Device Simulation for NANO MOSFET and Scaling issues

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Abstract

For understanding of the device operations and its interaction with the circuit in the nano scale era, the device simulation has been extended to include the quantum transport effects, statistical effects and to be compatible with the circuit simulation environments. To do so, the full Newton scheme has been developed to fully integrate the Poisson equation, transport equation and the Schrodinger equation in the NANOCAD[1], which is the in-house developed program for the 2 and 3 dimensional device simulator. The method is applied to the nano scale Double Gate(DG) MOSFET structure showing that the quantum effect in the transport direction as well as in the vertical direction is important. Also, the CLESICO[2] system has been developed to treat the nodes in the device same as the nodes in the circuit, thereby the effects of the internal physics in the device on the circuits can be readily understood. The method is applied to understand the effects of the thermal noise of the MOSFET channel in the RF mixer and the local oscillator.

Introduction

As the MOSFET channel length is scaled down in the sub 40nm scheme, the quantum effects such as the quantum confinement effects in the vertical direction and the quantum tunneling effects lateral direction of the channel become more important. Also, the detailed physics in the device become more transparent to the circuit environments as the rail to rail voltage level is reduced while the noise level in the device is not scaled. The extension of the numerical device simulator to include the proper quantum transport effects and the coupled device/circuit simulation (mixed mode simulation) open the new horizon to the new paradigm of the device design and analysis for the MOSFET device and circuits in the nano scale regime.

For this, we have developed the NANOCAD software to find the a self-consistent solution of the Schr⁻odinger, Poisson, and carrier transport equations[1]. Also, the CLESICO system, the mixed mode simulation environment to solve the semiconductor equations and the circuit equation(KCL and KVL) using the harmonic balance techniques[2].

In the NANOCAD environment, a fully coupled Newton scheme [3] is applied to solve the Schrödinger, Poisson, and carrier transport equations simultaneously. In this way, the numerical error and difficulty(or slow) in the

numerical convergence in the decoupled method could be largely improved. In the next section, the application of the algorithm to 2DEG/DG(Density Gradient) mode analysis of the silicon based DG MOSFET will be presented, where the Schrödinger equation is solved in the confinement direction and the quantum corrected transport equation is solved in the transport direction.

In the CLESICO system, the devices are discretized as in the conventional device simulators. The semiconductor equations (i.e. Poisson equation and the electron and hole continuity equations) are solved in the frequency domain using the harmonics balance (HB) technique [4]. The iterative matrix solver, generalized minimum residual method (GMRES)[5], is exploited since the size of the system is too large to deal with the direct solver. We use the 'quasi-static Jacobian,' which neglects the time derivatives of the governing equations for the system including the semiconductor equations, as a prescaler. We find out that the method is very effective and numerically efficient in decoupling the components originated from different sampled components in the time domain up to a few hundreds GHz range. For the noise analysis in the CLESICO, the system is linearized to obtain the conversion Green's functions (CGFs) by an aid of the generalized adjoint approach [6]. As an example, we consider the RF mixer with the two-dimensional MOSFETs and will show that the simulations give the correlation between the detailed physics in the MOSFET's such as the noises and the circuit performances.

DG MOSFET simulation

As an example of the 2DEG/DG mode analysis of the DG MOSFET shown in fig.1, the two-dimensional Schr[•]odinger equation is divided into the confinement (*y*-coordinate) and transport (*x*-coordinate) directions. The electron density in each subband, $N_{\rm ki}$, is obtained by the quasi-Fermi energy ($E_{\rm kFi}$) and the quantum potential.

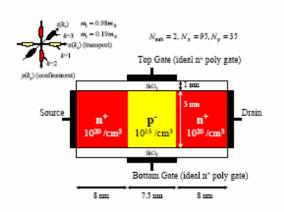


Fig. 1 Schematic of the thin body DGFET structure. The device and crystal coordinates are aligned. The same bias is applied to the top and bottom gates.

Fig. 2 shows the overall Jacobian matrix to stand for the system of equations in the coupled manner. The

unknowns are the variables, V, ψ_k , E_{ki} , $\sqrt{N_i^k}$, and E^{k}_{Fi} ,

which are the electrostatic potential, the waver function, energy eigenvalue, area density, and Fermi level (of kth subband), respectively.

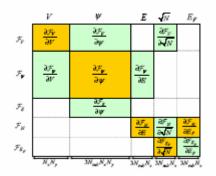


Fig. 2.Schematic of the Jacobian matrix. The total number of unknowns is $((1 + 3N_{sub})N_xN_y + 9N_{sub}N_x)$. Note that each block matrix is very sparse.

Fig. 3 and 4 show the area density of electrons and the energy level of the subbands along the channel. In the figures, the comparisons are made with the more comprehensive quantum transport model called the NEFG model[7,8]built in NANOCAD. It can be shown that the DG/DEG model accurately and efficiently simulate the internal physics as well as the IV characteristics(not shown in this paper).

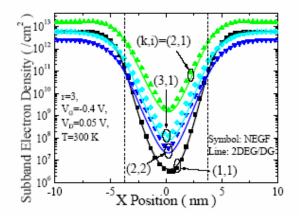


Fig. 3. Subband electron densities along the channel predicted by the 2DEG/DG (line) and NEGF (symbol) models.

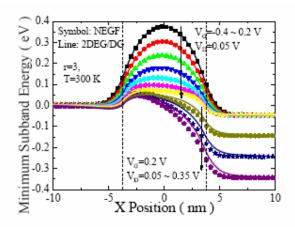


Fig. 4 Bias dependence of the minimum subband energy level predicted by the 2DEG/DG model (line) and the NEGF model (symbol). The gate bias is first increased from -0.4 V to 0.2 V with the drain bias fixed to 0.05 V, and then the drain bias is increased from 0.05 V to 0.35 V.

RF mixed mode simulation

As an example of the mixed mode simulation using the CLESICO system, the effects of the diffusion noise sources of the MOSFET channel to the RF mixer are simulated. The circuit considered in this work is the single-balanced RF CMOS mixer with 2 resistors and three MOSFETs as shown in Fig. 5. The output is taken as a differential voltage from drains of two LO transistors. The number of the unknowns per a sampling time is about 24,000. Since the number of the harmonics is set to 10, the whole system has about a half million unknowns. The magnitude and fundamental frequency of the LO signal is 0.15 V and 1 GHz, respectively. We found that the conversion gain from the 1.1 GHz RF signal to the output at 0.1GHz is 1.33.

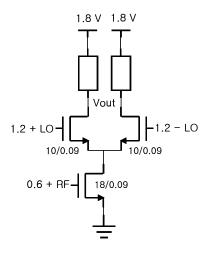


Fig. 5 Circuit schematic of the single-balanced downconversion mixer.

The CGF(Conversion Green Function) for the mixer output noise voltage at 0.1 GHz corresponding to the (modulated) electron noise source is calculated. Fig. 6 shows the CGF for 1.1 GHz noise source in the RF port MOSFET. The noise source in the drain side has strong impact on the mixer output noise. Fig. 7 also shows the same quantity in the left LO port MOSFET. Contrary to Fig. 6, the noise source in the source side has a strong impact on the mixer output noise since the frequency down-conversion from 1.1 GHz to 0.1 GHz takes place in the channel in the LO port MOSFET. Similar studies have been performed to understand the CGFs for other frequency components of the noise such as 0.1 GHz noise source (no frequency conversion) in the RF port and LO port MOSFET. The effect of the noise source only in the drain side of the LO port MOSFET is found to be dominant because the frequency conversion is not needed in this case.

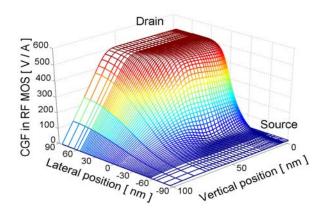


Fig. 6. CGF for 1.1 GHz noise source in the RF port MOSFET.

In Fig. 8 and 9, we plot the CGFs along the channel in the RF port MOSFET and LO MOSFET, respectively.

In this way, the detailed contribution of the noises originated from each device (and passive elements) to the output noise can be known. In this example, the power spectral density of the mixer output noise voltage is calculated to be $20.2 (\text{nV})^2/\text{Hz}$, among which 55 % comes from the RF port MOSFET and the other comes from the LO port MOSFETs (the noise from two resistors are not considered).

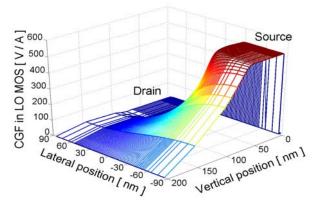


Fig. 7. CGF for 1.1 GHz noise source in the left LO port

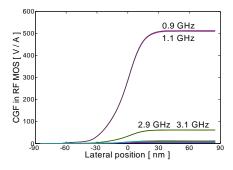


Fig. 8. CGFs along the channel in the RF port MOSFET.

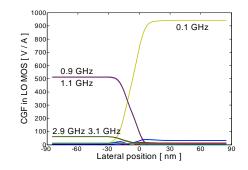


Fig. 9. CGFs along the channel in the left LO port MOSFET.

Conclusion

In this work, we have developed the coupled scheme for the Schrodinger equation, transport equations and the Poisson equation. The scheme is successfully applied to the modal approach for the DG MOSFET structures. Also, the physics based TCAD framework, CLESICO, is developed to perform the mixed mode simulation in the circuit environments. The method is applied to the mixer circuits used to down convert the RF signals. It is shown that the detailed internal physics in the devices and their interactions with the circuit node can be known. It is believed that the approaches will render more profound tool for the analysis and design of the nano scale MOSFET devices and circuits.

Acknowledgement

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References

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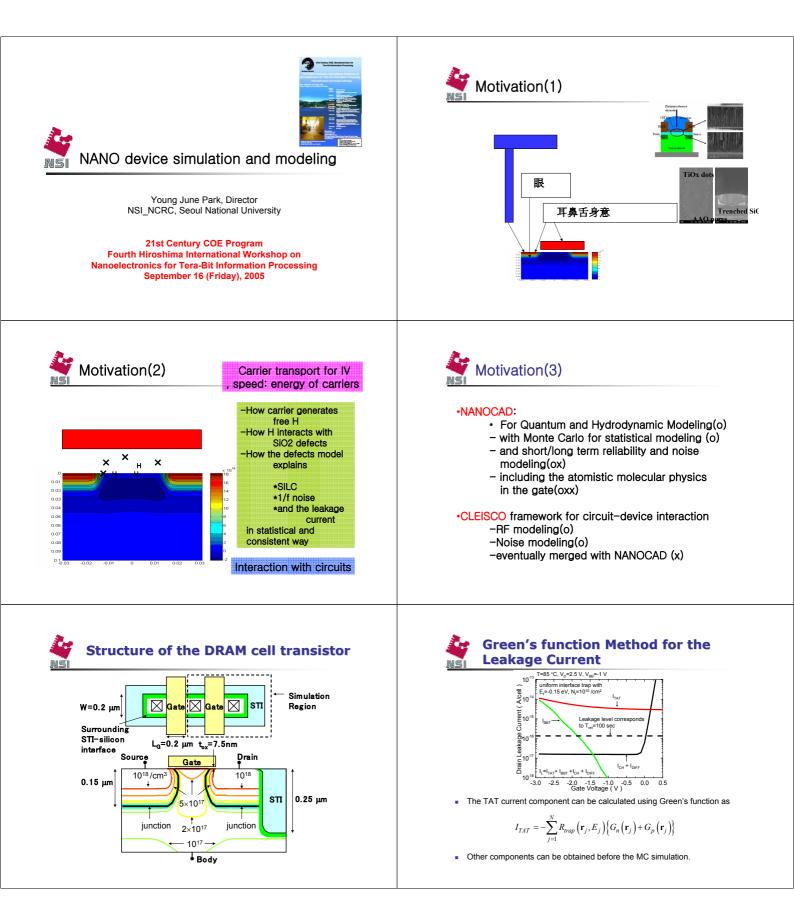
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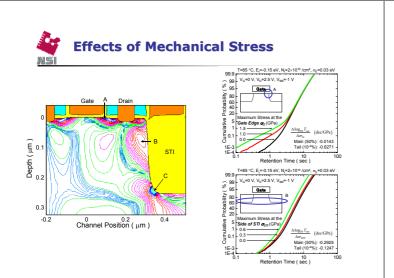
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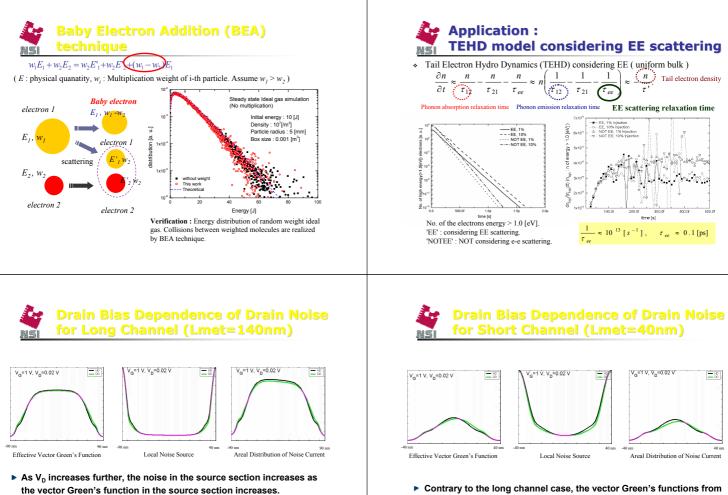
dissertation, Purdue Univ., West Lafayette, IN, USA, Dec. 2001.



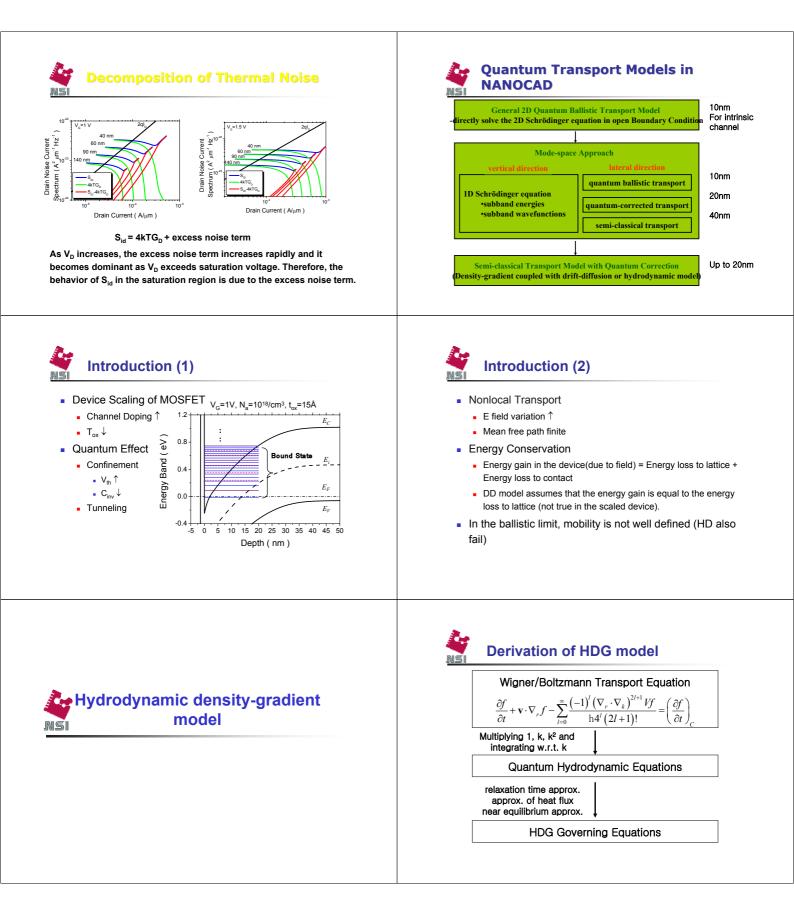


Monte Carlo (MC) modeling for Electron-Electron (EE) scattering

- ✤ EE scattering
 - $\, \ast \,$ a hot electron source of deep sub-micron device
 - * MC is the most effective method for EE scattering simulation
- Multiplication
 - * Split one MC electron into copied electrons
 - * Weights are aligned to all the copied electrons
- * Propose Baby Electron Addition (BEA) technique
 - * Technique for weight redistribution after EE scattering
 - The conservation of energy, momentum and charge is guaranteed by additional of an electron after scattering



- The difference of vector Green's functions between HD and DD models confined in the drain section, where the noise source are negligible.
- Contrary to the long channel case, the vector Green's functions from HD and DD models become very different in the entire region if V_D increases.



 After derivation, we obtain a very similar equation set to HD model, except the effective quantum potential term

$$\psi_{qn} = 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}}$$

Driving force in the drift term

$$F_{eff} = -\nabla \left(\psi_{qn} + \psi \right)$$



Electron Flux Density

$$\mathbf{F} = \mu n \nabla \left(\psi + \psi_q \right) - \mu \nabla \left(\frac{k_B T}{q} n \right)$$

• Electron Energy Flux Density $\mathbf{S} = -\kappa \nabla T + \frac{5}{2} k_B T \mathbf{F},$

Governing Equations (1)
Poisson Equation

$$-\nabla \cdot (\varepsilon \nabla \psi) - q(p - n + N_D^+ - N_A^-) = 0,$$

Electron Continuity Equation
 $\nabla \cdot \mathbf{F} + U = 0$
Energy Balance Equation
 $\nabla \cdot \mathbf{S} - q \nabla \psi \cdot \mathbf{F} + U \frac{3}{2} k_B T + n \frac{3}{2} k_B \frac{T - T_0}{\tau_w} = 0,$

• Quantum Potential Equation $\nabla \cdot (b\nabla \sqrt{n}) - \sqrt{n} \psi_q / 2 = 0$



$\psi_{\rm Si} = \psi_0 + V_{\rm bias}$	Poisson's equation				
$n = n_0$	Electron continuity equation				
$\psi_{qn} = 0$	Quantum potential equation				
$T_{\rm n} = T_{\rm 0}$	Energy balance equation				

Penetrating Boundary Condition for Si/SiO₂ Interfaces

 ${\, \bullet \,}$ The electron density penetrated into oxide by x from the Si/SiO_2 interface can be approximated as

$$n(x) = n(0) \exp\left(-2x / x_p\right),$$

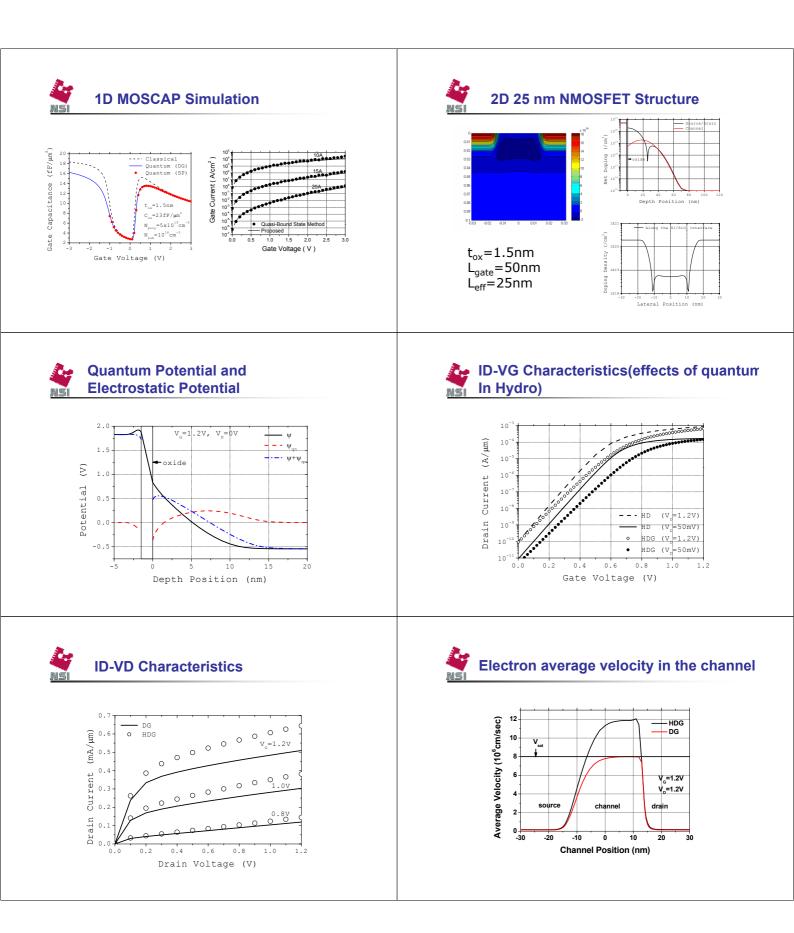
where n(0) is the electron density at the interface and

$$x_p = \frac{h}{\sqrt{2m_{ox}\Phi_B}}$$

is the characteristic penetration depth calculated from WKB approximation.



$\psi_{\rm Si} = \psi_{\rm SiO_2}$	Poisson's equation			
$\mathbf{n}\cdot\mathbf{F}=0$	Electron continuity equation			
$\mathbf{n} \cdot b_{\mathrm{ox}} \nabla \sqrt{n} = -(b_{\mathrm{ox}} / x_{\mathrm{p}}) \sqrt{n_0}$	Quantum potential equation			
$\mathbf{n} \cdot \mathbf{S} = 0$	Energy balance equation			





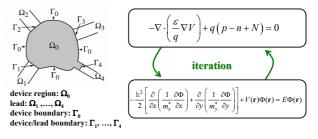
Quantum mechanical model

-Full Quantum and ballistic

- -Mode Space approach with
 - * Drift diffusion
 - * Hydro dynamic

2D Quantum Ballistic Transport Model

 Directly solve the coupled Poisson and Schrödinger equation using the finite element method for arbitrary shaped device domain in open B.C.



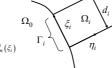
2D Quantum Ballistic Transport Model

Boundary condition at the leads

$$\Phi(\eta_{i},\xi_{i}) = \sum_{1}^{N} \chi_{m}^{i} \left[a_{m}^{i} e^{-ik_{m}^{i}\eta_{i}} + b_{m}^{i} e^{ik_{m}^{i}\eta_{i}} \right] + \sum_{N=1}^{\infty} \chi_{m}^{i} \left[a_{m}^{i} e^{\kappa_{m}^{i}\eta_{i}} + b_{m}^{i} e^{-\kappa_{m}^{i}\eta_{i}} \right]$$

• where χ_m is the solution of the coupled 1-D Poisson and Schrödinger equations at the lead *i*

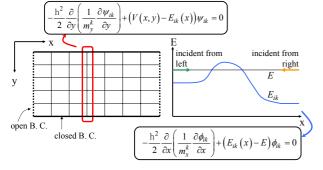
 $\begin{cases} -\frac{d}{d\xi_i} \left[\varepsilon(\xi_i) \frac{dV(\xi_i)}{d\xi_i} \right] = \rho(\xi_i) \\ -\frac{h^2}{2} \left[\frac{d}{d\xi_i} \left(\frac{1}{m_{\xi_i}^*} \frac{\partial \chi_m^i(\xi_i)}{\partial \xi_i} \right) \right] + V(\xi_i) \chi_m^i(\xi_i) = E_m^i \chi_m^i(\xi_i) \end{cases}$



The local coordinate system in lead *i* region

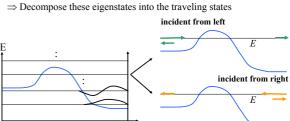


 The 2-D Schrödinger equation is divided into the confinement (y) and transport direction (x).



2D Quantum Ballistic Transport Model

• Sampling of the Density of State: Calculate sine and cosine like bound states (standing wave solution) and eigenenergies (Laux et al.)



Calculation of the Sine-like bound states

Sin-like bound state is decomposed into traveling wavefunctions

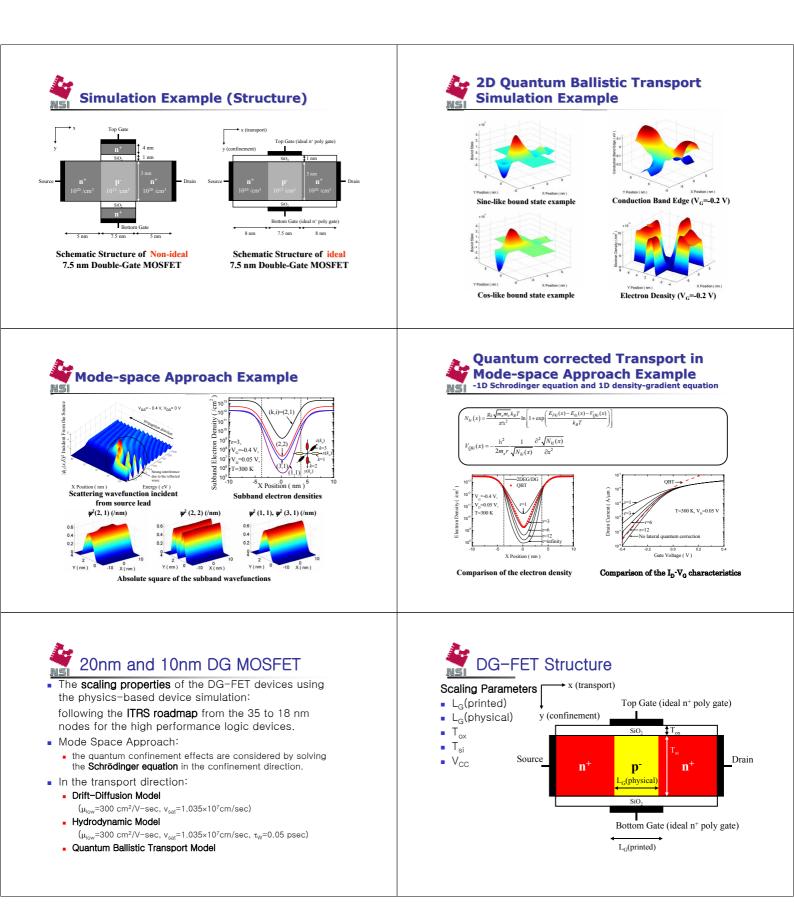
Semi-classical Transport with Quantum Correction

■ Effective quantum potential is derived from the Wigner distribution function ⇒ its gradient acts as a driving force

$$\psi_{qn} = 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}}$$

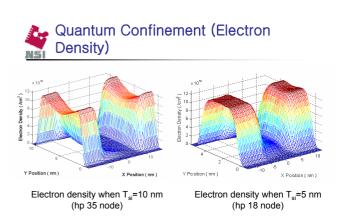
$$F_n = \mu_n n \nabla \left(\psi + 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} \right) - \mu_n \nabla \left(\frac{k_B T_n}{q} n \right)$$

 It is an approximate approach, which gives reasonable results when the quantum confinement effects are dominant.

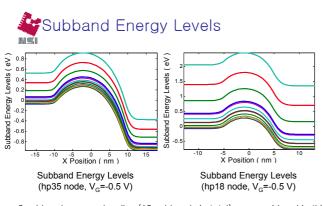


Scaling of DG-FET (ITRS Roadmap)									
Year of production	2012	2013	2014	2015	2016	2017	2018		
MPU 1/2 pitch (nm)	35	32	28	25	22	20	18		
Printed gate length (nm)	20	18	16	14	13	11	10		
Physical gate length (nm)	14	13	11	10	9	8	7		
EOT (physical) (nm)	0.7	0.6	0.6	0.6	0.5	0.5	0.5		
EOT(including poly dep.)	0.9	0.8	0.8	0.8	0.7	0.7	0.7		
Power supply voltage (V)	0.9	0.9	0.9	0.8	0.8	0.7	0.7		
Silicon thickness (nm)	10	9	8	7	6.5	5.5	5		

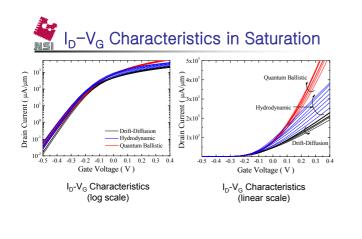
- Silicon thickness is chosen to half of the printed gate length.
- Poly gate depletion effects are approximately taken into account by adding 0.2 nm to the EOT.

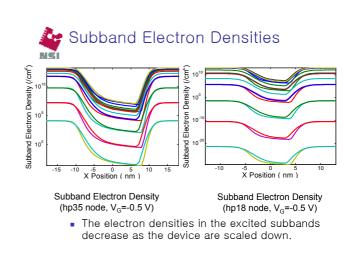


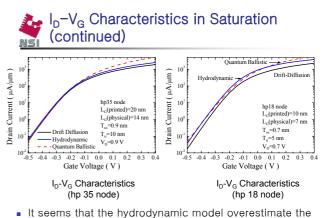
 Electron density near the interface decreases rapidly due to the quantum confinement effects.



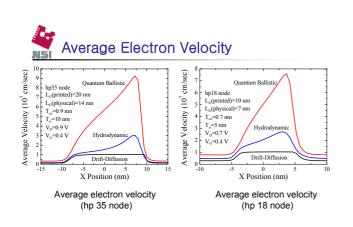
- 6 subbands per each valley (18 subbands in total) are considered in this work.
- Note that the spacing between the levels increases as the device is scaled down.







It seems that the hydrodynamic model overestimate the drain current in the sub-threshold region (especially in the short-channel device)



 $-G \mid I_{N,N} \mid 0 \mid \delta I$

0

 $0 \quad I_{N,N} \quad \delta V$

 $J_{dev}\delta\varphi + J_V\delta V = 0$

 $\delta I = G \delta \varphi$

 $\delta V = \delta V_{cir}$

0

0

[2] K. Mayaram, and D. O. Pederson, IEEE TCAD, vol. 11, pp. 1003-1012, 1992

 $I_{N,N}$ $-G_{eq}$ δI

 $0 I_{N,N}$

 $J_{dev}\delta\varphi + J_V\delta V = 0$

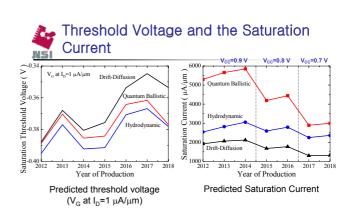
 $\delta I = G_{eq} \delta V$

 $\delta V = \delta V_{cir}$

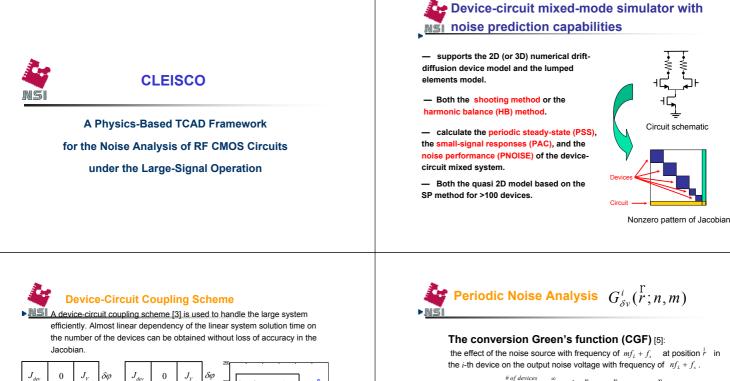
δV

Linear system solution time

versus the number of inverter

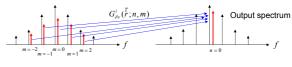


 The difference in the threshold voltage between the drift-diffusion and quantum ballistic models increases as the scaling proceeds due to the source-to-drain tunneling effect.

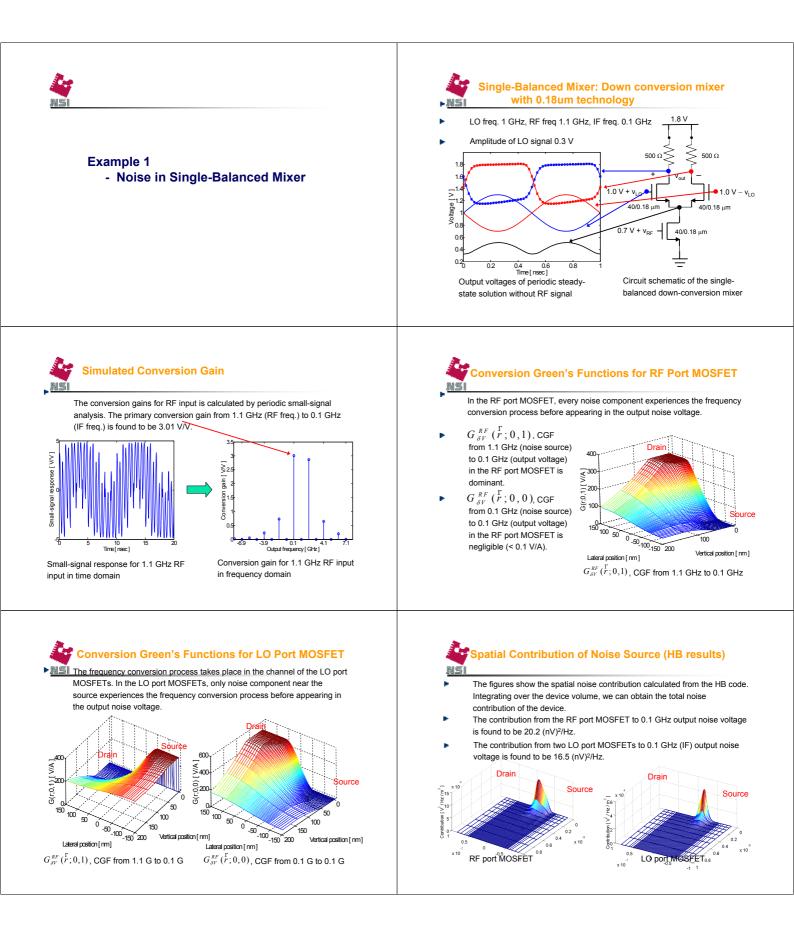


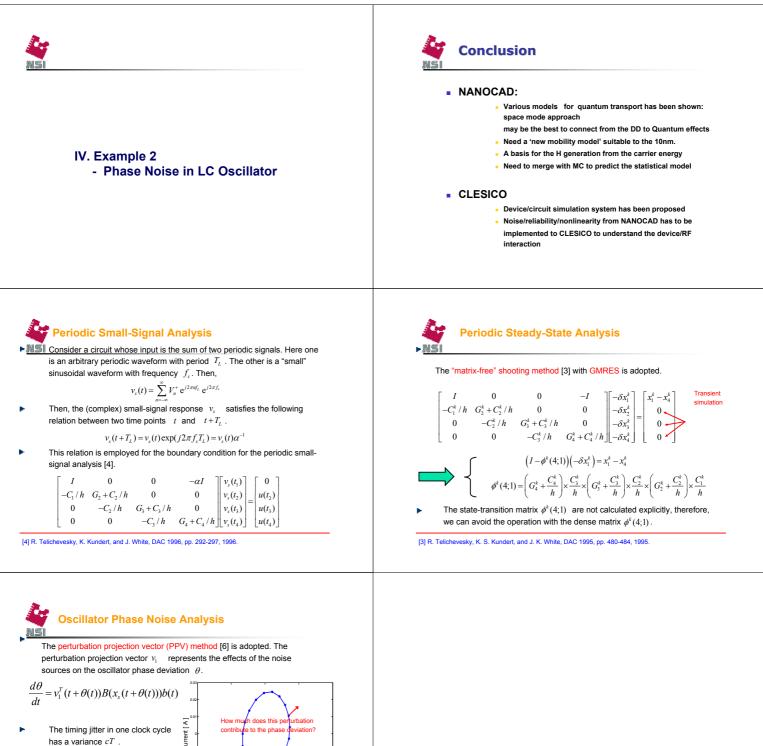
$$\delta v(nf_L + f_s) = \sum_{i=1}^{\# of \, devices} \sum_{m=-\infty}^{\infty} \int_{V} d\vec{r} G^i_{\delta v}(\vec{r}; n, m) s(\vec{r}; mf_L + f_s)$$

Noise source



[5] F. Bonani, S. D. Guerrieri, G. Ghione, and M. Pirola, IEEE TED, vol. 48, pp. 966-977, 2001.





cT =

 $\int_0^T v_1^T(\tau) B(x_s(\tau)) B^T(x_s(\tau)) v_1(\tau) d\tau$

[6] A. Demir, and J. Roychowdhury, IEEE TCAD, vol. 22, pp. 188-197, 2003