



Simulating Hydrogen Transport and Single-Event Transients

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RUTGERS



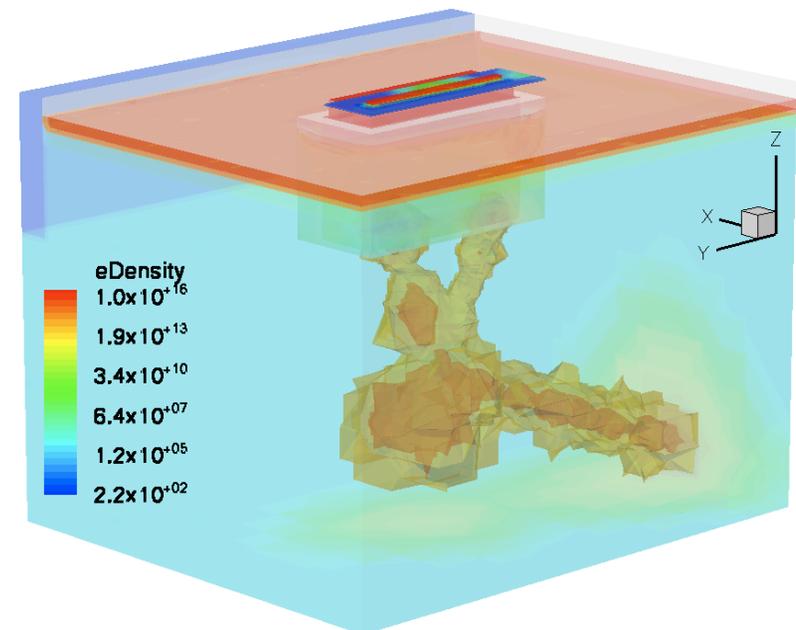
FEAR THE SWAMP

ONLY GATORS GET OUT ALIVE



Objectives and Outline

- Provide device simulation environment for rad-hard applications (both SET and degradation)
- Address Rad-Hard specific issues
 - Numeric - discretization, parallel
 - Physics - strain, mobility
 - Coupled Device / Defect



FLOOPS / FLOODS / FLOORS

- Multi-dimensional, Object-oriented codes
- P = Process / D = Device 90% code shared
- Scripting capability for PDE's - Alagator
- Commercialized - ISE / Synopsys
 - Sentaurus - Process is based on FLOOPS
- Licensed at over 300 sites world-wide
- Fick's Second Law of Diffusion
 - $\text{ddt}(\text{Boron}) - 9.0\text{e-}16 * \text{grad}(\text{Boron})$
 - $\partial C(x,t) / \partial t = D \partial^2 C(x,t) / \partial x^2$
- All physics is defined on the command line
- Rapidly evolve models for new devices / materials / physics

FLOOXs User Guide (Wiki)

- New FLOOPS/FLOODS user guide is under development
- The website will include:
 - Device and process simulation examples
 - Alagator scripting language and command examples
 - Code development section

Address:

<http://www.flooxs.ece.ufl.edu>

The screenshot shows a Wiki page titled "FLOOXs Manual" from the University of Florida SWAMP Center. The page has tabs for "page", "discussion", "view source", and "history". The main content area is titled "Device Examples" and contains a "Contents [hide]" section with a numbered list of links: 1 Resistor, 2 P-N Diode, 3 Bulk-Si MOSFET, 4 FinFET, 5 BJT, and 6 Other Useful Resources. Below this, there are sections for "Resistor", "P-N Diode", "Bulk-Si MOSFET", "FinFET", and "BJT", each with a list of example links (e.g., "Resistor example (1D)", "Resistor example (2D)", "PN diode example (1D)", etc.). On the left side, there is a "navigation" menu with links like "Main Page", "Community portal", "Current events", "Recent changes", "Random page", and "Help". Below that is a "search" box with "Go" and "Search" buttons. At the bottom left is a "toolbox" with links like "What links here", "Related changes", "Upload file", "Special pages", "Printable version", and "Permanent link".

Laser-Induced Current Transients in Strained-Si Diodes (NSREC09)

- Single event transients (SETs) and single event upsets (SEUs) are related to collection of radiation-generated charge at sensitive circuit nodes
- Due to the widespread adoption of strained-Si technology, it is important to understand how mechanical stress affects these transient pulses.
- A pn diode is a good representation of the source/drain junctions that are responsible for charge collection in MOSFETs.
- Uniaxial strain engineering has the potential to control the shape of single event transients and collected charges in devices.

Reverse biased
pn diode
(NSREC 09)



Strained
CMOS
(Fall 09)

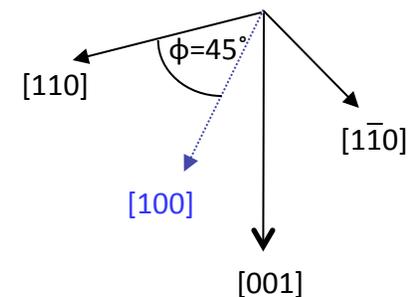
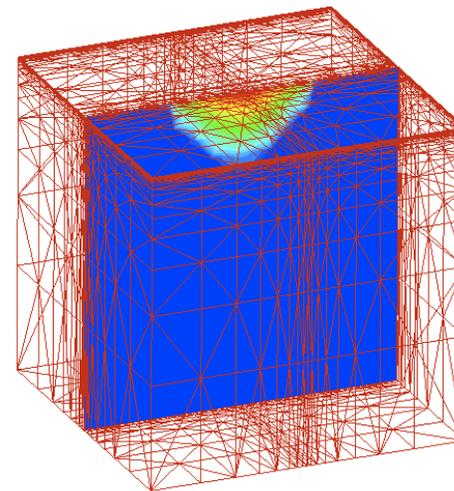
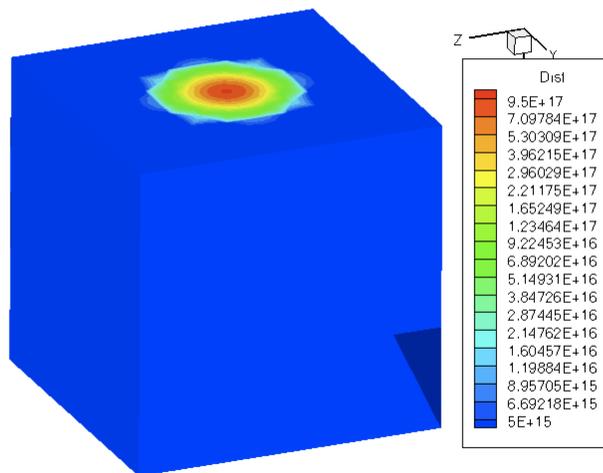


Mixed-mode
CMOS
(2010)

Simulation Setup

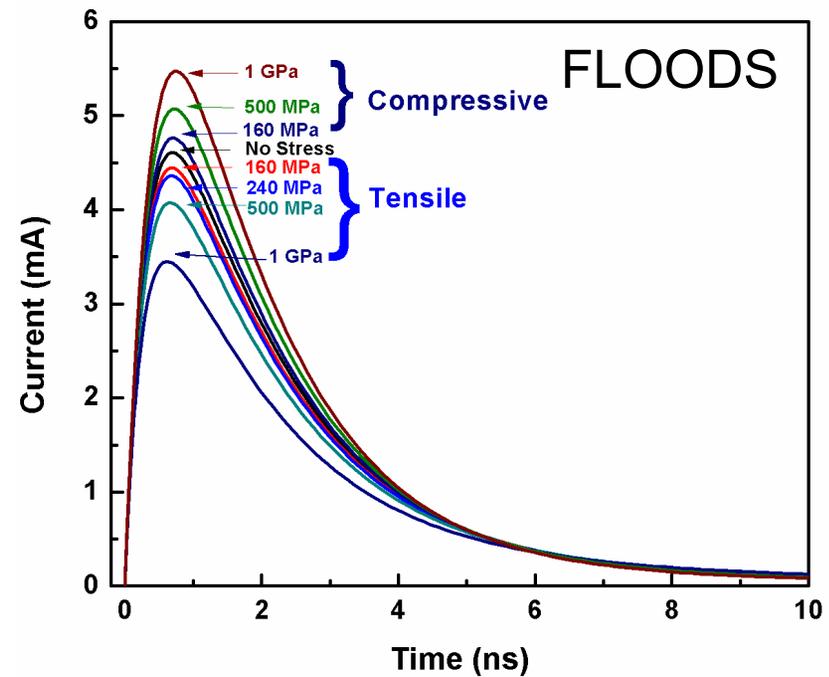
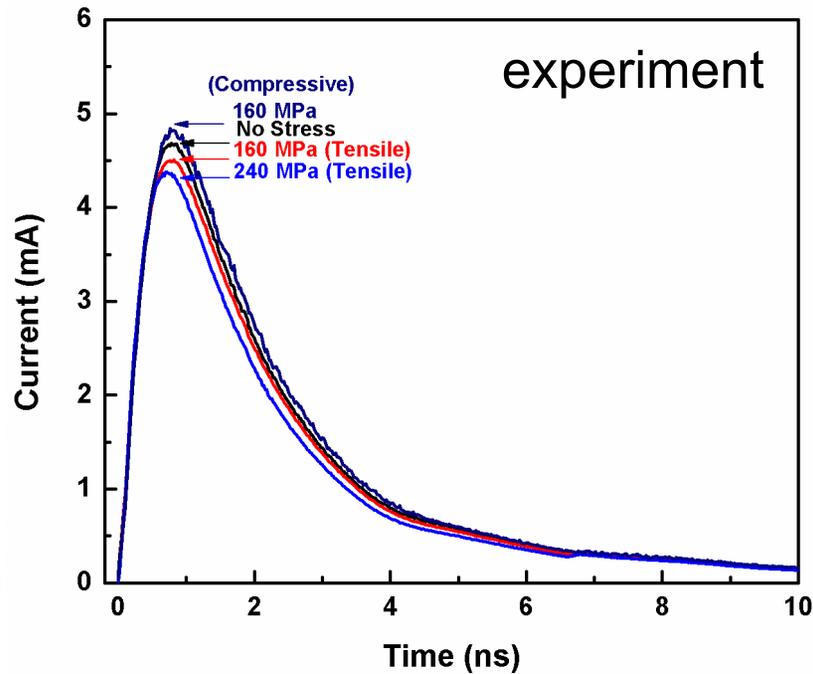
- A reverse-biased n+p diode of dimensions 40 x 40 x 40 μm was created
- Advanced mobility models (Masetti, Brooks-Herring) and recombination models (SRH, Auger) were used
- The number and distribution of electron-hole pairs generated by the laser pulse are calculated by a single photon absorption (SPA) equation.
- The SPA parameters are matched to the values of the laser used for the experiment
- Uniaxial mechanical stress along the $\langle 110 \rangle$ direction was applied

$$N_{1p}(z) = \frac{\alpha}{\hbar\omega} \exp(-\alpha z) I(r, z)$$



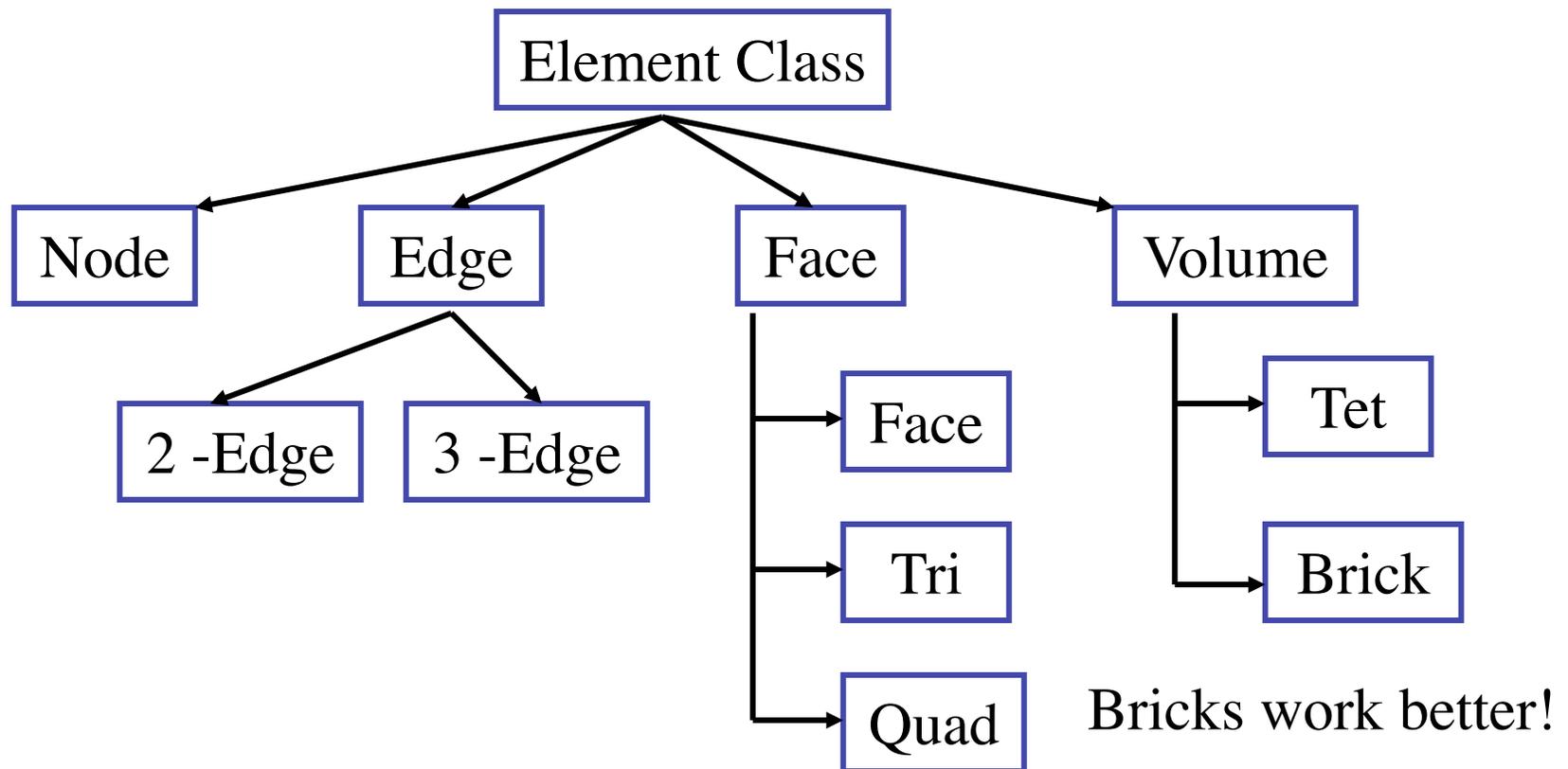
Simulation Results

- FLOODS simulation output shows the same trend as the experimental data
- The change in the collected charge under mechanical stress can be explained by a change of electron mobility in the $\langle 001 \rangle$ direction ($\Delta\mu_n^\perp$)
- The FLOODS predicts that the amount of charge collected under 1 GPa of tensile stress is 22% less than that collected in an unstressed device.



Object Oriented

- Derived Specific Geometry Elements
- Common properties so code is independent

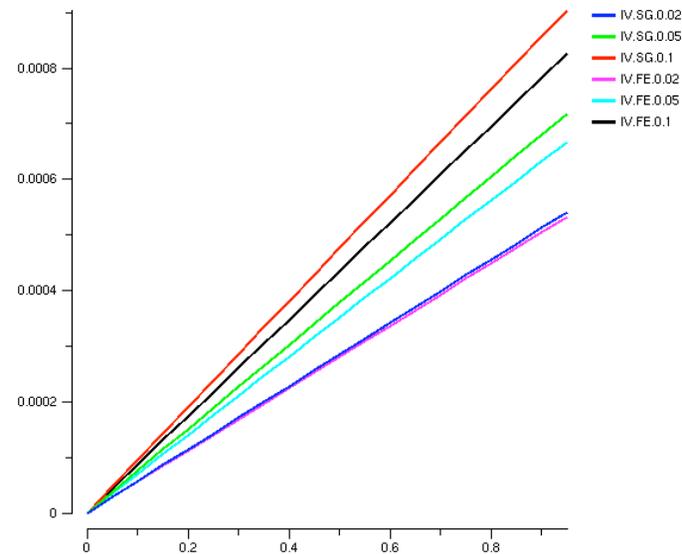
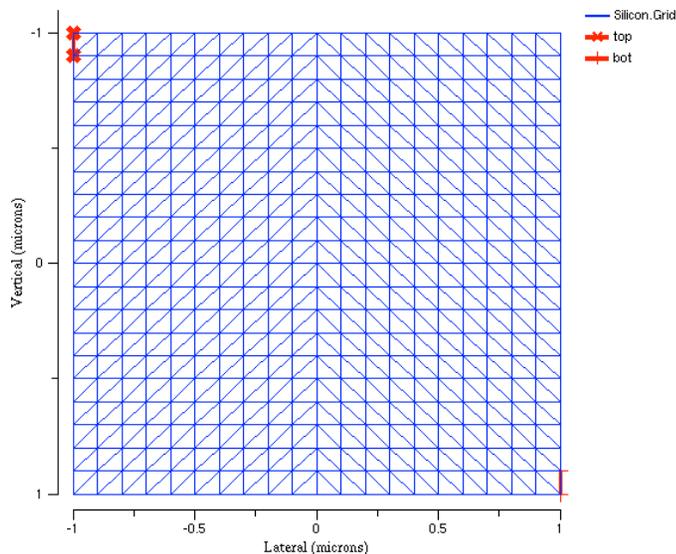


Comparison of Discretization Methods

- Commercial tools use finite volume Scharfetter-Gummel (n, p, ψ) current edge
- Experimental finite element quasi-Fermi levels ($\varphi_n, \varphi_p, \psi$) current continuous

$$J_n = qn\mu_n E + qD_n \nabla n = -q\mu_n n \nabla \phi_n$$

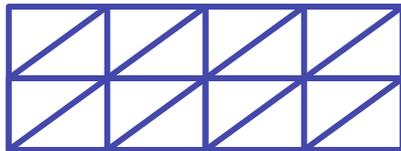
- SG requires grid alignment for accurate answers - not possible in generic rad strike



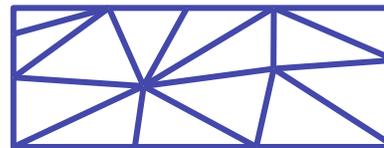
Mesh Element Types

- The quasi-Fermi method takes the $\text{Grad}(Q_f)$ over the element to calculate current density, thus current flow in the QF method is not defined on the edges is in the Scharfetter-Gummel method -> may be better for particle strike transients
- The follow elements were tested using the different discretization methods:

Quad-Diagonal
(FLOODS Default)



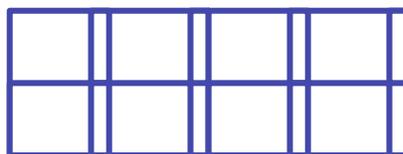
Randomized
Quad-Diagonal



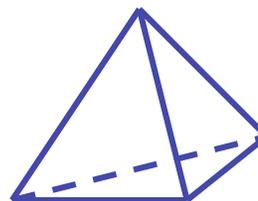
Quad



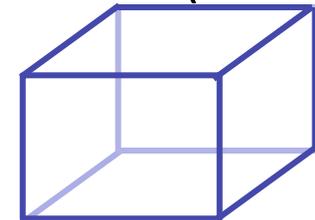
Uneven Quad



Tetrahedron



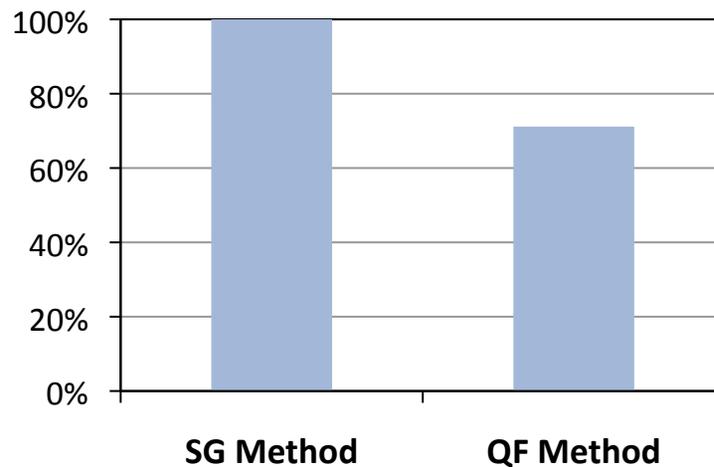
Hexahedron (Brick)



Results Summary

- For 3-D simulations, brick elements offer better solution converge than tetrahedra elements (DC and transient)
- The quasi-Fermi method requires fewer Newton steps to converge for each time step during 3-D charge collection transients. This results in a shorter total simulation time.
- The improved stability of the FEQF method for 3-D charge collection transients may be due to a better handling of isotropic current flow.

**Average 3-D Transient Simulation Time
(normalized)**



FE QF might parallelize better than FV SG

Philips Mobility Model

The Philips mobility model is of an empirical form derived from the Masetti^[2] model (eqn. 20 in ref. [1]).

$$\mu_{e,D+A+j}(N_D, N_A, n, p) = \mu_{e,N} \left(\frac{N_{e,sc}}{N_{e,sc,eff}} \right) \left(\frac{N_{ref,1}}{N_{e,sc}} \right)^{\alpha_1} + \mu_{e,c} \left(\frac{n+p}{N_{e,sc,eff}} \right) \quad [20]$$

$$N_{e,sc,eff} = N_D + G(P_e)N_A + p / F(P_e)$$

Where:

The G and F terms are quantum-mechanic scattering parameters. F varies from 1 to 5 and $\mu_{e,c}$ and $\mu_{e,N}$ are mobility constants.

When $n=p \gg N_D$ or N_A , as in the case of a radiation strike, equation reduces to the following:

$$\mu_{e,D+A+j} \approx \mu_{e,c} \cdot F(P_e) \cdot 2 \quad - > 500$$

Proposed mobility model

The new model reduces mobility with increasing e-h carrier concentration. The proposed mobility model is a modified version of the Klaassen / Masetti^[2] model (lattice and ionized impurity scattering) and is coupled with a classical electron-hole scattering model.

Doping dependent majority

$$\mu_{e,L,I,maj} = \mu_{\min} + \frac{\mu_{\max} - \mu_{\min}}{1 + (N_j / C_R)^{\alpha_1}} - \frac{\mu_1}{1 + (C_S / N_j)^{\alpha_2}}$$

Doping dependent minority

$$\mu_{e,L,I,min} = \mu_{\min} + \frac{\mu_{\max} - \mu_{\min}}{1 + \left(\frac{N_j}{C_R}\right)^{\alpha_1}} - \frac{\mu_1}{1 + \left(\frac{C_S}{N_j}\right)^{\alpha_2}} + \frac{\mu_2}{1 + \left(\frac{N_j}{C_T}\right)^{\alpha_3}}$$

Weighted average approach

$$\mu'_{e,L,I} = \left(\frac{N_D}{N_D + N_A}\right) \cdot \mu_{e,L,I,maj} + \left(\frac{N_A}{N_D + N_A}\right) \cdot \mu_{e,L,I,min}$$

Conwell-Weisskopf^[3,4] e-h scattering
(Brooks-Herring also an option):

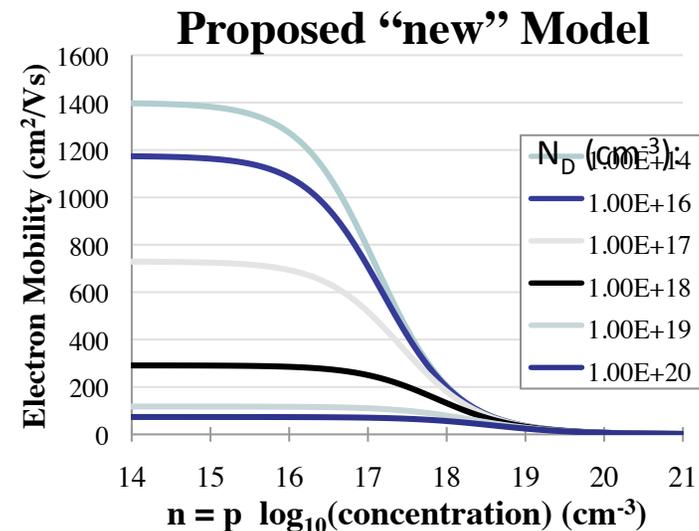
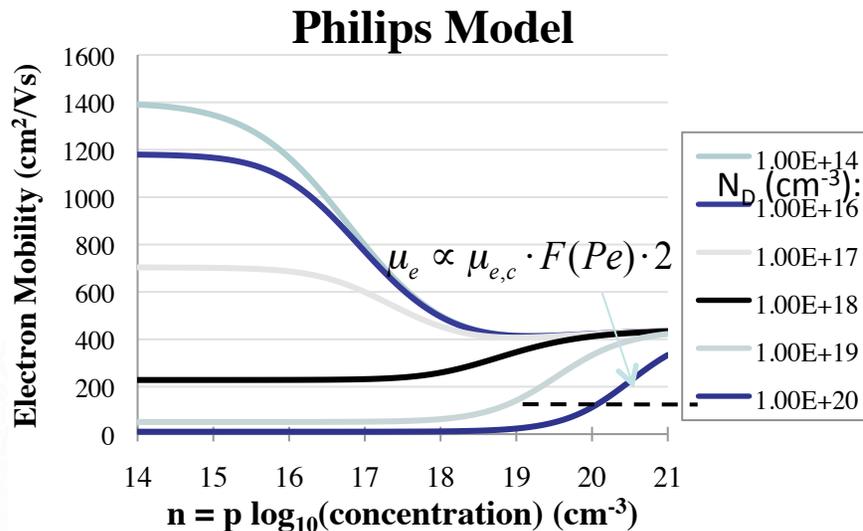
$$\mu_{eh} = \frac{D \left(\frac{T}{T_0}\right)^{3/2}}{\sqrt{np}} \left[\ln \left(1 + F \left(\frac{T}{T_0}\right)^2 (pn)^{-1/3} \right) \right]^{-1}$$

Final Result:

$$\mu_{e,L,I,eh} = \left[\frac{1}{\mu'_{e,j,L,I}} + \frac{1}{\mu_{eh}} \right]^{-1}$$

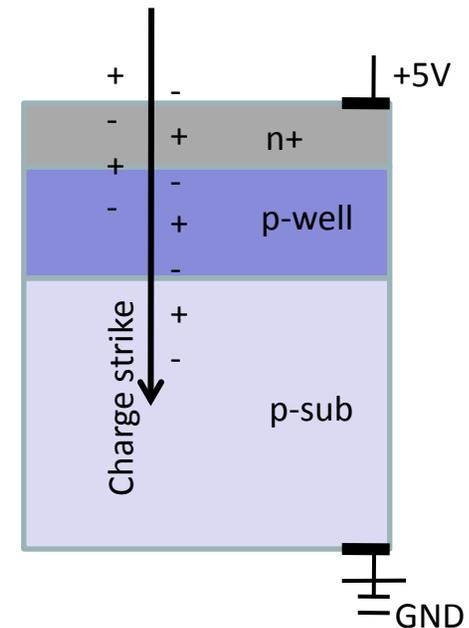
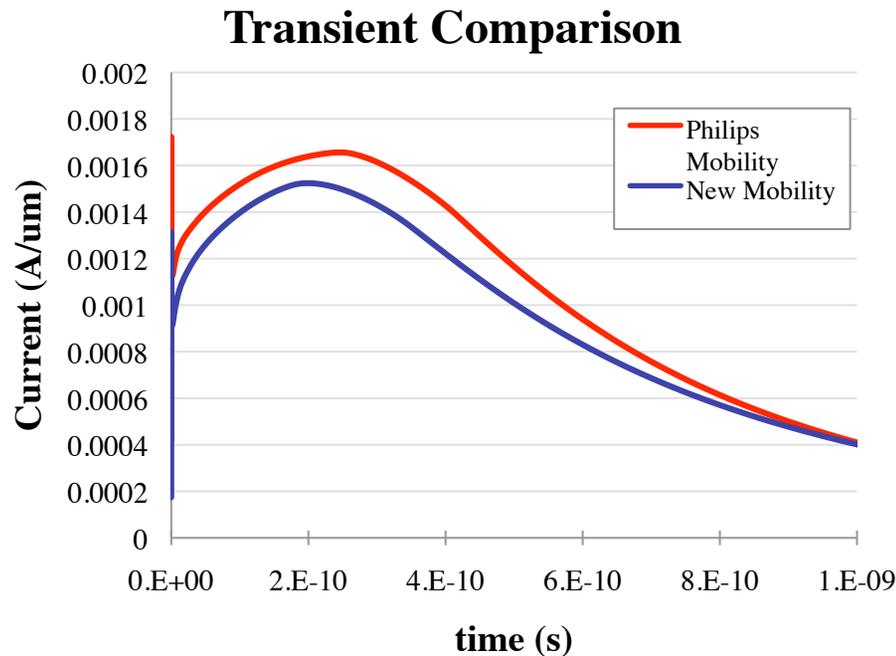
General Comparison

- The Philips mobility model predicts an increase in mobility if $n, p \gg N_D, N_A$ for doping levels more than $\sim 1e18 \text{ cm}^{-3}$
- The below graphs show how the different models treat electron mobility for a varying N_D concentration and increasing $n=p$ carrier levels. $N_A = 1e14 \text{ cm}^{-3}$ is held constant.



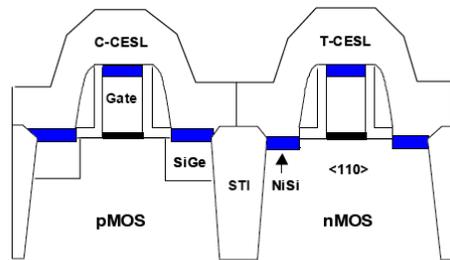
Charge collection simulation

To compare how the models collect charge, a simple 2D reverse-biased diode was simulated in FLOODS. As expected, the higher mobility predicted by the Philips model results in a larger amount of charge collected.

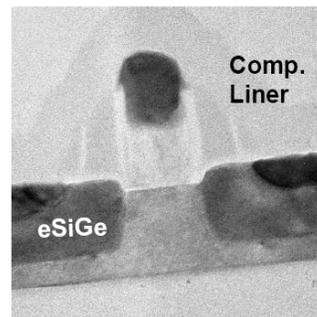


Strained CMOS Devices

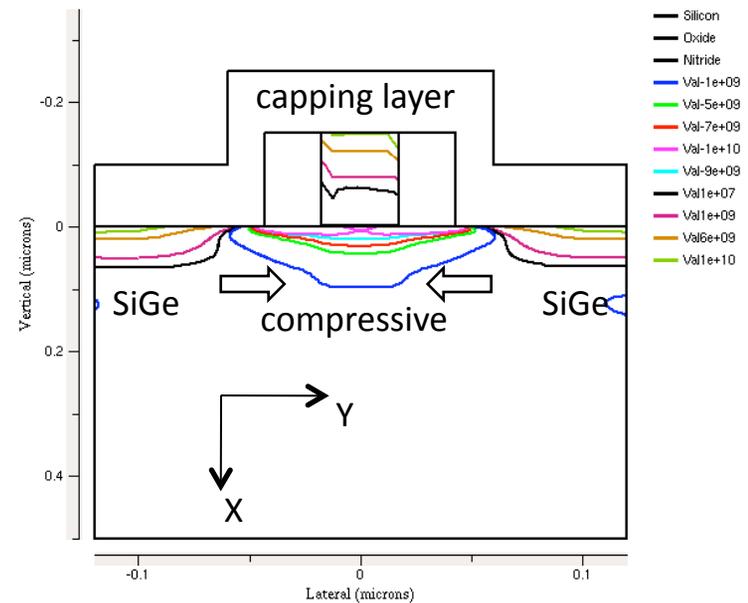
- Following the conclusion of the strained diode work, strained CMOS devices will be looked at in greater detail
- 3-D Strained CMOS devices are now working in FLOODS
- Examining possibility of a mixed-mode SRAM cell simulation (stressed vs. unstressed)
- Mixed-mode option will require new coding



Cheng, et al. IEDM 2007



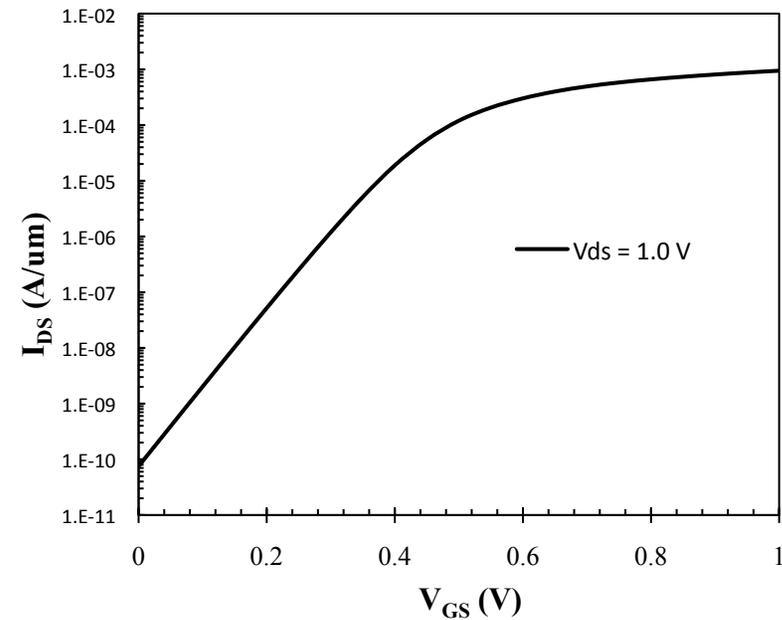
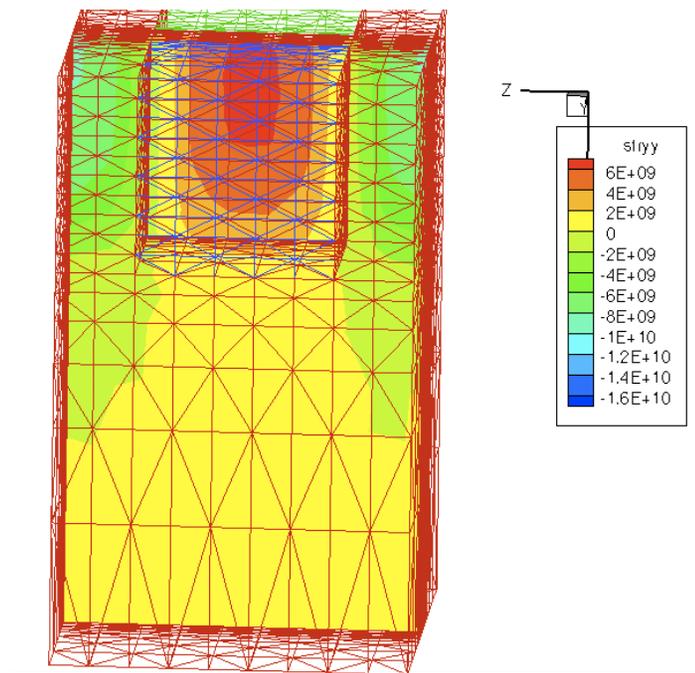
Horstmann, et al. IEDM 2005



FLOODS predicted stress profile [dyne/cm²]
(Y component) ~1 GPa in channel region

Strained Double-Gate FinFET

- In addition to 3-D strained CMOS, 3-D Strained double-gate FinFETs are now working in FLOODS



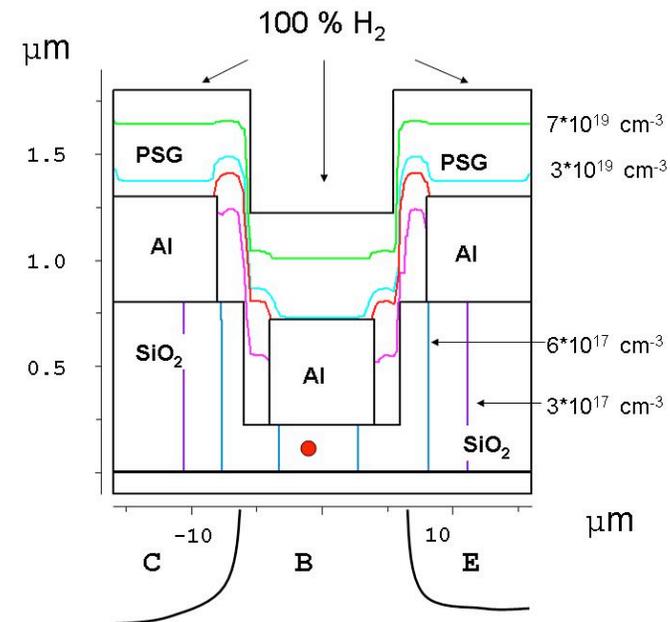
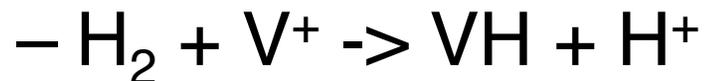
nFinFET I-V characteristic

Hydrogen Trapping Simulation

TNS, TBP

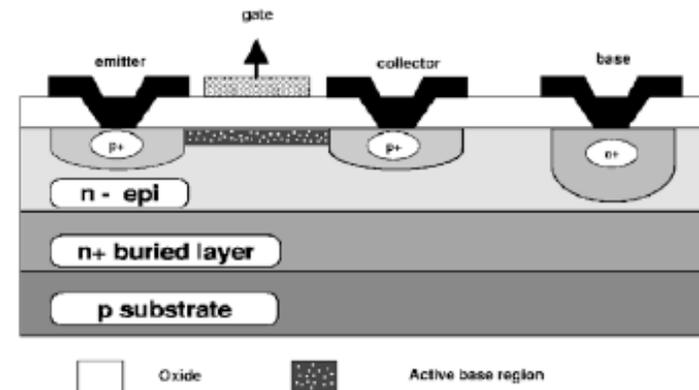
Vanderbilt + UF

- Simulate in Quasi-Steady State
 - Hydrogen Soak Anneals
- Simulate Hole / Hydrogen / Vacancy Interactions in Oxides
 - Simple first order reactions
 - Diffusion + Field Transport
 - Issues with the Chen model
- Build Equations for Proposed Reactions (Tuttle)

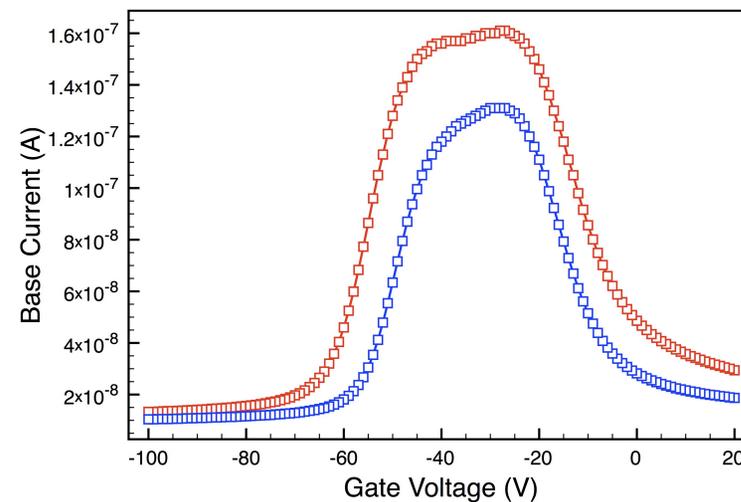


Hydrogen Simulation Development

- Implemented Equations
- TNS Paper Last Year
- Refine the model
- Developed
 - Reaction Add Routine
 - Equation Builder
- Working on right Eqn's
- Collaborate w/ Vandy
 - Hughart's Experiments



Picture from Ball et al., IEEE TNS, 49(2002) p.3185



Summary

Continuing Work:

- Quasi-Fermi method testing, need to understand transient simulation time savings
 - QF method coupled with parallelized code may offer good simulation time benefit
- Non-linear piezoresistive stress model (Hyunwoo Park)
 - Biaxial stress modeling
 - Optimum stress type to minimize SET

Future Work:

- Parallelization of Code using PETSc
- Mixed-Mode Simulation