Progress in PROPHET Project and QM Modeling

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- Features available and under development in PROPHET for device simulation
- Density gradient (DG) approach to QM corrections
- Hybrid empirical approach to QM corrections

Team in PROPHET Project

- Stanford University
- Bell Labs, Lucent Technologies (Dr. C. Rafferty)
- UT Austin (Prof. G. Carey)
- NASA Ames Res. Center (Dr. B. Biegel)
- Naval Res. Lab. (Dr. M. Ancona)

Chronicles in Device Simulation of PROPHET†

(†abbr. device effort)

- Nov. 1996, prototyping thermal diffusion eq. solver in PROPHET. Worked out transformation of $J \cdot E$ term at steady state
- April to Aug. 1997, Dr. Conor Rafferty of Bell Labs stationed in Stanford to formally launch the device effort.
- April 1997, Scharfetter-Gummel current

discretization scheme implemented (Dr. A. Pardhanani)

- July 1997, input file format/syntax has been overhauled, resulting in more natural language interface
- July 1997, electro-thermal system completed and tested for steady state analysis. Resistor and pn diode examples are demonstrated.
- August 1997, the device effort together with results from electro-thermal analysis was introduced in a seminar to HP Labs and in a

presentation of NASA workshop.

- Nov. 1997, dynamic trapping analysis capability has been completed by including the rate eq.
- Nov. 1997, transient analysis of thermal diffusion eq. solver passed test.
- Dec. 1997, for the first time DG model is implemented in 2D analysis and the results for MOS cap/fet analysis are qualitatively correct (e.g. carrier confinement in the inversion layer with repulsive boundary condition at Si/SiO_2).
- Feb. 1998, applied the code with DG model to

MOS capacitor with t_{ox}=31Å. The C-V simulation results agree with those from Poisson/ Schroedinger eq. solver (Bell Labs) almost perfectly and fit measured data quite well.

- April 1998, extensive test with MOS caps. of t_{ox} ranging from 21 to 79Å provided by HP Labs. The results are excellent in re-producing the general trend and caps. in inversion/accumulation regions. The discrepancy in threshold is under investigation.

Available Device Simulation Features in PROPHET

- Drift-diffusion carrier transport (two-carrier continuity eqs. + Poisson's)
- Electro-thermal system with lattice temperature dependence of physical parameters (e.g., mobilities, thermal conductivity, bandgap, effective density of states, and etc.)
- Dynamic trapping analysis by solving trap rate eq.
- Density-gradient transport (quantum potential) for QM corrections.

Features under Development

- Heterostructure
- Mobility degradation due to electric field (both transverse and longitudinal)
- Schroedinger eq. solver
- Hydro-dynamic model
- AC analysis (small signal)
- Circuit boundary conditions (lumped R/L/C)
- Noise analysis

Electro-thermal System Simulation

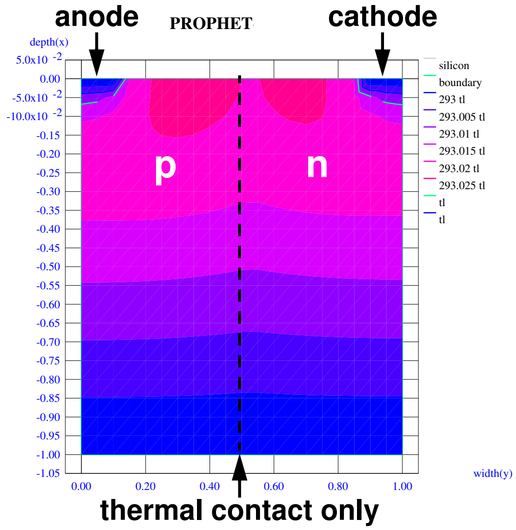
- Transformation of $J \cdot E$ term

$$J \cdot E = \psi(\nabla \cdot J) - \nabla \cdot (\psi J) = -\nabla \cdot (\psi J)$$

The last equality holds only at the steady state, but considerably simplifies the implementation (need only introduce new flux ψJ.

- Independent specification of electrical and thermal boundary conditions

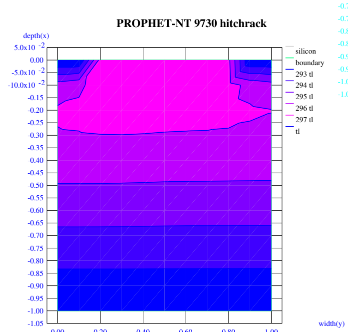
Asymmetric Temperature Distribution in a Symmetric pn Diode

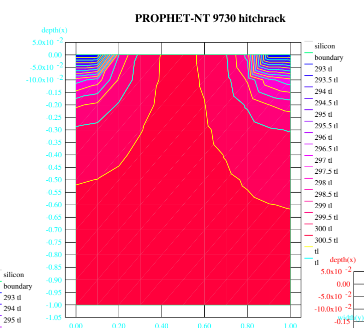


The asymmetry can be explained by the mobility difference for holes and electrons. Due to the higher resistivity in the p-region, the lattice temperature should be higher than that in n-region.

Vertical pn Junction @Vdd = 2V with Different Number of Thermal Contacts

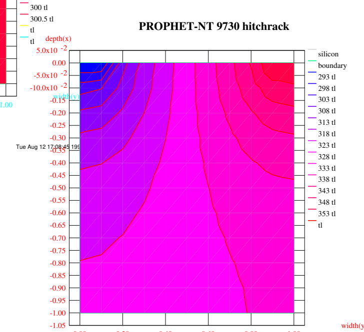
With three thermal contacts: two top and one bottom





Only two top corners are thermal contacts

With only one thermal contact on the top-left corner



Density Gradient (DG) Transport

- Model for carrier flux

$$F_n = n\mu_n \nabla\psi - D_n \nabla n + 2b_n n\mu_n \nabla\left(\frac{\nabla^2\sqrt{n}}{\sqrt{n}}\right)$$

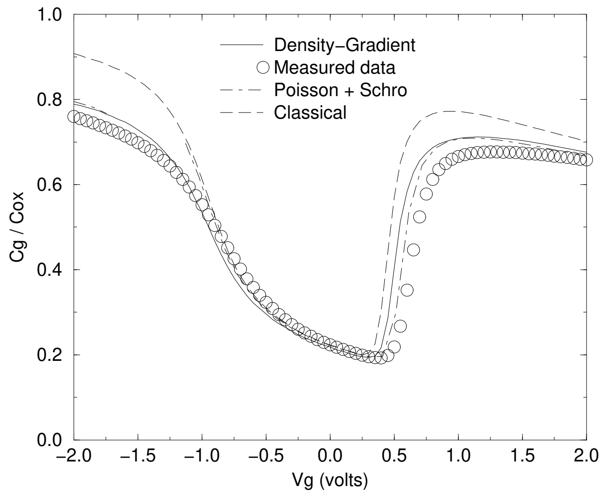
  where $b = \bar{h}^2/(12qm^*)$ representing QM effect and the term $2b_n\nabla^2\sqrt{n}/(\sqrt{n})$ can be identified as "quantum potential".

- The complete system consists of five equations and is to solve for five variables: ψ, n, p, ϕ_n, ϕ_p (ϕ for quasi-Fermi level)

DG System Description

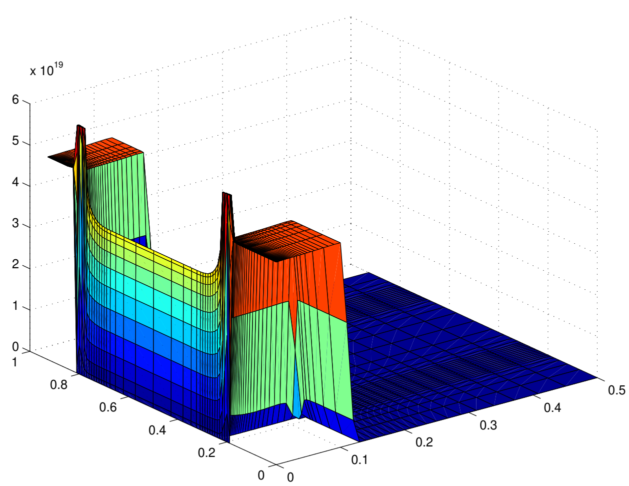
$$\begin{aligned}
-\nabla \cdot (\varepsilon \nabla \psi) &= q(p - n + N_D^+ - N_A^-) \\
\nabla \cdot (n\mu_n \nabla \phi_n) &= g - r \\
\nabla \cdot (-p\mu_n \nabla \phi_p) &= g - r \\
\phi_n - \psi + \frac{kT}{q}\ln\frac{n}{n_i} &= 2b_n\left(\frac{\nabla^2\sqrt{n}}{\sqrt{n}}\right) \\
\phi_p - \psi - \frac{kT}{q}\ln\frac{p}{n_i} &= 2b_p\left(\frac{\nabla^2\sqrt{p}}{\sqrt{p}}\right)
\end{aligned}$$

C-V Simulation of MOS Capacitor with tox=31Å (0.18µm CMOS)



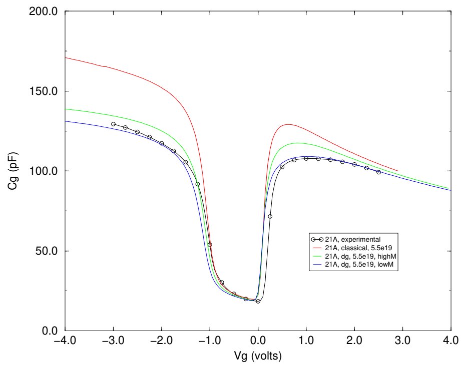
Data provided by HP Labs, and the Poisson/ Schroedinger (P/S) solver from Bell Labs. Note that P/S solver fails to converge in the weak accumulation region. Otherwise, DG provides essentially the same results as does P/S except at the threshold. Both simulations agree with data reasonably well.

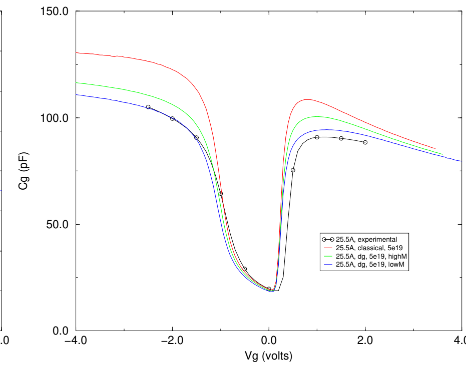
DG Simulation of MOSFET



Bird eye's view of electron distribution under bias of V_{GS}=2V and V_{DS}=0.1V.

Validation Over Tech Generations

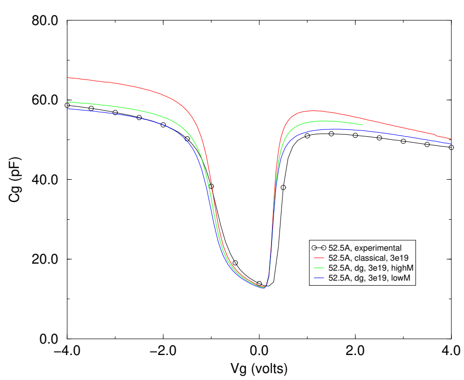


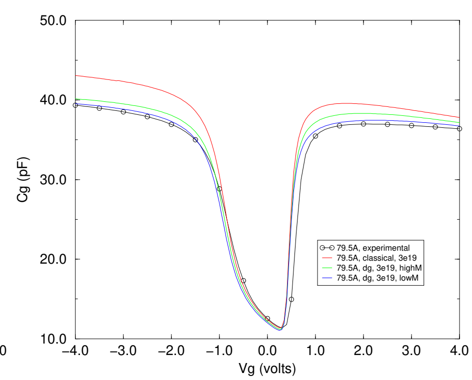


t_{ox} = 21Å, corresponding to <u>0.1µm</u> or below CMOS technology.

t_{ox} = 25.5Å, corresponding to <u>0.13 µm</u> CMOS technology.

Validation (cont'd)





t_{ox} = 52.5Å, corresponding to <u>0.25µm</u> or below CMOS technology.

t_{ox} = 79.5Å, corresponding to <u>0.35 µm</u> CMOS technology.

Hybrid Empirical Approach to QM Corrections

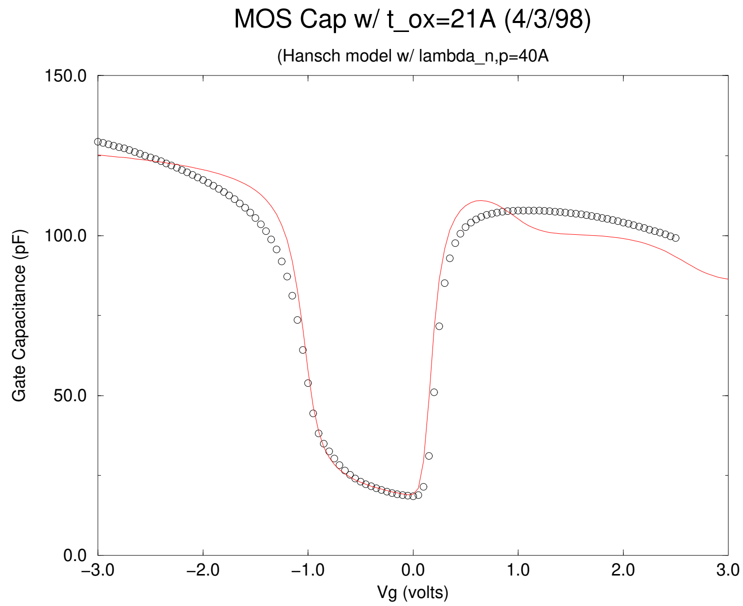
- The manifestation of QM effects in device characteristics:
  - Gate capacitance
  - Threshold voltage
- Two physical mechanisms responsible to these corrections
  - Energy band quantization in the surface potential well
  - Repulsive boundary condition for carriers in Si/SiO2 interf.

Existing Empirical Models and Their Deficiencies

- Hansch's model (1989)
  - Ad hoc shape of carrier profile to model the repulsive boundary condition

$$n(z) = n_{\text{classic}}(1 - e^{-z^2/\lambda^2})$$

  - Smooth C-V in all bias region. However,
  - Characteristic length, λ, is not a function of surface field
  - Not enough correction to the threshold voltage shift and simulated capacitance in accumulation region is flattened.



The trend of simulated capacitance in the accumulation region is not correct (flattened), reflecting the fact that λ in the model does not depend on the surface field. The ripple in the inversion region is an artifact due to lack of generation of minority carriers. It can thus be neglected. Note that the correction to threshold voltage is not enough.

- van Dort's model (1994)
  - Use bandgap broadening to model energy quantization
  - Correction is correlated to the surface transverse field

$$\Delta E_g = \kappa\beta F_S^{2/3}$$

  - With κ as fitting parameter, simulated C-V can fit data very well in both inversion and accumulation regions and threshold voltage shift is adequate
  - The biggest problem is that the model has singularity in the flatband region ($F_S = 0$)

$$\Delta C_g^{QM} \propto F_S^{-1/3}$$

  - Carrier profile follows classical picture (peaked at the Si/SiO_2 interface)

Hybrid Empirical Model

- Eliminate the singularity in van Dort model

$$F_S^{2/3} \rightarrow \frac{F_S^2}{a\exp\left(-\frac{F_S^2}{\sigma^2}\right) + F_S^{4/3}}$$

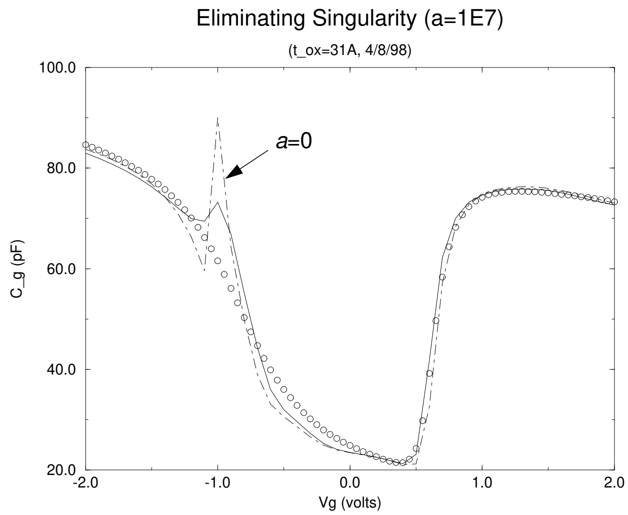
  where $a \neq 0$ and there is no singularity in the entire bias range. Both *a* and σ are adjusting parameters.

- Apply both van Dort and Hansch models at the same time. Advantages:
  - ✧ Cover both physical mechanisms: quantization & repulsive

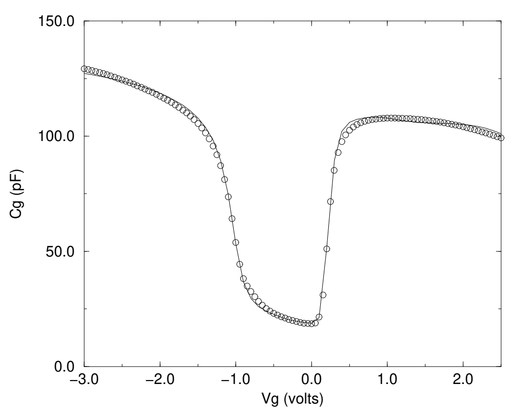
  - ✧ κ is close to 1 (more physical)
  - ✧ Enough correction to threshold shift (important in simulating I-V characteristics)
  - ✧ Correct channel carrier profile

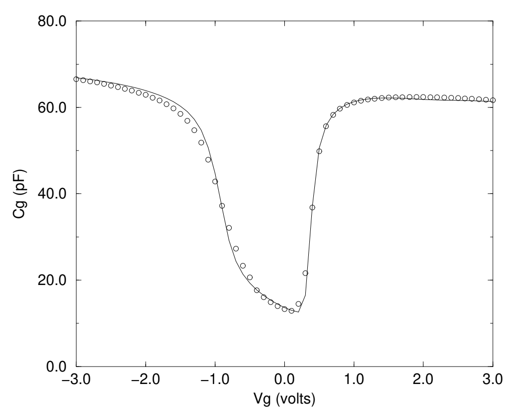
- Model accuracy and robustness have been validated across several generations of CMOS technologies (0.35 to 0.1μm)

Singularity with Dort Model and Its Remedy



Validation of Hybrid QM Model





Comparison between measured data (symbols) and simulation results (line) using hybrid model for t_{ox}=21Å.

Comparison for t_{ox}=44Å

Planned Work

- Complete device simulation capabilities in PROPHET
- Extend the application of device simulation for RF device/circuit analysis
- Explore the possibility for optoelectronic device analysis