540891

2D QUANTUM SIMULATION OF MOSFET USING THE NON EQUILIBRIUM GREEN'S FUNCTION METHOD

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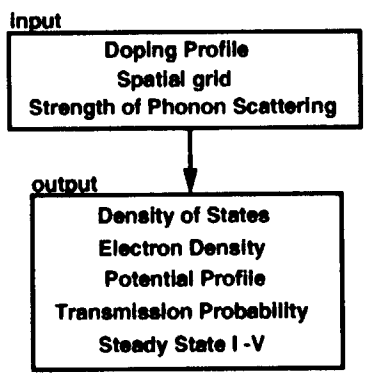
MOTIVATION

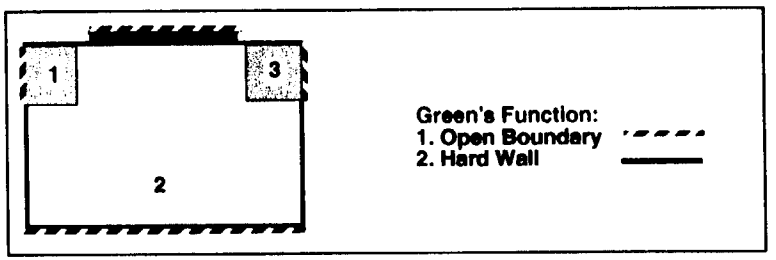
- Develop a quantum mechanical simulator for ultra short channel MOSFET simulation: Theory, Physical approximations, and computer code
- Explore physics that is not accessible by semiclassical methods
- Benchmarking of semiclassical & classical methods
- Study other 2D device and molecular structures
  - Discretized Hamiltonian ------> Tight-binding Hamiltonian

STATUS

- Prototype two dimensional simulator
  - NEGF-Poisson Equations
  - Conduction Band: Three band model
  - Valence Band: Parabolic band and drift diffusion



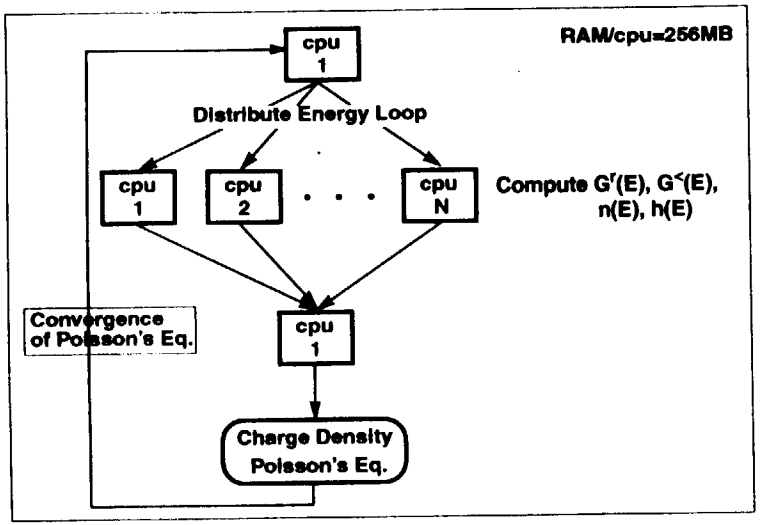
BOUNDARY CONDITIONS



Electron Density:

Regions 1 and 3	$n(r,E) = -(1/\pi)\ \mathrm{Im}[G^r(r,E)]\ f(r,E)$ (DOS * Fermi function)
Region 2	$n(r,E) = -iG^<(r,E)$

ARCHITECTURE / SOLUTION PROCEDURE



ALGORITHMS

The computational challenge lies in evaluating G^r and $G^<$ (electron density), a number of times as demanded in a self-consistent solution. These quantities are obtained by solving a matrix equation of the form:

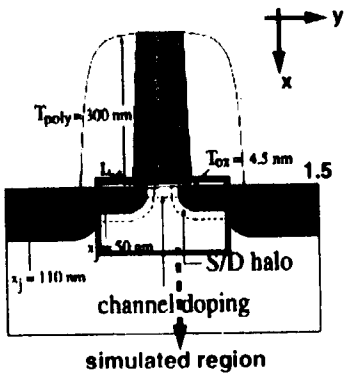
$$A\,G^{\alpha} = F,$$

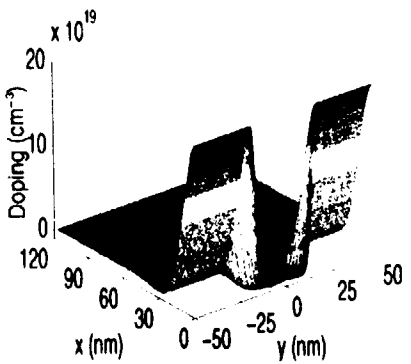
where $\alpha = r, <$ and A is block tridiagonal matrix.

$$\begin{bmatrix} A_1 & U_1 & & & & \\ U_1 & A_2 & U_2 & & & \\ & U_2 & x & & & \\ & & & x & x & \\ & & & x & x & U_{N-1} \\ & & & & U_{N-1} & A_N \end{bmatrix}$$

- For G^r, F = Identity matrix, and a known recursive algorithm is used.
- For $G^<$, F = Full matrix. We have developed a special recursive method to compute $G^<$.

MIT-25 nm MOSFET (http://www-mtl.mit.edu:80/Well)

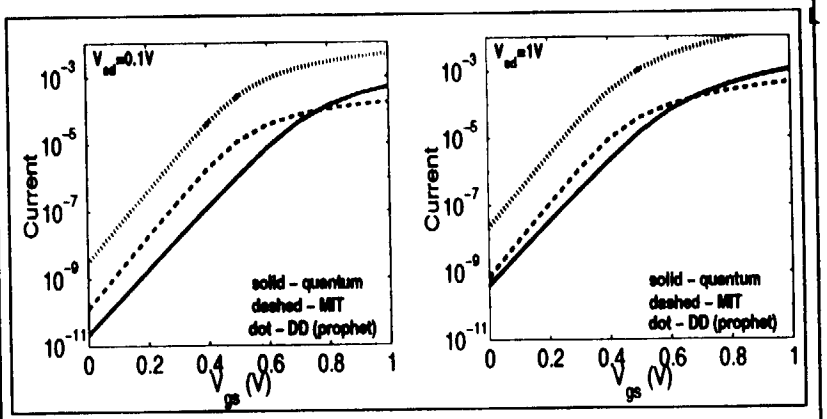




* $\lambda \sim 3$ nm
* Transit time ~ 10^{-14} s

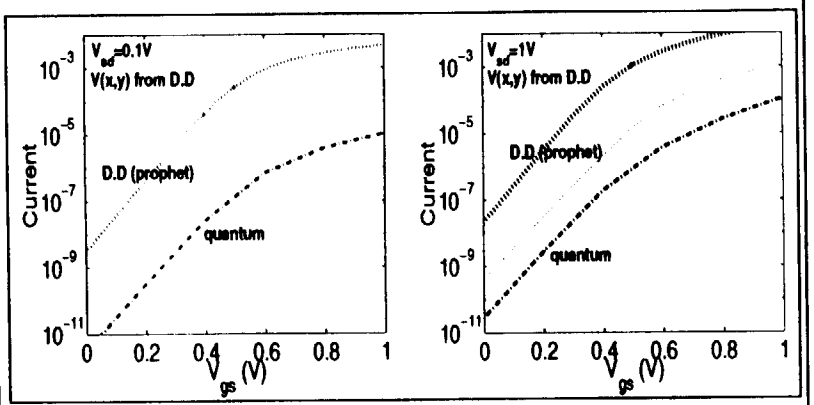
DRAIN CURRENT - COMPARISON OF DIFFERENT METHODS

- Potential profiles are calculated self-consistently by the respective simulators.



- DD (prophet) - two orders of magnitude larger current
- MIT (MEDICI with quantum corrected) - current is 3-5 time larger than our computed currents.

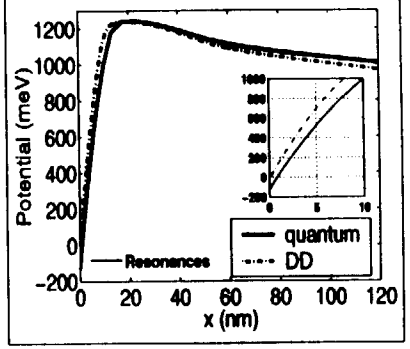
To ensure that the above results are not artifacts of different convergence criteria used by the simulators, we compare the current calculated by prophet and our quantum simulator, for the DD potential profile:



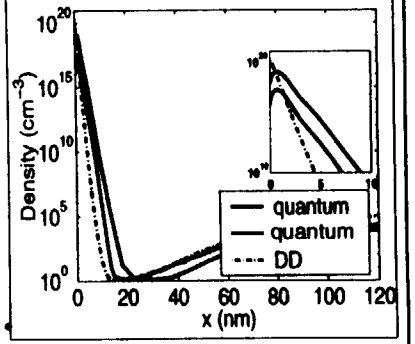
These results are in accordance with the findings above but the quantum current is smaller. This is because the calculated barrier height in the quantum case is larger than in DD.

POTENTIAL PROFILE AND DENSITY - COMPARISON OF DD AND QUANTUM

Self-consistent potential profile at mid channel for V_{gs}=1V and V_{sd}=0

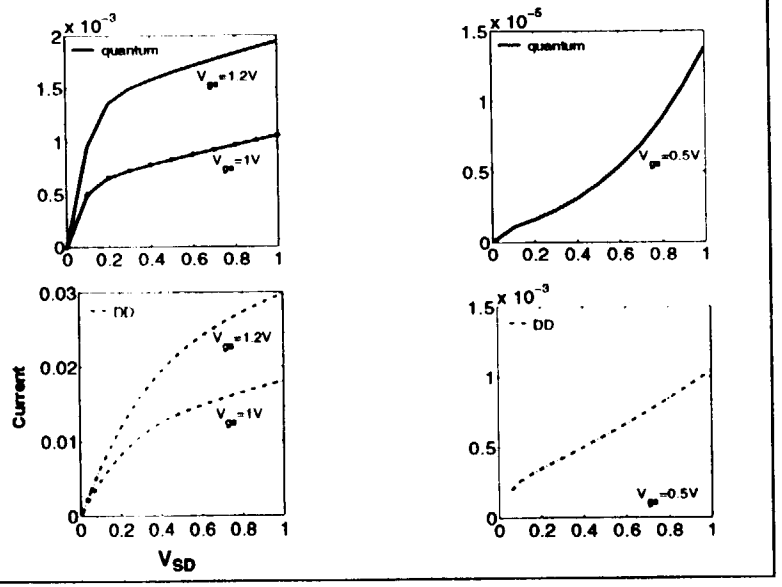


Corresponding density (blue and red), and the density calculated by our simulator using the DD potential profile (green).



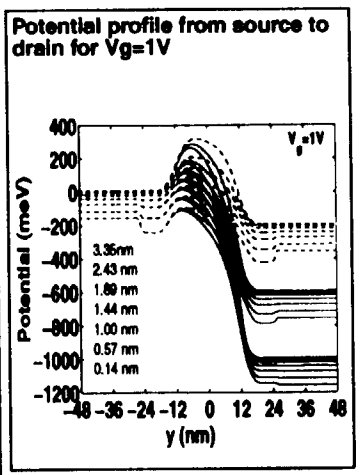
Classical (DD) potential profile is unsuitable to calculate the density and current in the quantum case as shown in the above plots.

Current versus V_{SD}

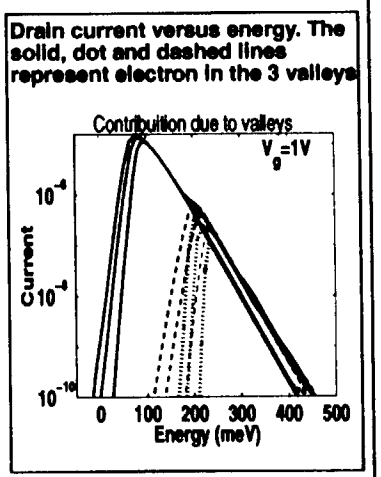


CURRENT VERSUS ENERGY

Potential profile from source to drain for Vg=1V



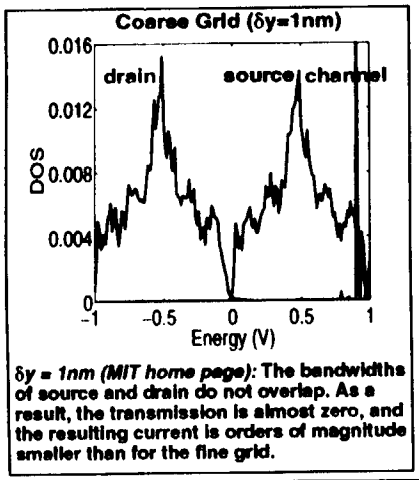
Drain current versus energy. The solid, dot and dashed lines represent electron in the 3 valleys



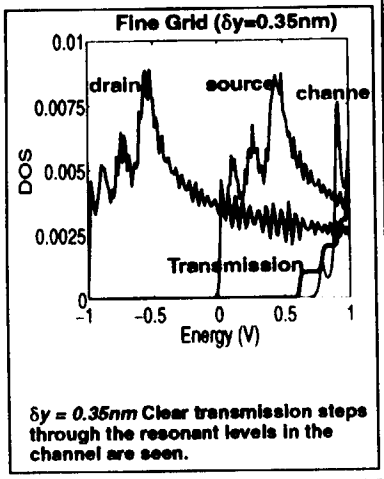
Vd=0.2V Vd=0.6V Vd=1V

SPURIOUS REFLECTION DUE TO GRID

- Energy Bandwidth = $2h^2/m\delta y^2$, where δy is the grid spacing. A coarse grid can result in order of magnitude smaller current due to spurious reflection of charge.



δy = 1nm (MIT home page): The bandwidths of source and drain do not overlap. As a result, the transmission is almost zero, and the resulting current is orders of magnitude smaller than for the fine grid.



δy = 0.35nm Clear transmission steps through the resonant levels in the channel are seen.

SUMMARY

We have developed a simulator to calculate ballistic current in ultra short channel MOSFETs. The main challenge lies in the self consistent solution of Poisson's equation and the Green's function equations (with open boundary conditions).

The drain current and electron density are calculated using potential profiles from: (i) drift-diffusion simulations (prophet, without quantum corrections) and (ii) our Green's function simulator. We find that the drift-diffusion current is about 100 times larger than that calculated by our simulator. Thus emphasizing the need to compute the potential profile self-consistently.

For a specific device, namely the MIT 25nm MOSFET, the quantum corrected (classical) drain current computed by MEDICI is only a factor of 3-5 larger than the drain current calculated by our simulator.

At large applied drain biases, an appropriate choice of spatial grid is important in obtaining correct drain currents. A coarse grid leads to spurious reflection of electrons incident from the source.

Work to include realsitic scattering mechanisms is in progress.