into New Testing Strategies, Better Lifetime Prediction and Scaling, Improved Device Behavior and Design

Research Goal
FLOOPS / FLOODS

• Object-oriented codes
• Multi-dimensional
• P = Process / D = 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 (building a wiki manual)
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 flow</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**
  - \( \text{ddt}(\text{Boron}) - 9.0\times10^{-16} \times \text{grad}(\text{Boron}) - K \times (\text{Boron} - \text{Trap}) \)
  - \( \frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2} \)
Outline

- Modeling Overview
- Strain Effects
- Noise Modeling
- Device Simulation Development
- Directions
Simulation Capability—Band Structure

- **Tight binding method.**
  - relatively simple and gives whole band structure
  - straightforward microscopic picture of how strain affects inter-atomic interactions

- **k·p method.**
  - semi-empirical parameters for greater accuracy at the Γ point
  - physical parameters such as momentum-matrix elements and eigen-energies
  - strain effect incorporated through deformation potential

We heavily use k·p method \([1]\) since it is semi-empirical and more accurate provided accurate deformation potentials are used.

- effective mass
- mobility enhancement
- threshold voltage shift
- gate leakage change

The Hamiltonian

\[ H = H_0 + \frac{\hbar^2 k^2}{2m_0} + H_{so} + \frac{\hbar}{m_0} k \cdot p + H_{strain} \]

Conduction and valence bands Hamiltonian

- Conduction band
  \[ H^c (k_l, k_z) = \left( \frac{\hbar^2}{2} \right) \left( \frac{k_l^2}{m_e^l} + \frac{k_z^2}{m_e^z} \right) + E_c + H_{strain} \]

- Valence band
  \[ H_{6\times6}^v (k) = \begin{bmatrix} H_{3\times3}^U (k) & 0 \\ 0 & H_{3\times3}^L (k) \end{bmatrix} + H_{strain} \]

where

\[ H_{3\times3}^U (k) = \begin{bmatrix} F & K & -iH_i \\ K & G & \Delta - iH_i \\ iH_i & \Delta + iH_i & \lambda \end{bmatrix} \]

and

\[ H_{3\times3}^L (k) = \text{conj}(H_{3\times3}^U (k)) \]


Deformation potential basis to construct the strain Hamiltonian
**Inverse Piezoelectricity**: Strain actuated by applied electric field

1) Applied electric field $E_{\text{ext}}$

2) $E_{\text{ext}} \rightarrow$ Polarization $P_z$

3) $P_z \rightarrow$ In-plane strain $\epsilon_{xx}$

\[
\begin{pmatrix}
P_x \\
P_y \\
P_z
\end{pmatrix} =
\begin{pmatrix}
0 & 0 & 0 & e_{15} & 0 \\
0 & 0 & 0 & e_{15} & 0 \\
e_{31} & e_{31} & e_{33} & 0 & 0
\end{pmatrix}
\begin{pmatrix}
\epsilon_{xx} \\
\epsilon_{yy} \\
\epsilon_{zz} \\
\epsilon_{yz} \\
\epsilon_{zx}
\end{pmatrix}
\]

\[
\epsilon_{xx} = \epsilon_{yy} = \frac{C_{33}}{2(e_{31} C_{33} - e_{33} C_{13})} P_z
\]

GaN: $e_{31} = -0.32$, $e_{33} = 0.63$

AlN: $e_{31} = -0.38$, $e_{33} = 1.29$

Under typical HEMT operation bias ($V_{DG} \sim 20V$), additional strain induced by inverse piezoelectricity is around 0.1% (500MPa).

[JAP, vol. 84, pp. 4951, 1998]
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)
Piezoresistance example

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

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

- **No Strain**
- **Strained**

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

- **No Strain**
- **Strained**
Inverse Piezoelectric Effect Calculation

- Mechanical Simulation with Piezo Terms
- Simple test case - MOS Cap on Piezo Material
- Asymmetry in the strain due to change in direction in the horizontal field across the gate
Outline

- Modeling Overview
- Strain Effects
- Noise Modeling
- Device Simulation Development
- Directions
Noise Simulation Progress to date

The current version of FLOODS was upgraded, with the help of Juan Sanchez PhD, to include:

- Small signal AC simulation for calculating channel and transfer impedance and transconductance
- Velocity fluctuation and defect noise simulation
- External circuit elements
Modeling of defects

- Random carrier transitions between continuum states \((E_C, E_V)\) and localized defect states.

**Shockley-Read-Hall Model**

Four basic equations with one trap level added, 3+N with N trap levels:

\[
F_\psi = -\frac{d^2 \psi}{dr^2} - \frac{q}{\varepsilon} \left[ p - n + N_D^+ - N_A^- - n_t \right] = 0
\]

\[
F_n = \frac{dn}{dt} - \frac{1}{q} \nabla \cdot J_n - g_n + r_n - \gamma_n(r,t) = 0
\]

\[
F_p = \frac{dp}{dt} + \frac{1}{q} \nabla \cdot J_p - g_p + r_p + \gamma_p(r,t) = 0
\]

\[
F_{n_t} = \frac{dn_t}{dt} + g_n - r_n - g_p + r_p - \gamma_t(r,t) = 0
\]
Noise terms

- Fluctuations in $\mathcal{A}$ perturbs the charge in the system
  - Add noise terms to trapped electron continuity equation
- Fluctuations in $n$ and $p$
  - Add noise terms to both the electron and hole continuity equations
- Noise source terms are expressed in defect activation energy, defect density and capture cross-section.
- G-R noise source strength in each differential volume is mapped to the external contact using scalar Green's function (in contrast with Diffusion and Hooge noises which use vector Green's function)

$$
S_{V,gr} = \sum_{i=1}^{N_{trap}} \sum_{\alpha=\psi,n,p} \tilde{G}_\alpha K_{\gamma_{ai},\gamma_{ai}} \tilde{G}_\beta^* \, dr
$$
Noise Source Mapping

$S_{V,gr}$

$K_{\gamma,gr}$

$\tilde{G}$
Noise Decomposition Normal S-D Operation

Noise Fitting ($V_{DS}=0.060$)

GR Noise and 1/f Noise

$$S_{ID}(f) = \frac{q\mu \alpha_H I_D V_{DS}}{L^2 f}$$

Approximate Hooge Parameter $\alpha_H = 2.56 \times 10^{-3}$

Characteristic Relaxation Time ($\tau_c$) for GR Noise

<table>
<thead>
<tr>
<th>Trap 1</th>
<th>Trap 2</th>
<th>Trap 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>14.4 ms</td>
<td>132.7 µs</td>
<td>1.06 µs</td>
</tr>
</tbody>
</table>
Brute Force Approach: Start with a 4x4 Jacobian matrix system with 1 trap level, or a (3+N) x (3+N) system with N trap levels. The noise Jacobian matrix becomes

\[
\begin{bmatrix}
\frac{dF_\psi}{d\psi} & \frac{dF_\psi}{dn} & \frac{dF_\psi}{dp} & \frac{dF_\psi}{dn_t} \\
\frac{dF_n}{d\psi} & \frac{dF_n}{dn} & \frac{dF_n}{dp} & \frac{dF_n}{dn_t} \\
\frac{dF_p}{d\psi} & \frac{dF_p}{dn} & \frac{dF_p}{dp} & \frac{dF_p}{dn_t} \\
\frac{dF_{n_t}}{d\psi} & \frac{dF_{n_t}}{dn} & \frac{dF_{n_t}}{dp} & \frac{dF_{n_t}}{dn_t} + j\omega
\end{bmatrix}
\begin{bmatrix}
\vec{\psi} \\
\vec{n} \\
\vec{p} \\
\vec{n_t}
\end{bmatrix} =
\begin{bmatrix}
0 \\
\vec{\gamma}_n \\
-\vec{\gamma}_p \\
\vec{\gamma}_{n_t}
\end{bmatrix}
\]
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.
Outline

• Modeling Overview
• Strain Effects
• Noise Modeling
• Device Simulation Development
• Directions
HEMT Structure

A 21st Century Approach to Reliability
Quasi-Fermi Approach

- Quasi-Fermi levels are energy levels used to specify the carrier concentrations under *none*quilibrium conditions
  - Similar to Fermi level for equilibrium conditions
  - Two energy levels
    - \( Q_{fn} \): Quasi-Fermi level for electrons
    - \( Q_{fp} \): Quasi-Fermi level for holes
- Streamlined approach for heterostructure device simulation
  - Helps define electron and hole concentrations continuously across the interface
  - Quasi-Fermi level that varies with position indicates current flow
- Affects:

  \[
  \begin{align*}
  p &= N_v e^{(E_V - Q_{fp})/kT} \\
  n &= N_c e^{(Q_{fn} - E_V)/kT} \\
  \frac{dp}{dt} &= \mu_p p \nabla Q_{fp} \\
  \frac{dn}{dt} &= \mu_n n \nabla Q_{fn}
  \end{align*}
  \]
A 21st Century Approach to Reliability

At equilibrium
\[ V_G = 0 \text{V} \quad V_D = 0 \text{V} \]

After gate bias
\[ V_G = -1 \text{V} \quad V_D = 0 \text{V} \]

Reverse bias at Schottky G contact
Bands bend up to achieve pinch-off
Mobility Model

Future work on strain-induced polarization demands a robust mobility model which includes field dependence.

  - Low-field mobility
    - Drift-diffusion
      - Influence of temp (T) and ionized impurity concentration (N)
      - $\mu_{\text{max}}, \mu_{\text{min}}, \alpha, \beta_{1-4}$
        - Parameters from Farahmand
      
  
  - High-field mobility
    - Low-field + field dependent mobility
      - E: Electric field
      - $E_c, v_{\text{sat}}, a, n_1, n_2$
        - Parameters from Farahmand

\[
\mu_0(T, N) = \mu_{\text{min}} \left( \frac{T}{300} \right)^{\beta_1} \\
+ \frac{(\mu_{\text{max}} - \mu_{\text{min}}) \left( \frac{T}{300} \right)^{\beta_2}}{1 + \left[ \frac{N}{N_{\text{ref}} \left( \frac{T}{300} \right)^{\beta_3}} \right]^\alpha(T/300)^{\beta_1}}
\]

\[
\mu = \frac{\mu_0(T, N) + v_{\text{sat}} E^{n_1-1}}{1 + a \left( \frac{E}{E_c} \right)^{n_2} + \left( \frac{E}{E_c} \right)^{n_1}}
\]
Interface Charge Effect

- Interface charge added with easy single command line
- Positive charge at interface draws in electrons
- Increased interface charge leads to larger 2DEG current and higher $v_{Dsat}$
- Link to strain calculations

Interface charge 1.2e13

Interface charge 2.0e13
Hydrogen Trapping 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
Material Flow Simulation

- Crude electromigration simulation
- Density is lowest where field is highest (corner)
- Field driven kickout mechanism
Conclusions

• Modeling Integrated
  – Fundamental Physics k•p feeds TCAD

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

• Connect strain calculations

• Temperature / Traps