TOSHIBA

Leading Innovation >>>

Resolving Individual Impurities in Statistical Variability Simulations

(Stable device simulation of random dopant fluctuation using long-/short-range separation treatments for impurity potentials)

Shuichi Toriyama

Advanced LSI Technology Laboratory

Toshiba Corporation

Outline

1. Objective
2. Introduction of the long/short (L/S) separation model and its comparison with the other models
3. Numerical examples using the L/S model
    1. (SOI-type) NAND FLASH memories --- L/S vs. CIC-DG ---
    2. Schottky contact resistance --- L/S vs. NGP --- (skip! →)
4. Open question: a limitation of the L/S model
5. Summary

Increasing Demands for RDF Simulation by DD

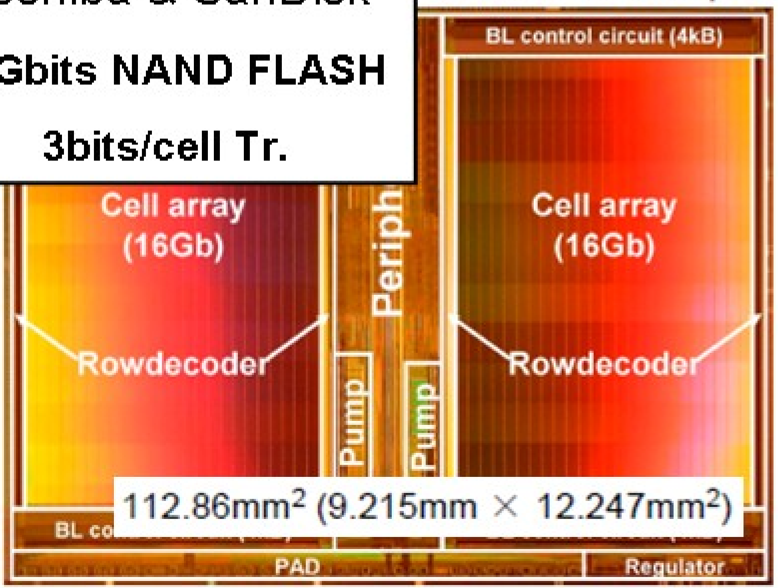
Intrinsic random (≠systematic) process vs. continuous scaling.

Toshiba & SanDisk

32Gbits NAND FLASH

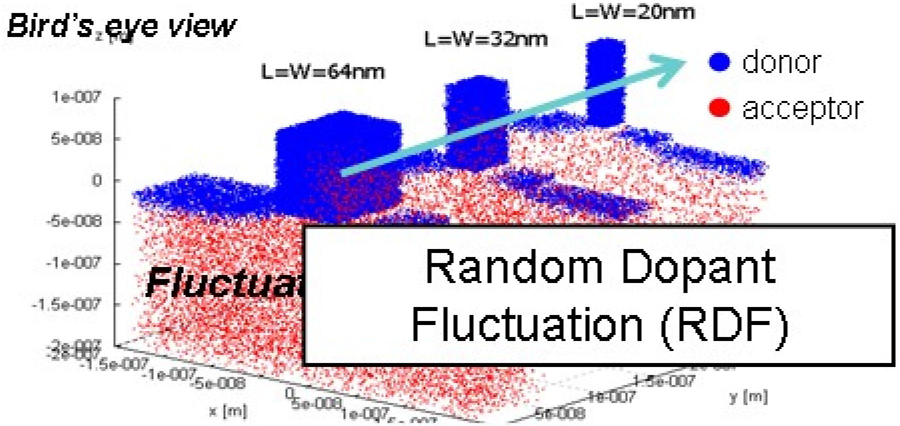
3bits/cell Tr.

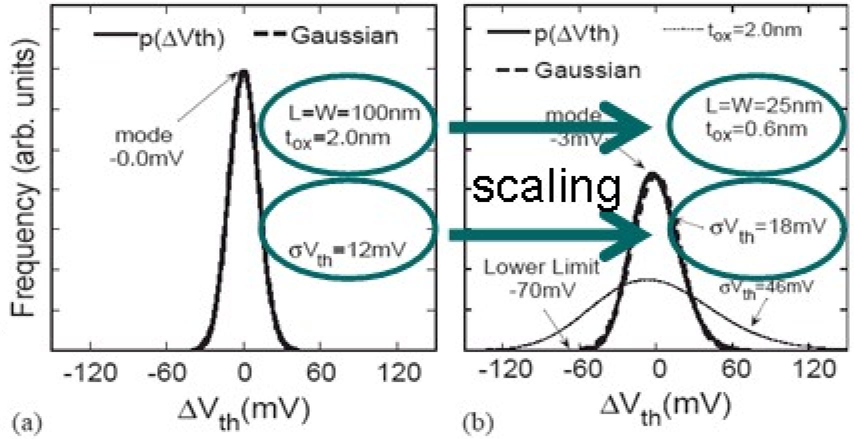
sub-35nm CMOS process



T. Futasuyama et al., 13.4, ISSCC2009

32Gb/(3b/Tr.) ≈10Billion Tr./chip

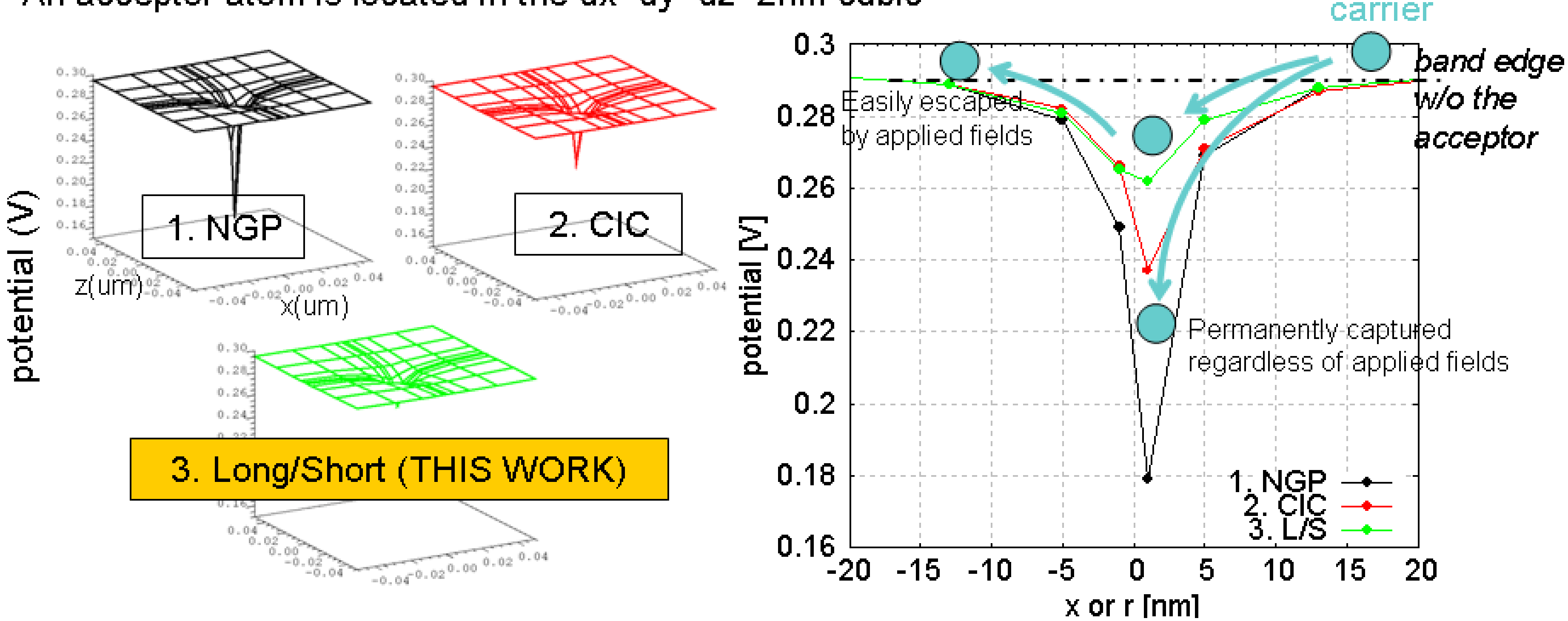




Calculating the RDF-impacts by using drift-diffusion-based (DD) TCAD both in advance of manufacturing chips and a posteriori, contributes to estimating the variation ranges and suggesting process optimizations.

Risks of Model-dependent Results

An acceptor atom is located in the dx=dy=dz=2nm cubic



The risks to be anticipated:

The device physics to be reproduced:

✓permanent carrier-capture	⟷	depletion condition
✓high resistivity	⟷	well-known impurity-limited μ

The potential using the model #3 (Long/Short) seems to be reasonable in terms of reproducing the physics. So, what is the Long/Short model?

Outline

1. Objective
2. Introduction of the long/short (L/S) separation model and its comparison with the other models
3. Numerical examples using the L/S model
    1. (SOI-type) NAND FLASH memories --- L/S vs. CIC-DG ---
    2. Schottky contact resistance --- L/S vs. NGP ---
4. Open question: a limitation of the L/S model
5. Summary

The Long/Short Separation Model (L/S model)[1]

Only the long-range components of impurity density are used in the charge term (ρ) of Poisson equation.

$$N_a(|\mathbf{r}-\mathbf{r_i}|) = \delta(\mathbf{r}-\mathbf{r_i})$$ (bare model; NGP)

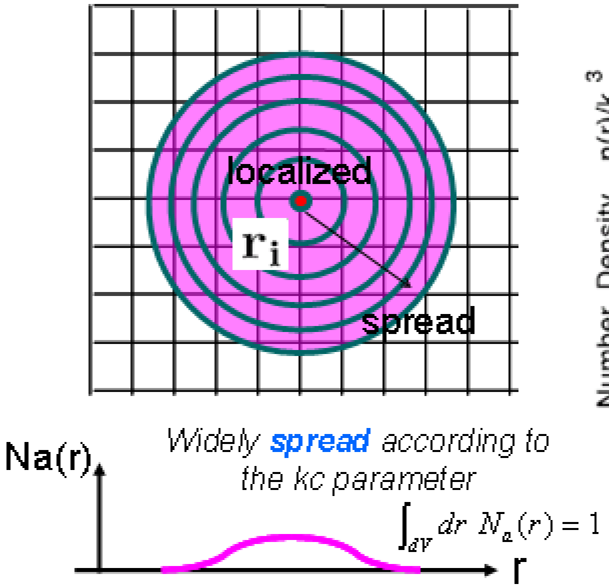
Fourier transform of the delta function leads to

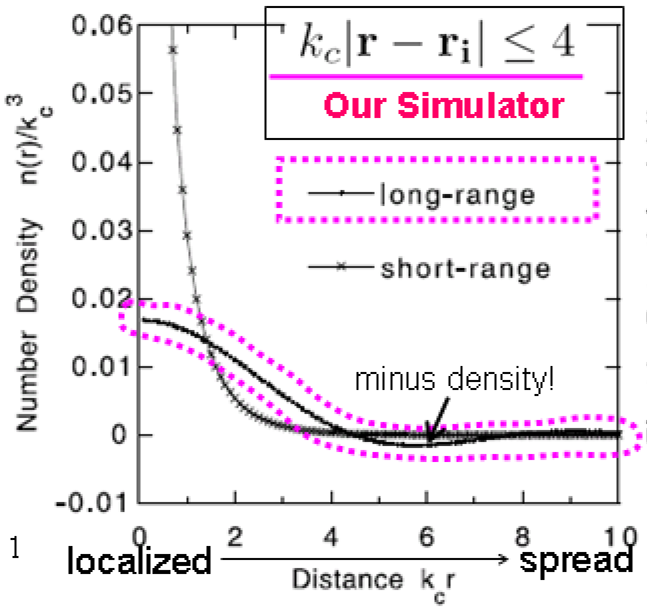
$$\rightarrow \quad N_a(|\mathbf{r}-\mathbf{r_i}|) = \frac{1}{V}\sum_{\mathbf{k}<\mathbf{k_c}} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r_i})}$$

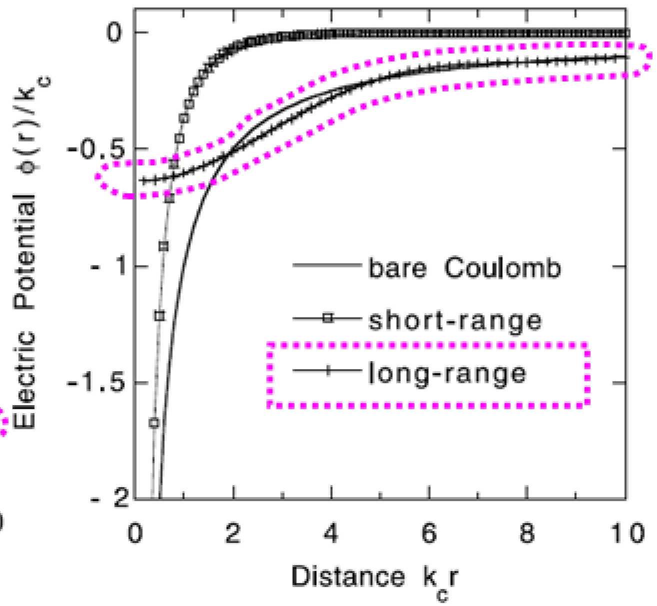
$$= \frac{k_c^3}{2\pi^2}\frac{\sin(k_c|\mathbf{r}-\mathbf{r_i}|) - (k_c|\mathbf{r}-\mathbf{r_i}|)\cos(k_c|\mathbf{r}-\mathbf{r_i}|)}{(k_c|\mathbf{r}-\mathbf{r_i}|)^3}$$ **(long-range)**

Cut-off parameter candidates:

$$k_c = \begin{cases} 2N_a^{1/3} & \text{(mean distance)} \\ \lambda_{DH}^{-1} & \text{(Debye-Huckel)} \\ \lambda_{TF}^{-1} & \text{(Thomas-Fermi)} \\ \text{fitting parameter} & \end{cases}$$



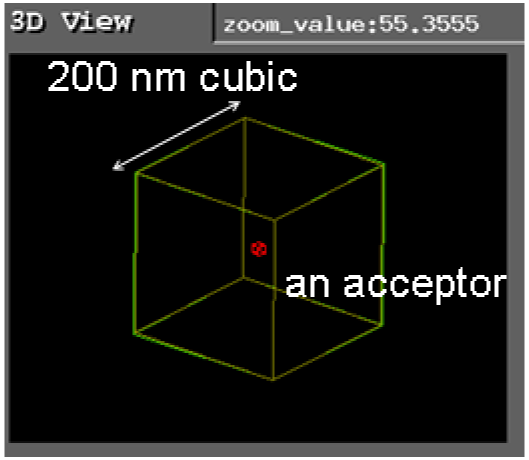


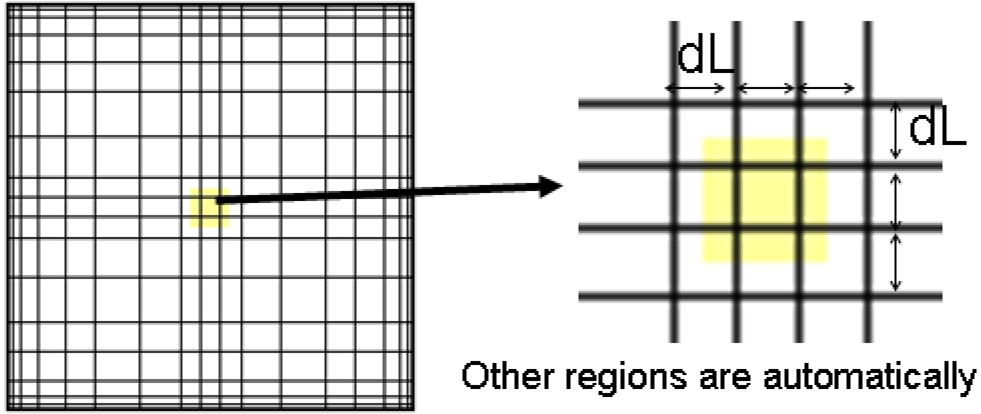


[1] N. Sano et al., Microelectron. reliab. **42**, 189 (2002).

Model Comparison

An impurity charge is located at the center of a Si bulk cubic in the dx=dy=dz =dL volume. In that condition, how does the potential shape become?





Other regions are automatically meshed.

index	Model	Refrence
1	**Nearest Grid Point (NGP)**	R. W. Hockney and J. E. EastWood, "Computer Simulation Using Particles", Institute of Physics Publishing, New York, 1987.
2	**Cloud-In-Cell (CIC)**	(same as above)
3	**Long/Short Separation (L/S)**	N. Sano et al., MicroElectron. Reliab. 42, 189 (2002). mean distance cut-off ver.
4	**Ezaki's modified L/S Model (Ezaki)**	T. Ezaki et al., IEICE Trans. electron. 86, 409 (2003).
5	**CIC with Density-Gradient (CIC-DG)**	for Density Gradient model, please refer to S. Odanaka, IEEE trans. Computer-Aided Design. 23, 837 (2004).

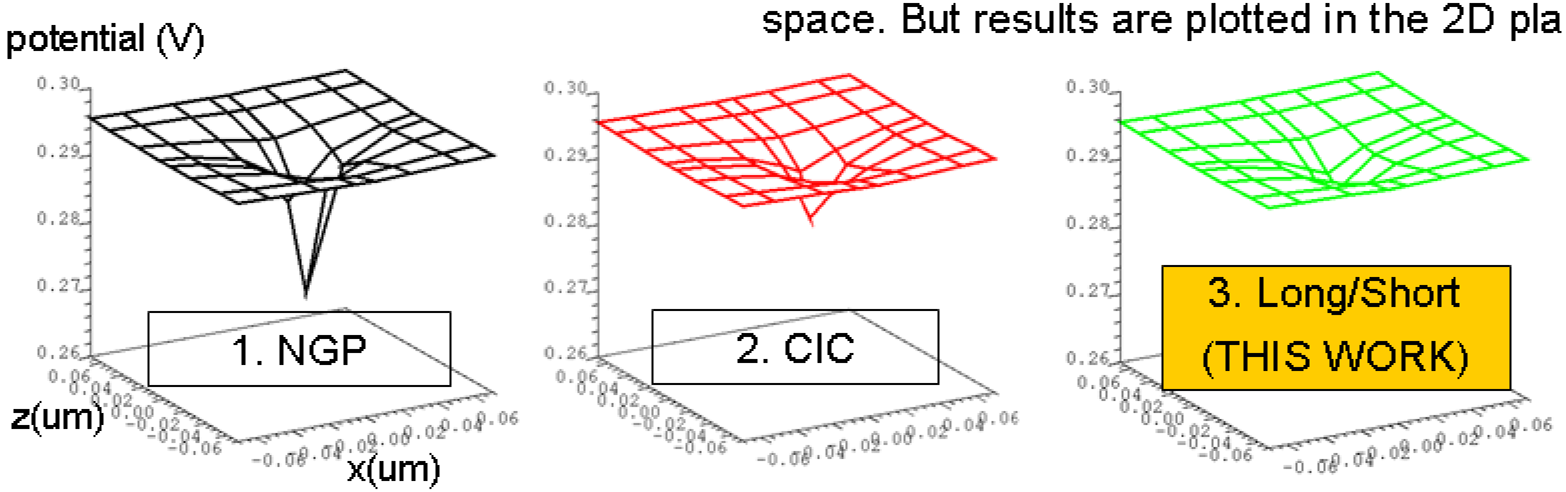
$$\rho(r) = \frac{ek_c^3}{2\pi^2}\frac{\sin(k_c r)}{(k_c r)^3}$$

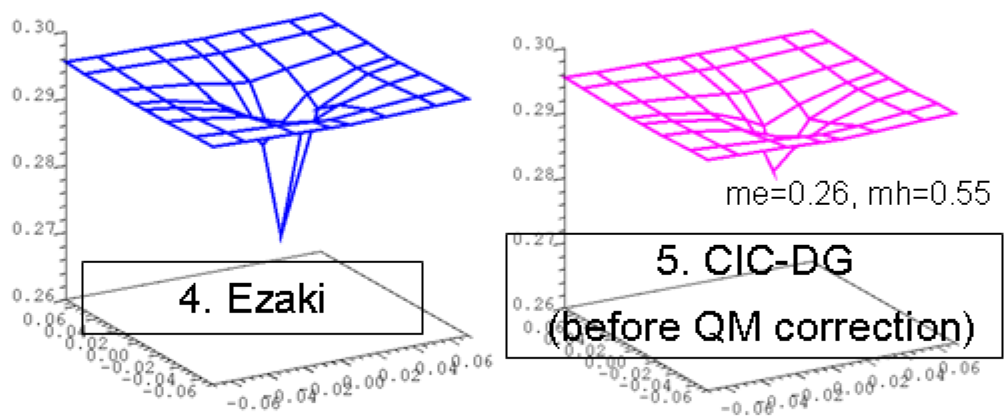
Ezaki

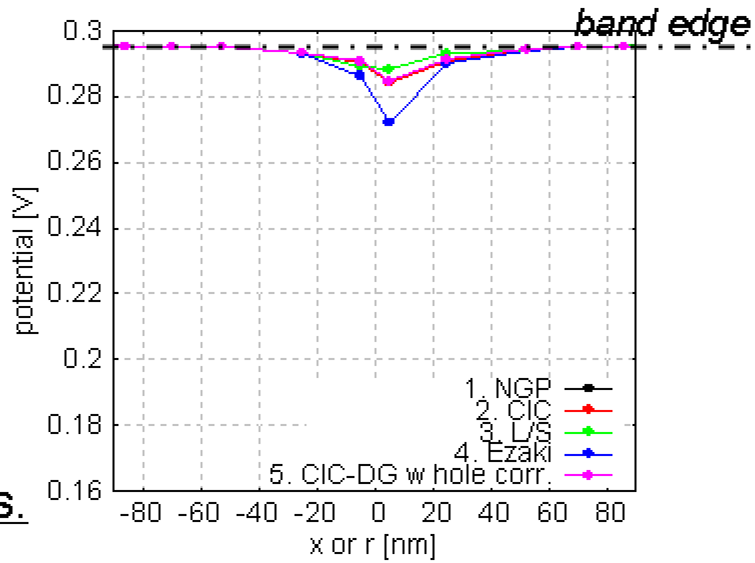
: omitting the 2nd term of L/S model to avoid "the minus density"

Atomistic Potentials with 10nm-grids

*All the stereo graphs below are calculated in the 3D space. But results are plotted in the 2D plane (y = 0).

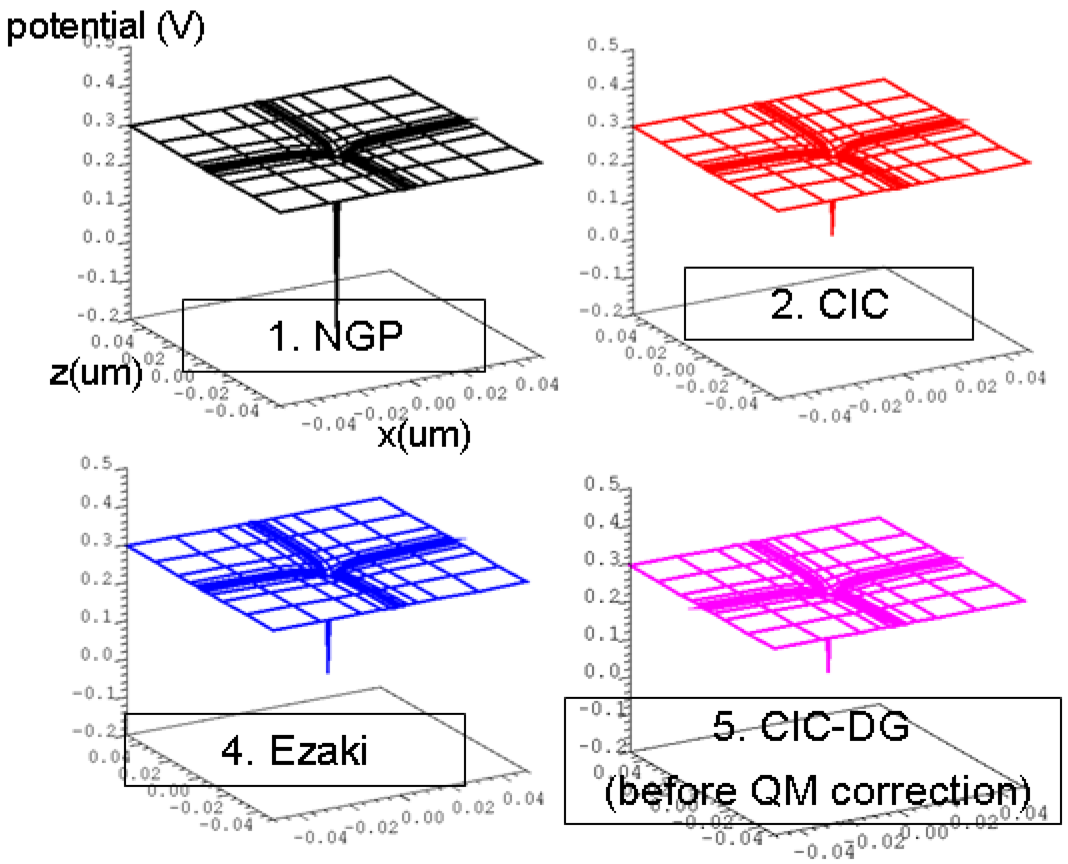


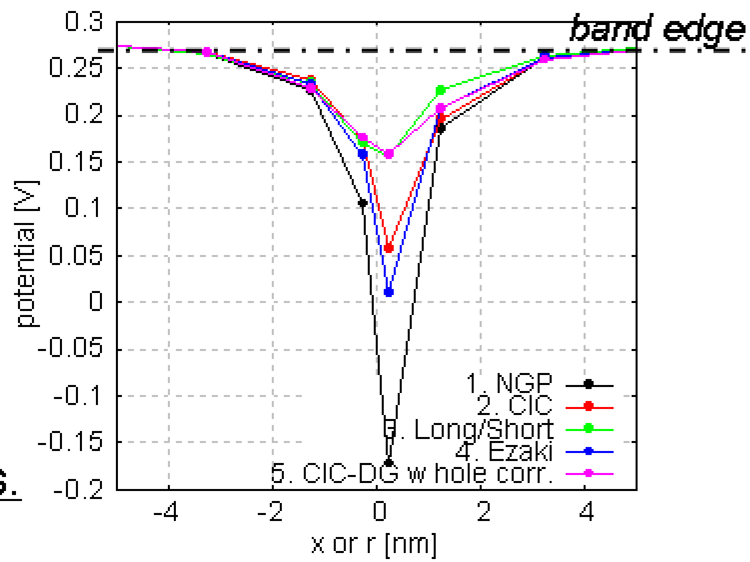




→ No special care is needed in rough mesh regions.

Atomistic Potentials with 0.5nm-grids

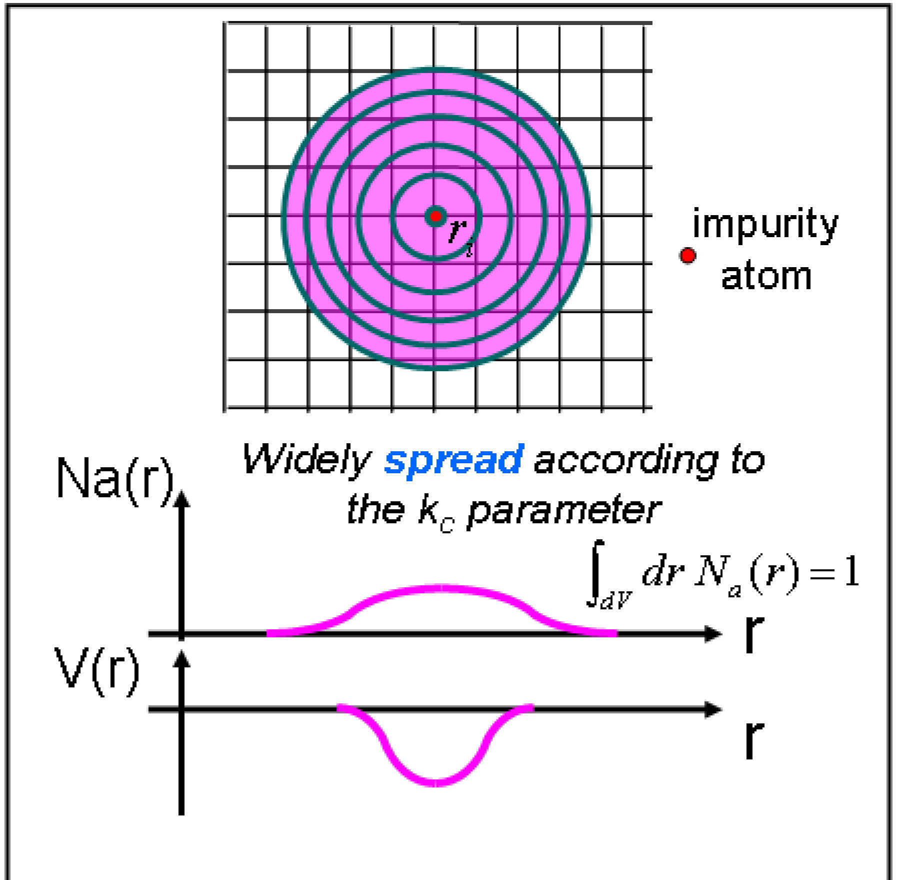




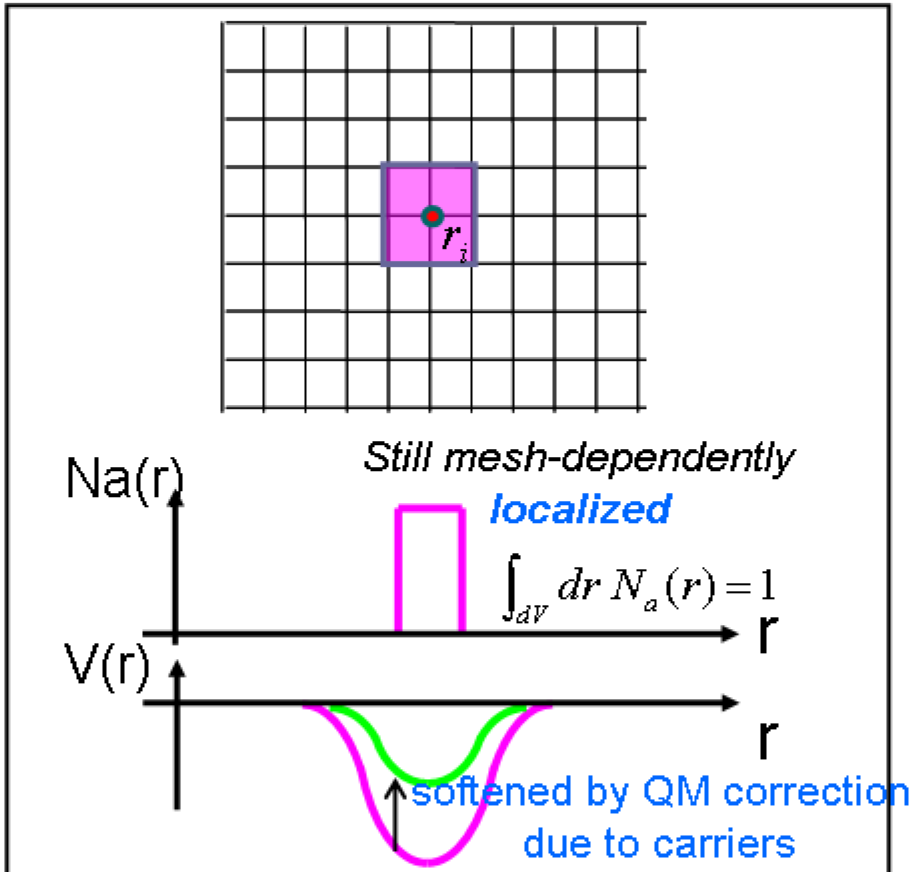
→ <u>Special care should be taken in fine mesh regions.</u>

In this case, the driven force for holes in “3” is similar to that in “5”.
But the concept is totally different, as is explained in the next slide.

Short Summary: Conceptual Difference



3. Long/short separation model



5. CIC with density-gradient

The "spreading" of L/S model definitely works well, especially at the contacts where dopant localizations cause the large decrease or increase in currents.

→ Let's see the SOI-NAND example

Outline

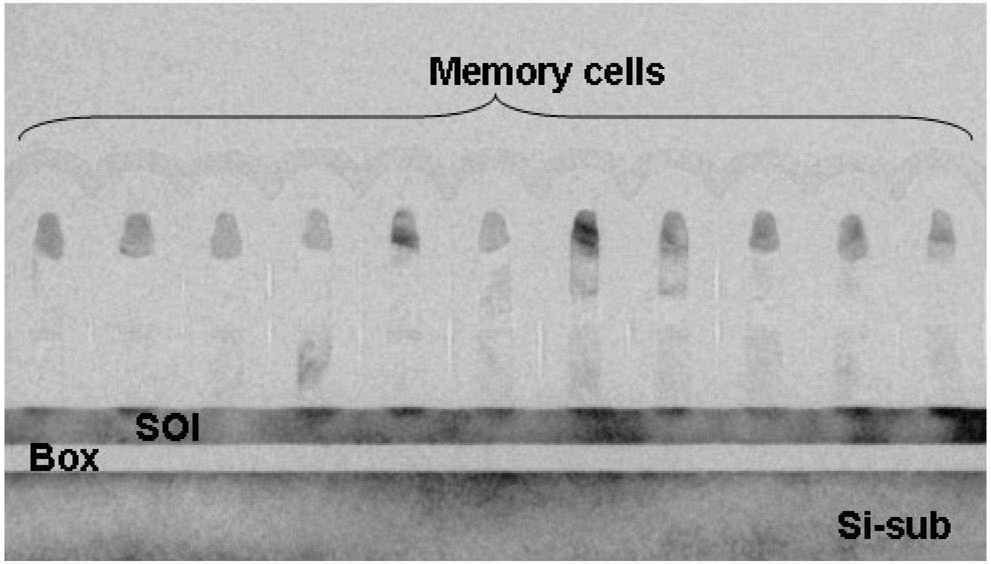
1. Objective
2. Introduction of the long/short (L/S) separation model and its comparison with the other models
3. **Numerical examples using the L/S model**
   1. (SOI-type) NAND FLASH memories --- L/S vs. CIC-DG ---
   2. Schottky contact resistance --- L/S vs. NGP --- (skip! →)
4. Open question: a limitation of the L/S model
5. Summary

SOI-type NAND FLASH Memories

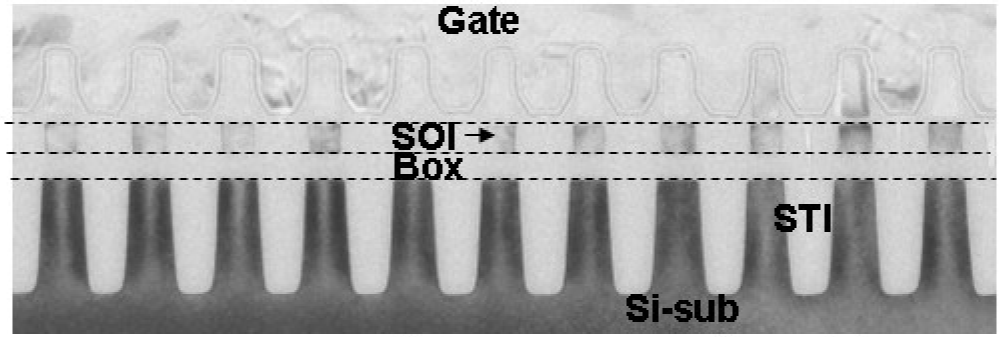
M. Mizukami et al., Jpn. J. Appl. Phys. 49, 04DD09 (2010).

Fabricated SOI NAND EEPROM TEM Image

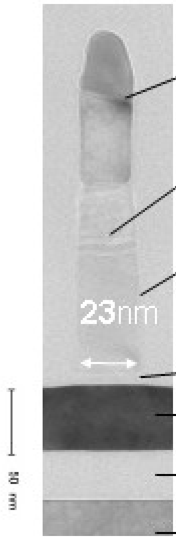
2Xnm cell size SOI EEPROM is fabricated

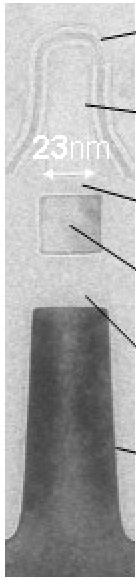


BL cross sectional image

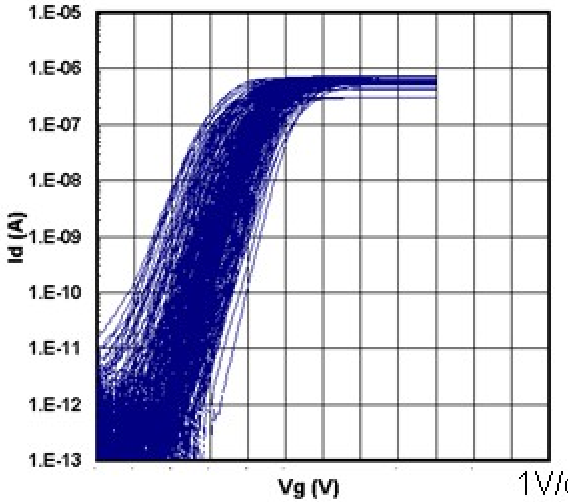


WL cross sectional image





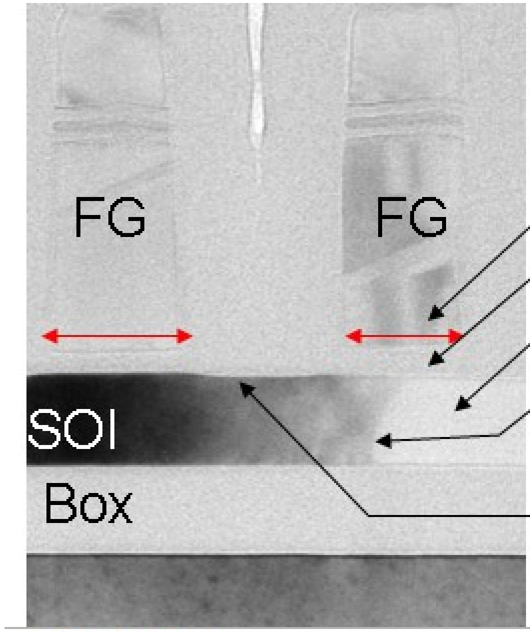
Electric Characteristics of the D-TOPS NAND EEPROM 3



D-ToPS cells' I-V curves

Initial Vth scattering of neutral cells
Back bias=0V, Vd=1.2V, Vread=all same

S-factor 558mV/dec(cent.). δVth = 4.1V ($\pm 6\sigma$)

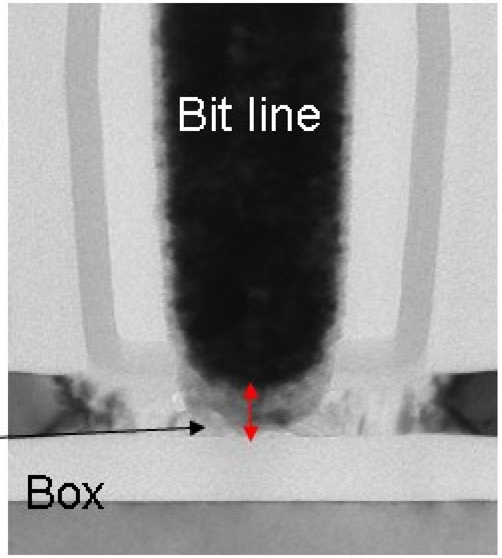


Vth scattering reason

- Channel length non-uniformity
- G_Ox thickness non-uniformity
- SOI thickness non-uniformity
- Si defect under FG

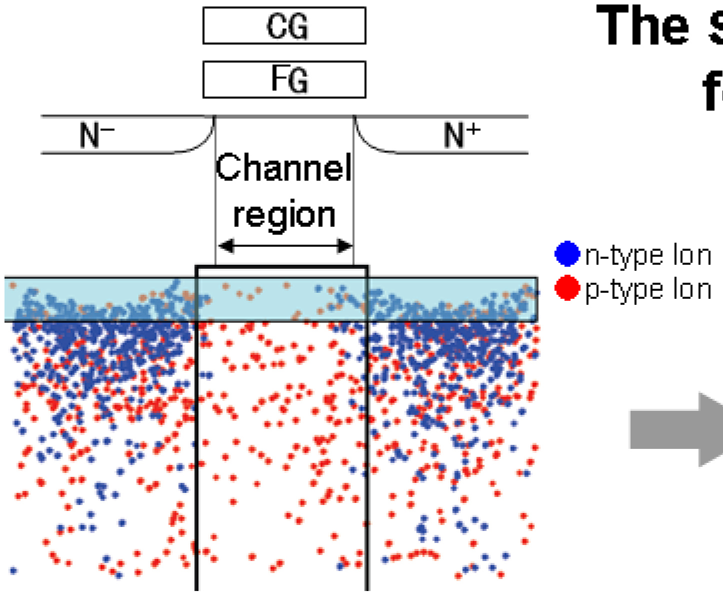
Icell difference reason

- Gauging
- Bit line contact non-uniformity

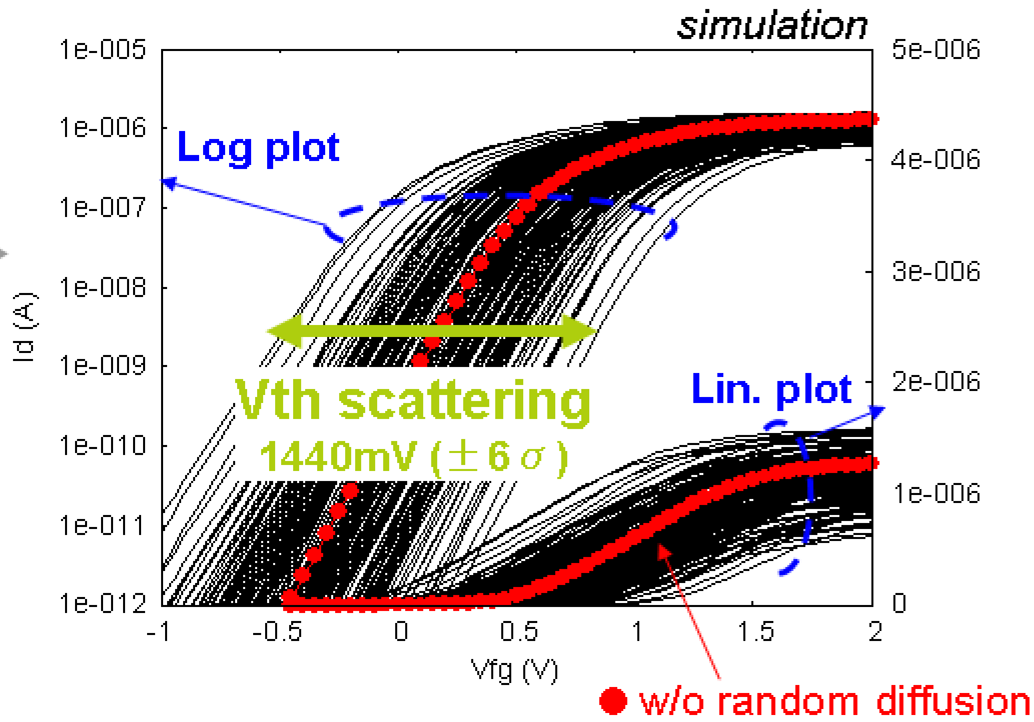


Conventional FG-NAND using Bulk Cell

The short channel effect is important issue for beyond 2Xnm cell NAND EEPROM!



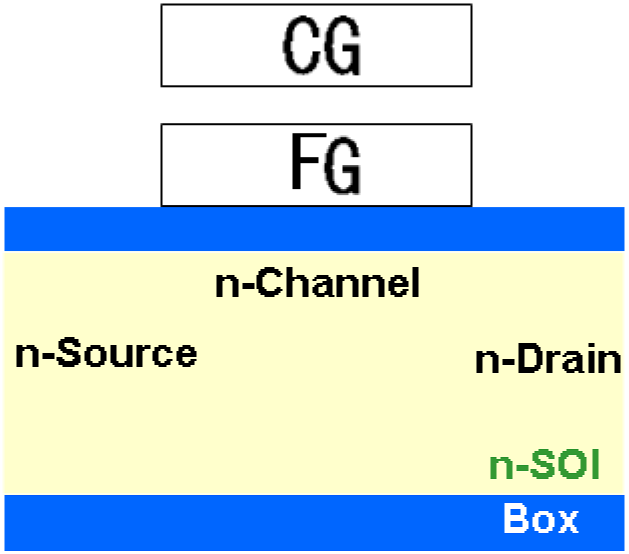
n-type impurities are diffused in the channel region randomly



Read-disturb is NOT avoided!!

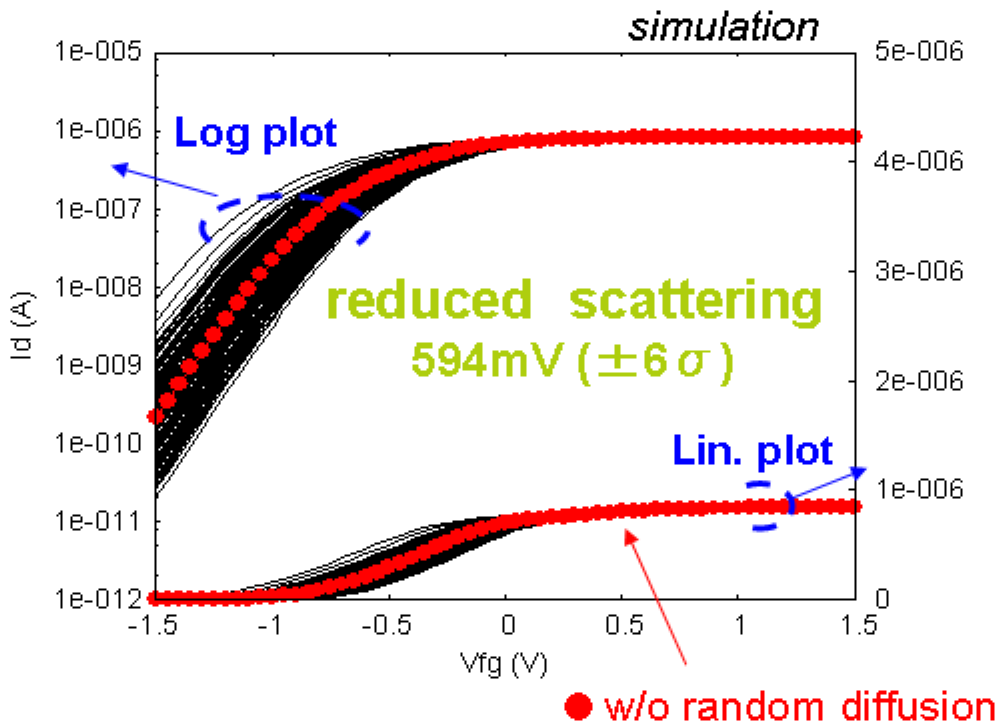
I-V simulation for 20nm cell size Tr. with random diffuse impurity effect

Proposed FG-NAND using SOI Cell



No different type impurities diffuse into the channel region

We propose a depletion-type cell Tr. on a self-manufactured SOI substrate for NAND EEPROM.



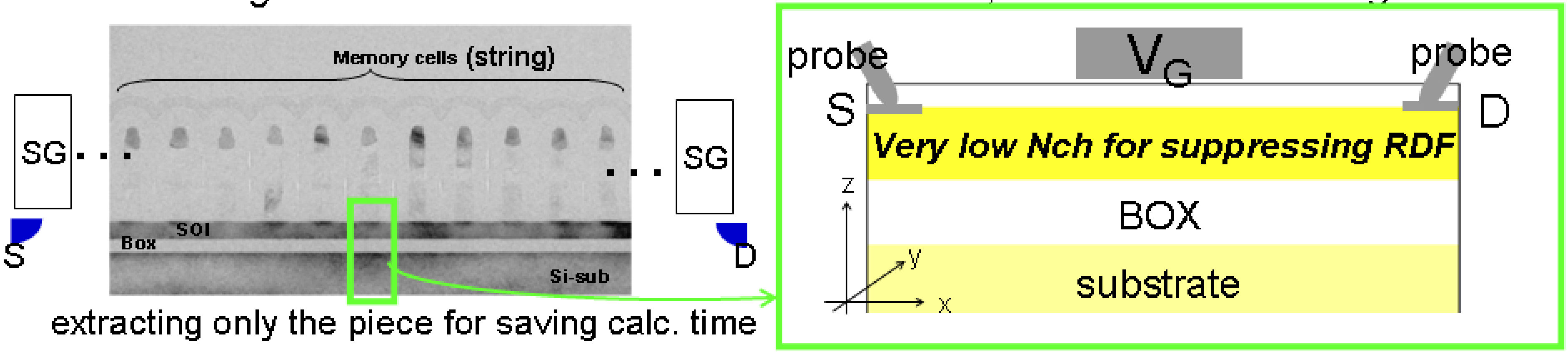
I-V simulation for 20nm D-type cell size Tr. with random diffuse impurity effect

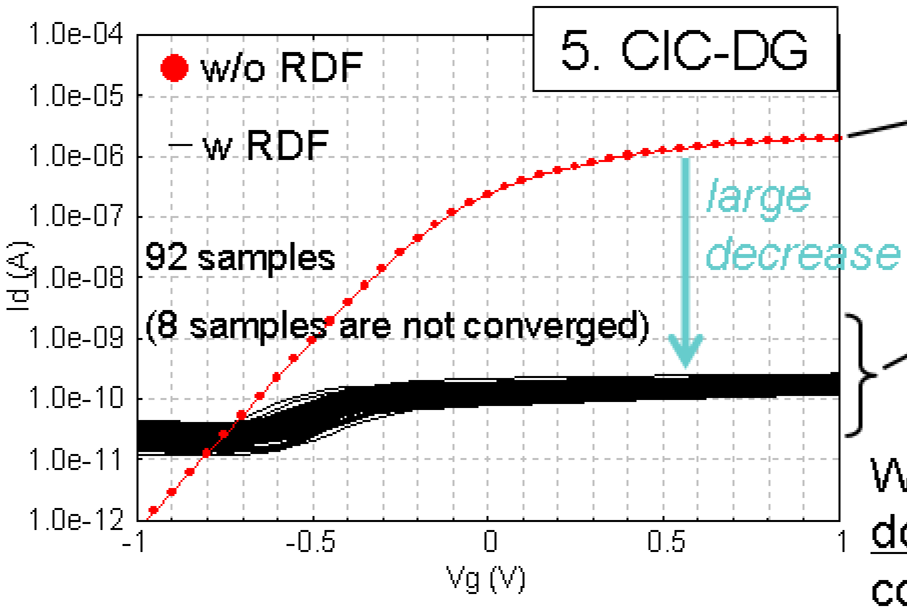
Short channel effect is reduced substantially

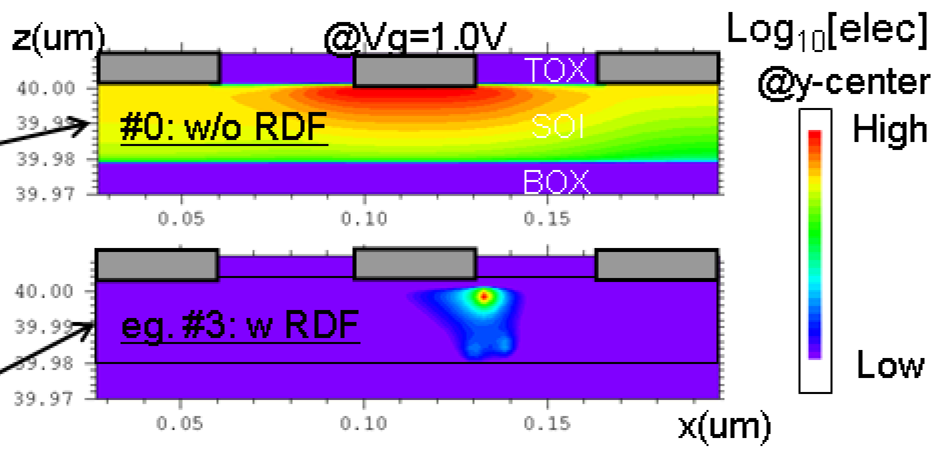
Adopting the CIC-DG Model to the SOI-NAND

Objective of simulation:

Just focusing on the characteristics of one cell Tr., not the entire string.



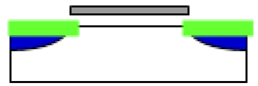




With RDF, electrons locally exist only at the few donor position. They do not flow in/out the S/D contacts; the device becomes highly resistive. What is the reason?

"Artificial Contact Starvation" caused by CIC-DG

The governing equations at the contacts (N-type ch.) are:



1. mass-action law

$$pn = n_i^{\,2}.$$

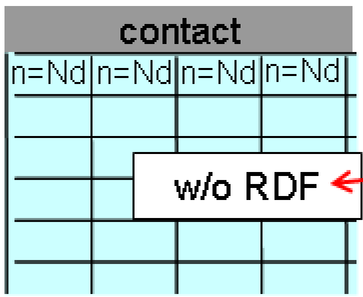
2. charge neutrality law

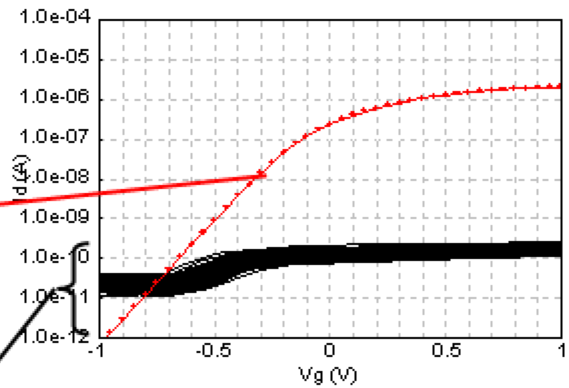
$$N_d + p - N_a - n = 0.$$

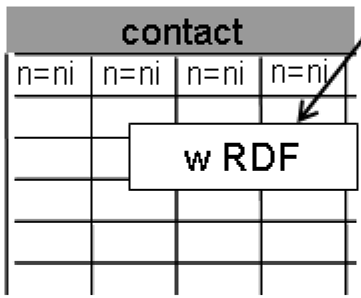
$$\therefore n = \frac{(N_d - N_a) + \sqrt{(N_d - N_a)^2 + 4n_i^{\,2}}}{2}$$

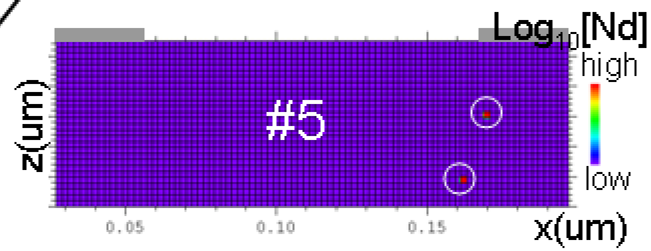
Mobile electron concentration at the contacts

If the mesh spacing is too fine in low impurity concentration structures, almost all the mesh grids show "Nd = 0, Na = 0". In that case, the quadratic equation returns the answer "**n = ni**". It results in the characteristics of intrinsic (no-doped) Si.





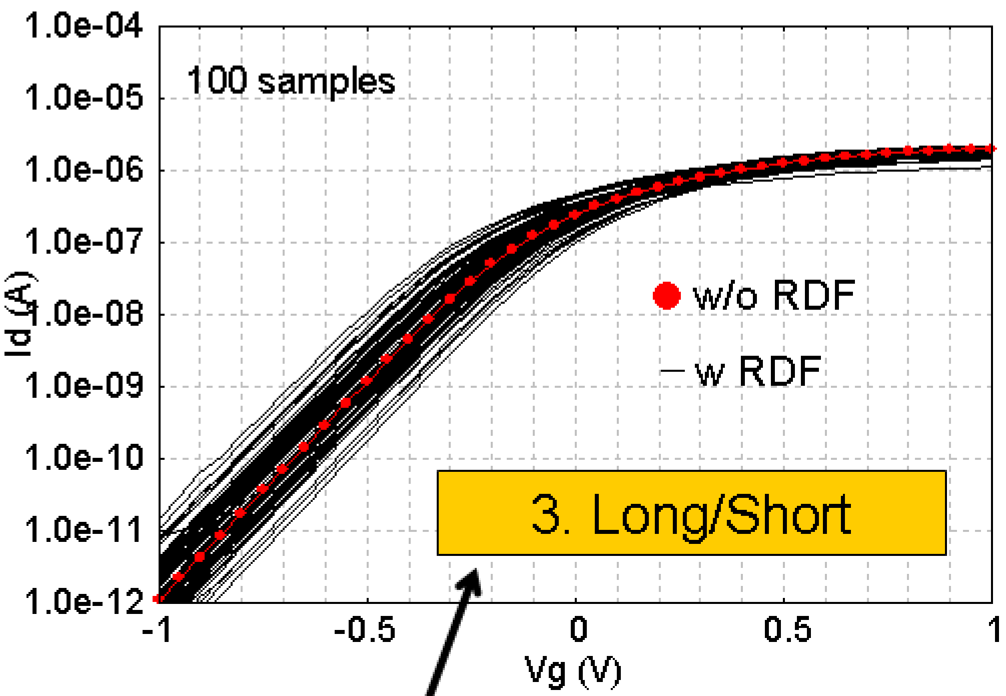


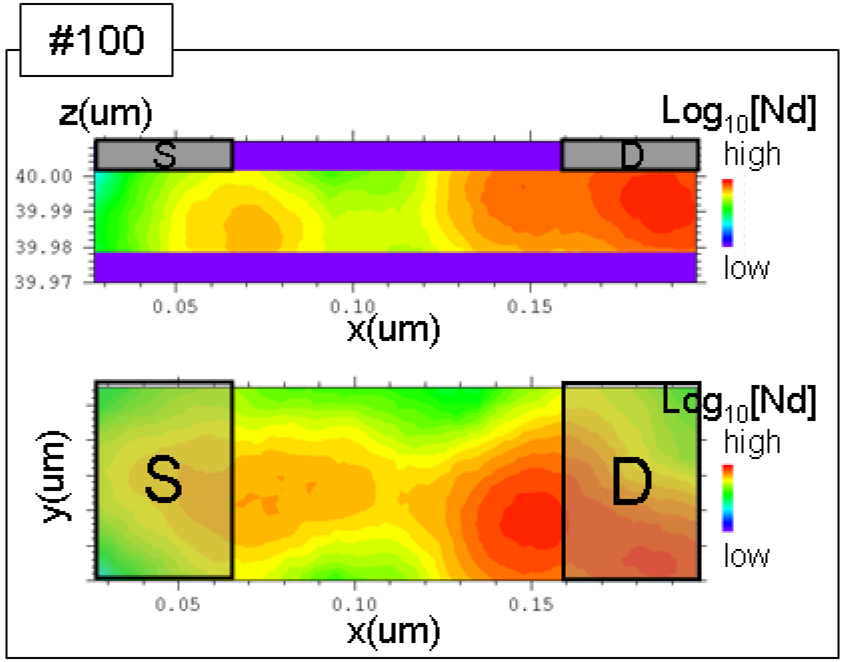


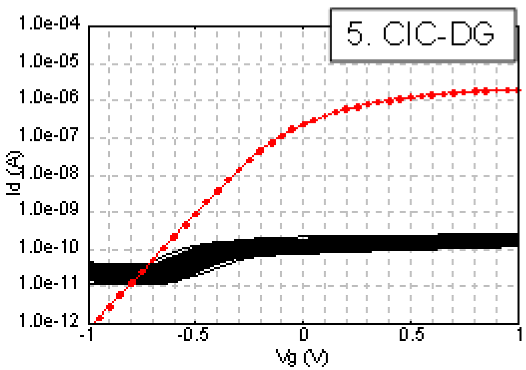
"artificial contact starvation"

Actually, no donor is found around the contacts.

The L/S Model Prevents the Artificial Starvation







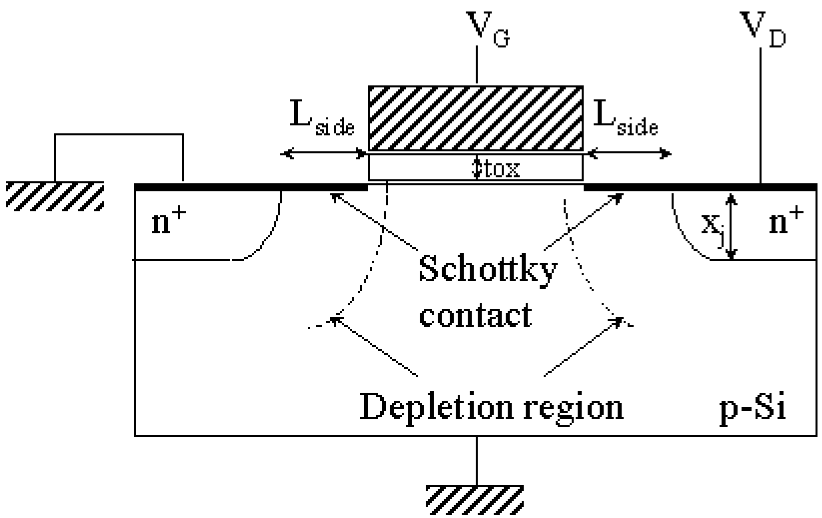
Non-zero impurity concentrations, representing the carrier concentration at the contacts, are ensured in the L/S model.

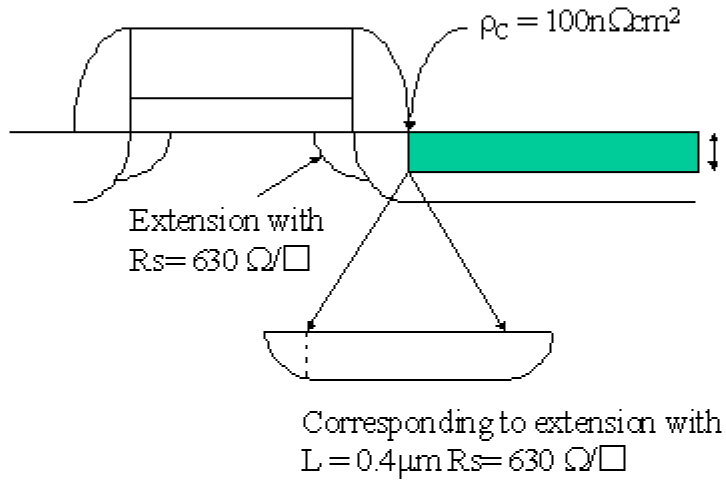
→ The L/S model prevents the *artificial* contact starvation.

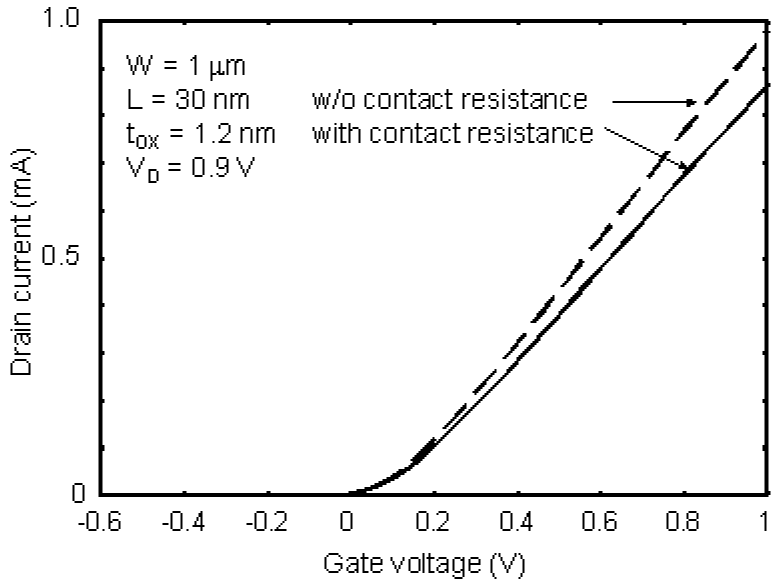
Variations of the Schottky Contact Resistances due to RDF

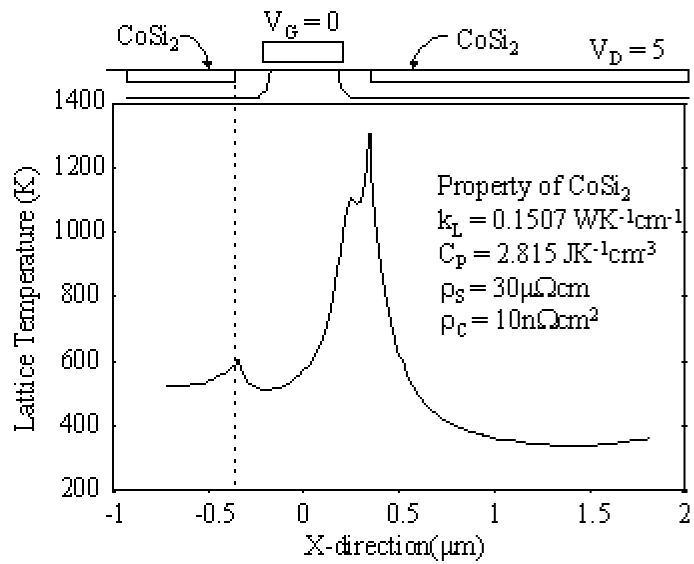
K. Matsuzawa et al., Proc. of SISPAD, 231 (2004)

Importance of the Metal-semiconductor Junction

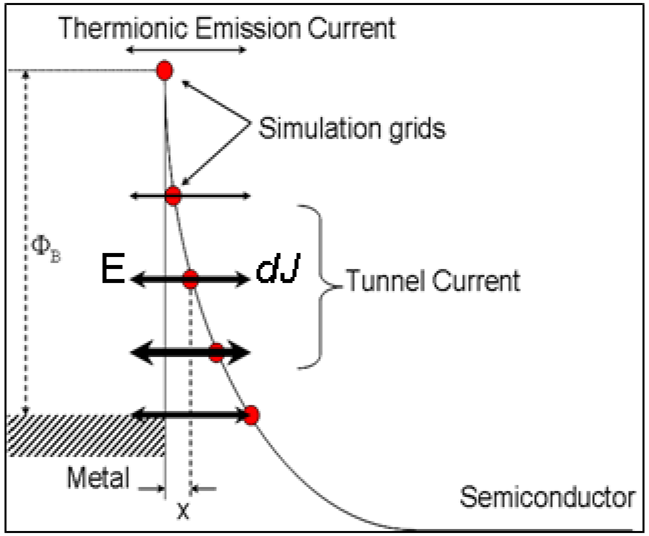


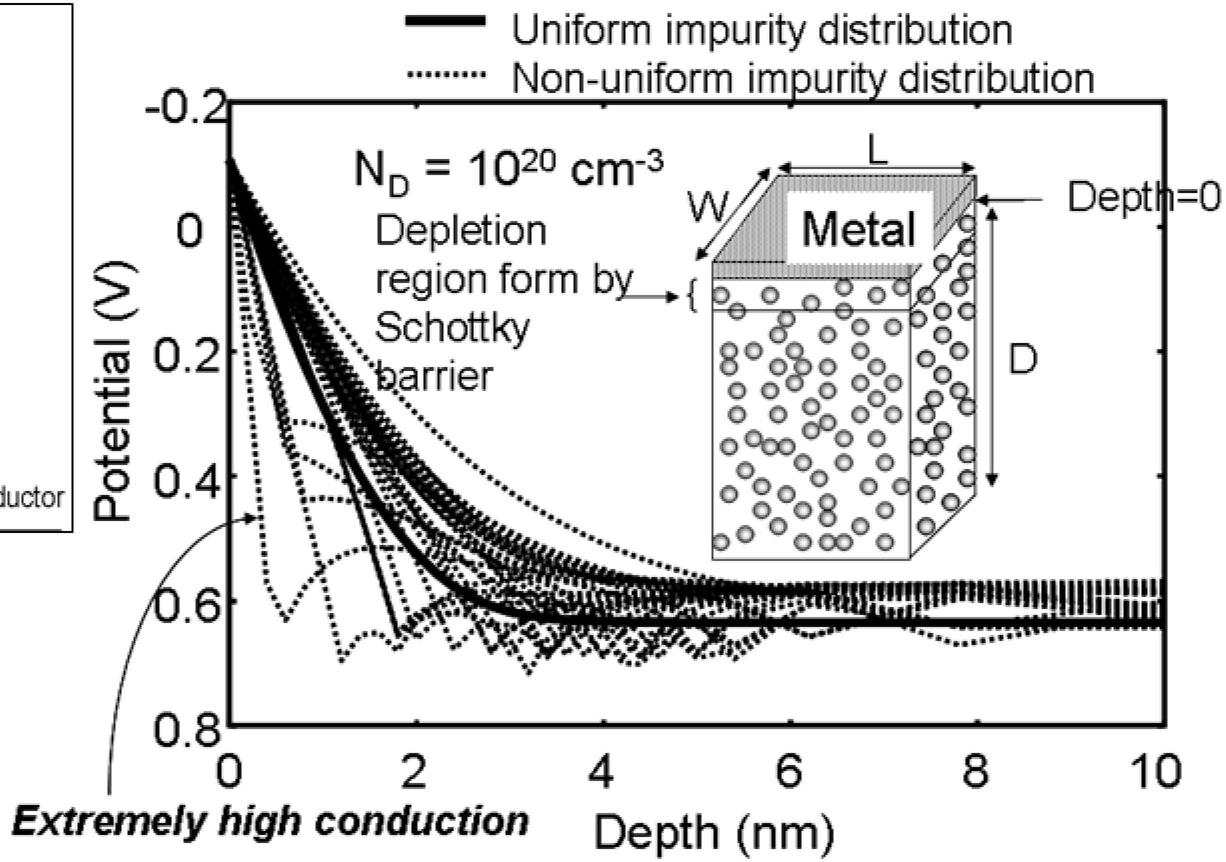


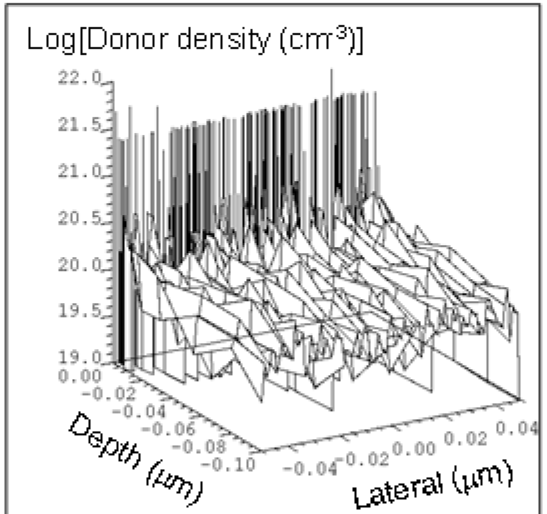




Schottky Barrier Variations using NGP





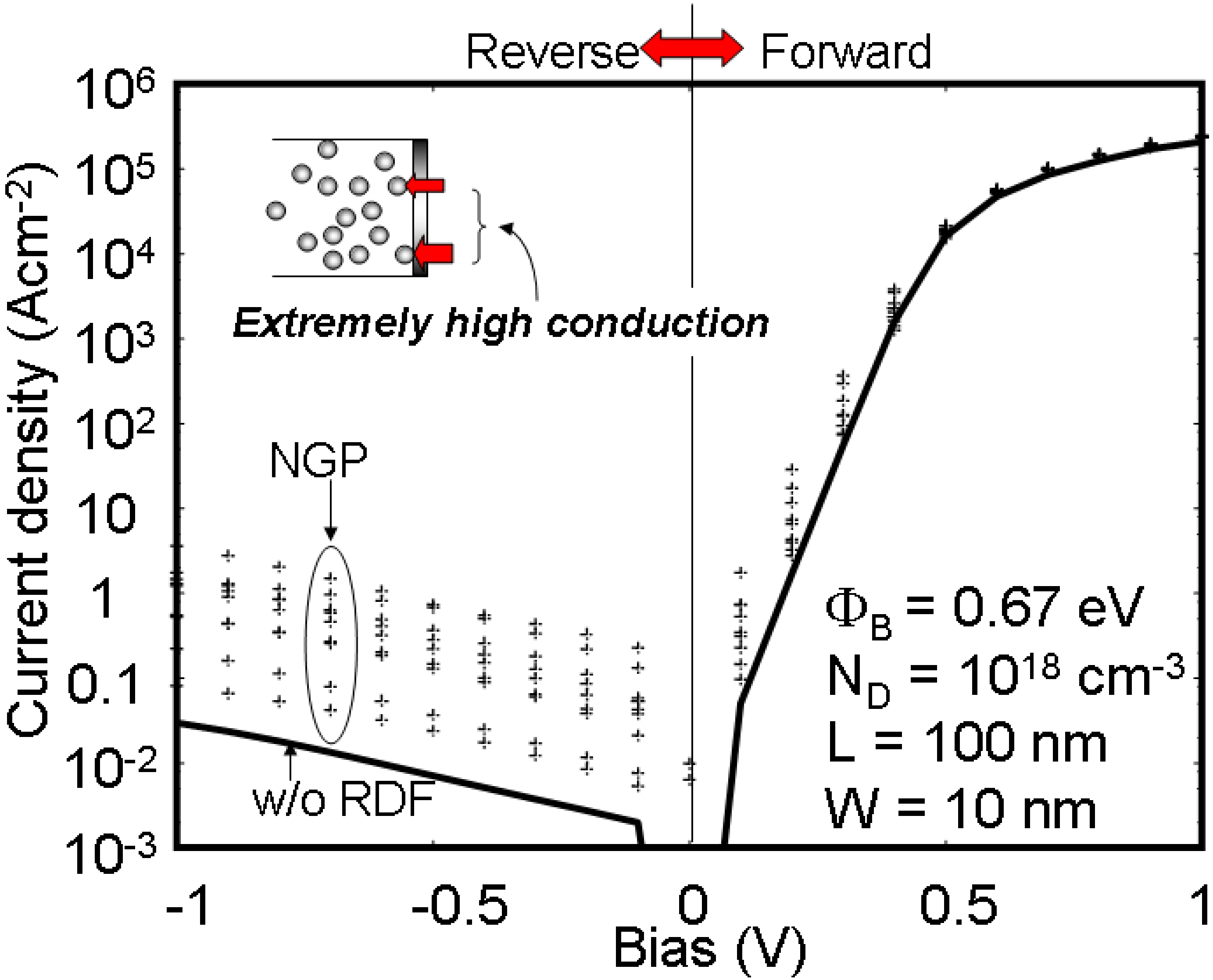


With NGP (both long&short components are included)

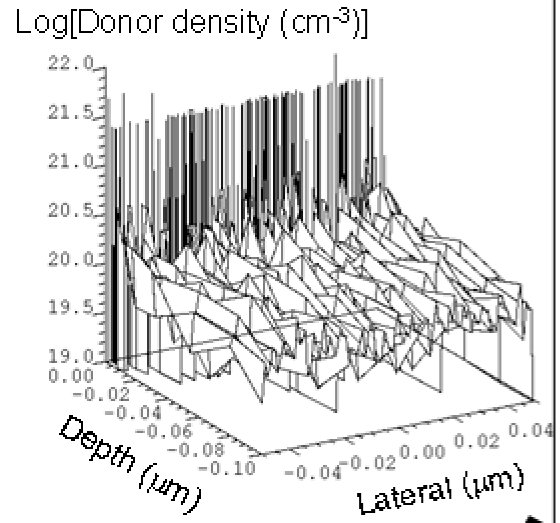
Tunneling currents (probabilities) depend on the integral area.

$$dJ \propto T_{WKB}(E) \approx Exp\left[-2\int_{in}^{out} dx \sqrt{\frac{2m_b}{\hbar^2}(V(x)-E)}\right]$$

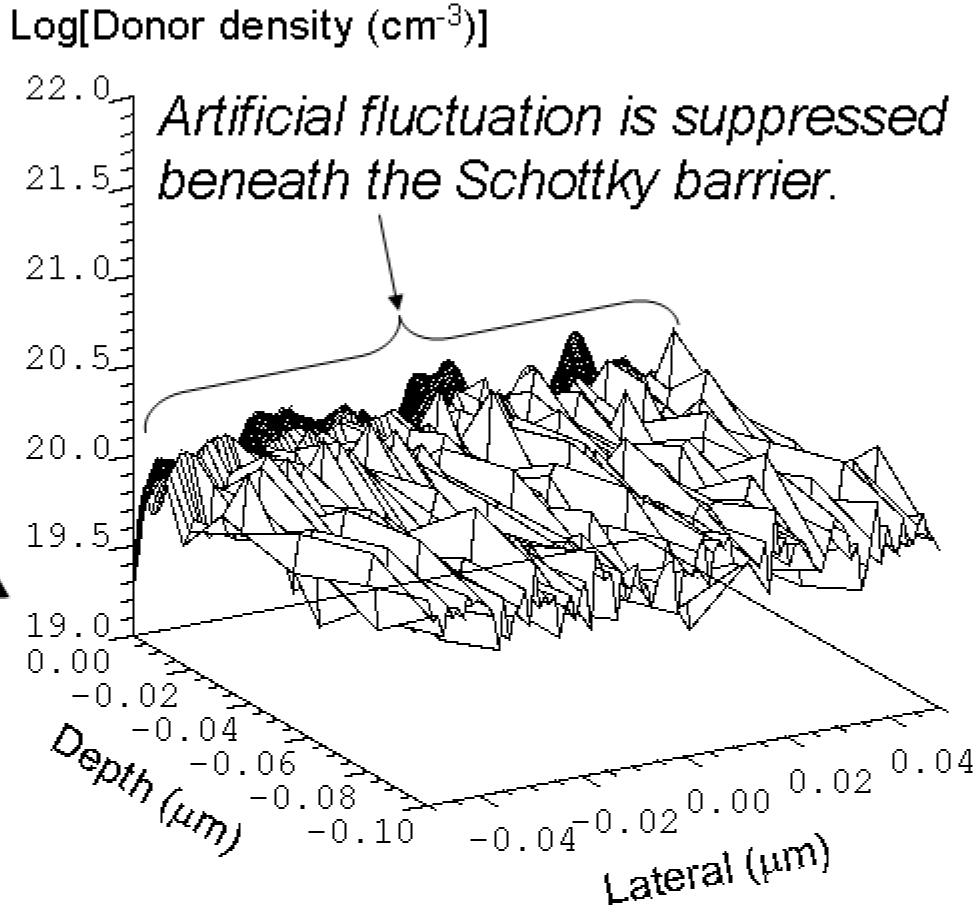
Artificially Low Contact Resistances by NGP



Adopting the L/S Model to Schottky Junctions

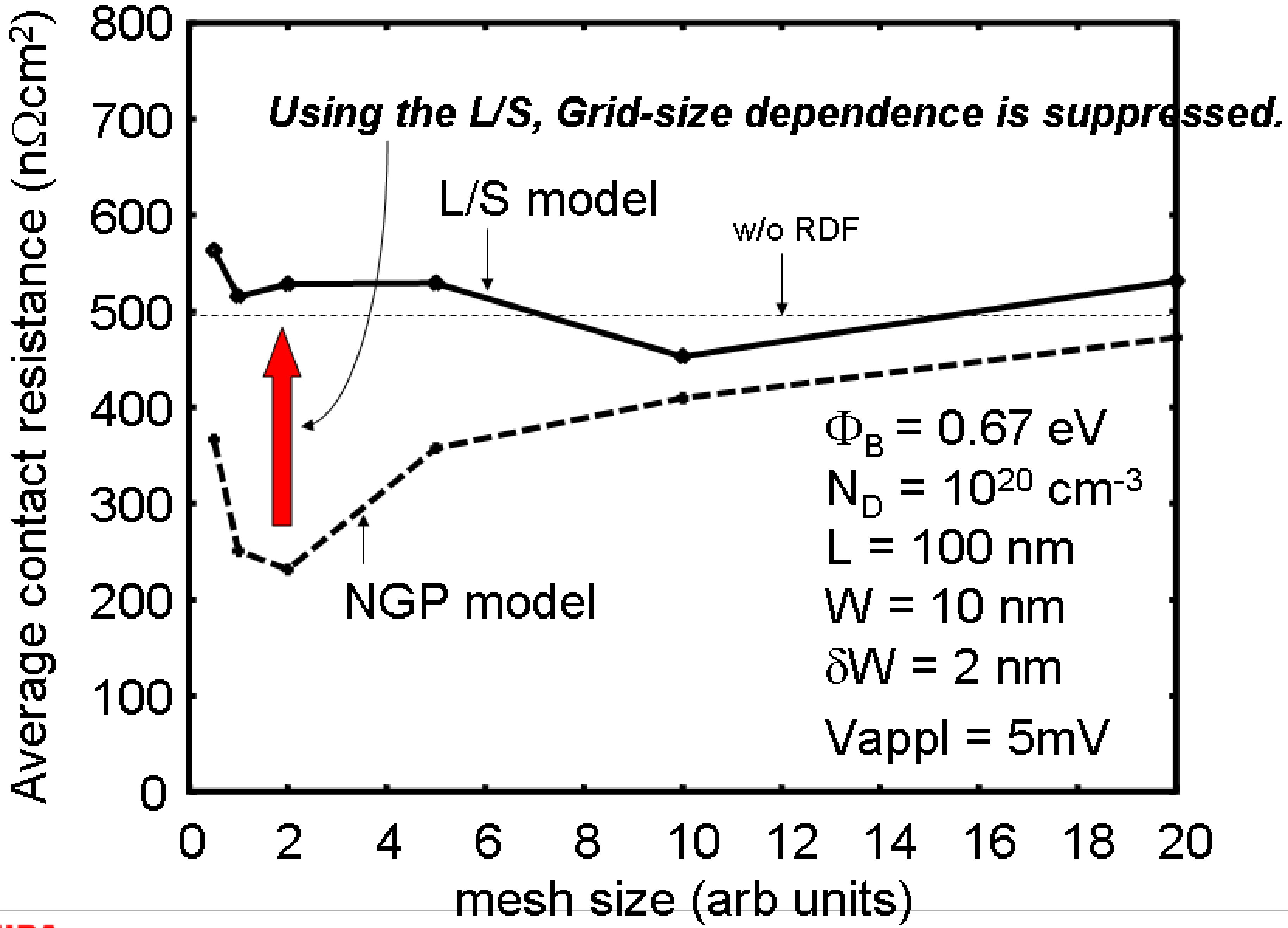


With NGP (both long&short components are included)



With the L/S model (=only the long-range components are considered)

Stable Results using the L/S Model

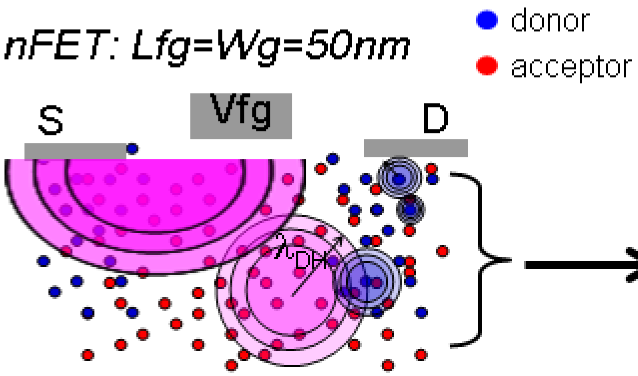


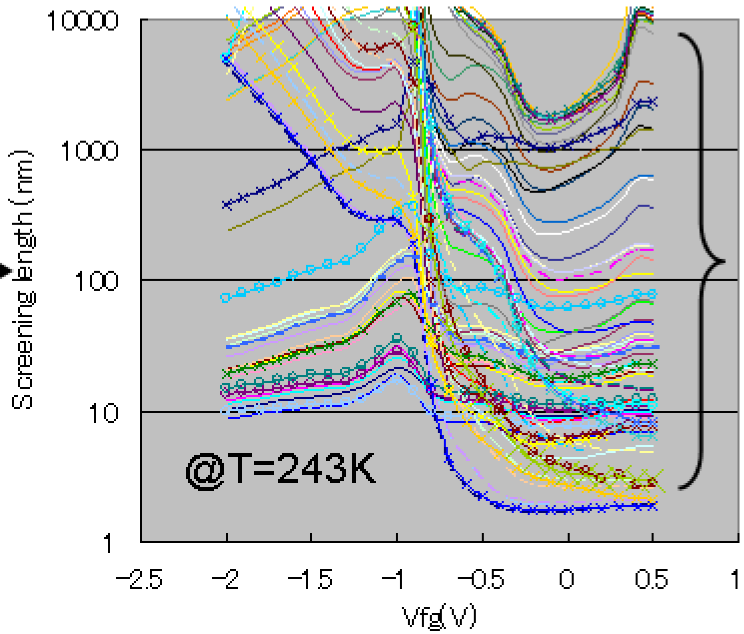
Outline

1. Objective
2. Introduction of the long/short (L/S) separation model and its comparison with the other models
3. Numerical examples using the L/S model
   1. (SOI-type) NAND FLASH memories --- L/S vs. CIC-DG ---
   2. Schottky contact resistance --- L/S vs. NGP ---
4. Open question: a limitation of the L/S model
5. Summary

Difficulty in the Determination of k_c in the L/S Model

In the depletion layer or near the pn-junction, the well-known Debye screening length expression returns unphysically long value. Those sometimes exceed the device size itself, because of low screening carriers.

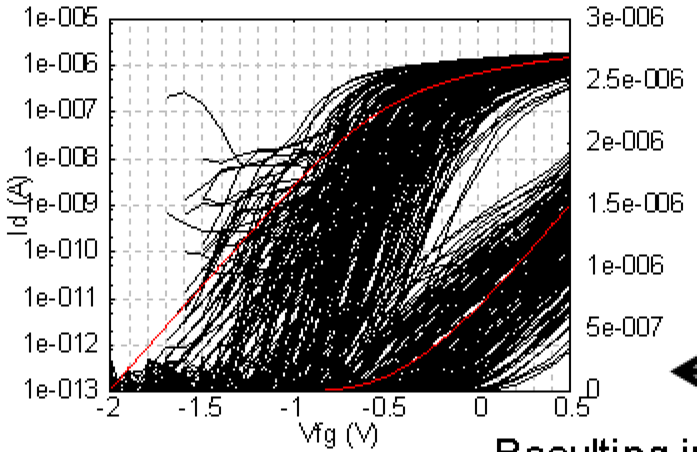




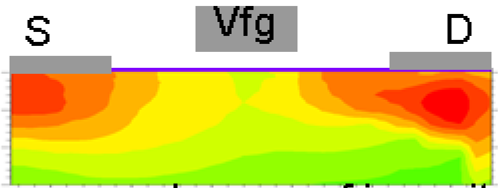
Each line represents the λ_{DH} around each impurities (both donor and acceptor) in the 50nm-nFET.

$$\lambda_{DH} = \sqrt{\frac{\varepsilon_{si} k_B T}{q^2 n_{screen}}}$$

$$k_c = \lambda_{DH}^{-1}$$



Resulting in strange (oscillating) Id-Vg curves.



The spread-range of impurity concentration significantly changes with the biases.

Derivation of Analytical λ_{DH}

Poisson Equation

$$\Delta(\delta\phi) = \frac{\delta Q}{\varepsilon} = q\frac{(\delta p - \delta n)}{\varepsilon} = \frac{q^2(p+n)}{\varepsilon k_B T}\delta\phi \quad ...(1)$$

Assuming local thermal equilibrium

$$n + \delta n = n_i \exp\left(-\frac{(E_c + q\delta\phi) - E_f}{k_B T}\right) = n\exp\left(-\frac{q\delta\phi}{k_B T}\right)$$

$$\rightarrow \delta n \approx n\exp\left(-\frac{q\delta\phi}{k_B T}\right) - n = n\left(1 + \frac{-q\delta\phi}{k_B T}\right) - n = -\frac{qn\delta\phi}{k_B T}.$$

$$p + \delta p = p\exp\left(\frac{q\delta\phi}{k_B T}\right)$$

$$\rightarrow \delta p \approx \frac{qp\delta\phi}{k_B T}.$$

Laplacian in the polar coordinate

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \quad ...(2)$$

Since eq. (3) satisfies with (1),

$$\delta\phi = \frac{q}{4\pi\varepsilon r}\exp\left(-\frac{r}{\lambda}\right) \quad ...(3)$$

↓ operating (2) to (3),

$$\Delta(\delta\phi) = \frac{1}{\lambda^2}\frac{q}{4\pi\varepsilon r}\exp\left(-\frac{r}{\lambda}\right) = \frac{\delta\phi}{\lambda^2} \quad ...(4)$$

↓ finally, we obtain

$$\lambda_{DH} = \sqrt{\frac{\varepsilon k_B T}{q^2(p+n)}}$$

Here, the analytical screening length expression is derived from the assumption that the potential attenuates to zero at infinity distance. ↔ Realistic device operation

Furthermore, the screening length in real device is not necessarily spherically-distributed. ↔ The L/S model (= spherical symmetry is assumed in principle)

Summary

■For the Long/Short (L/S) Separation Model

•The L/S model softens the acute potential around an impurity charge by means of spreading the charge concentration.

•The L/S model enables handling both highly doped concentration (e.g. Schottky contact) and extremely low concentration (e.g. SOI-NAND) cases.
=The L/S model can deal with the RDF around contacts in a unified way.

•The computational costs of the L/S is usually very low, compared with the DG model. We can run many samples within *tight R&D schedule*.

■For the most popular, CIC with Density-Gradient Model (CIC-DG)

•The CIC-DG model also softens the acute potential by QM corrections due to the mobile charges surrounding the singular point.

•However, since the impurity charge concentration is still localized, it causes "artificial starvation" at contacts, depending on the mesh sizes.
=Continuous (jellium) regions around the contacts are indispensable.

■Open Problems for the L/S model

•How does a TCAD user determine the cut-off parameter k_c?

Acknowledgement

This work is directly/indirectly supported by many collaborators:

•**Makoto Mizukami** (SOI-NAND), **Kazuya Matsuzawa** (Schottky), **Daisuke Hagishima** (Density-gradient), **Hiroyoshi Tanimoto**, **Toshiyuki Enda**, **Takashi Izumida**, **Nobutoshi Aoki**, **Shigeo Kondo**, **Shinya Naito**, **Michiru Hogyoku**, **Takeshi Shimane**, **Mitsutoshi Nakamura**, and **Naoyuki Shigyo**, all are belonging to Toshiba Corporation.

•Professor **Shinji Odanaka** of Osaka University.

•Professor **Nobuyuki Sano** of the University of Tsukuba.

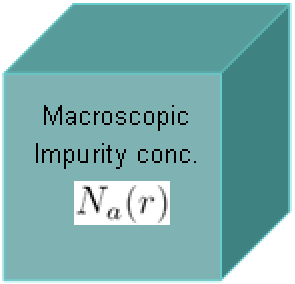
Appendix

How to Generate Atomistic Impurity Profiles

The number of impurity ⇒ Poisson random number.

The position of each impurity ⇒ uniform random number.

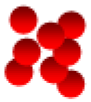
Stochastic variable: number n_a



δV Control Volume

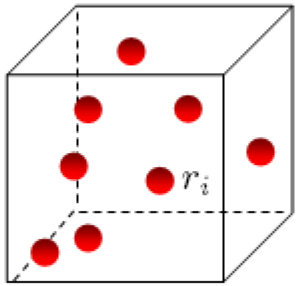
$$P(n_a) = \frac{e^{-\langle n_a \rangle} \langle n_a \rangle^{n_a}}{n_a!}$$

$$\langle n_a \rangle = N_a(r)\delta V$$



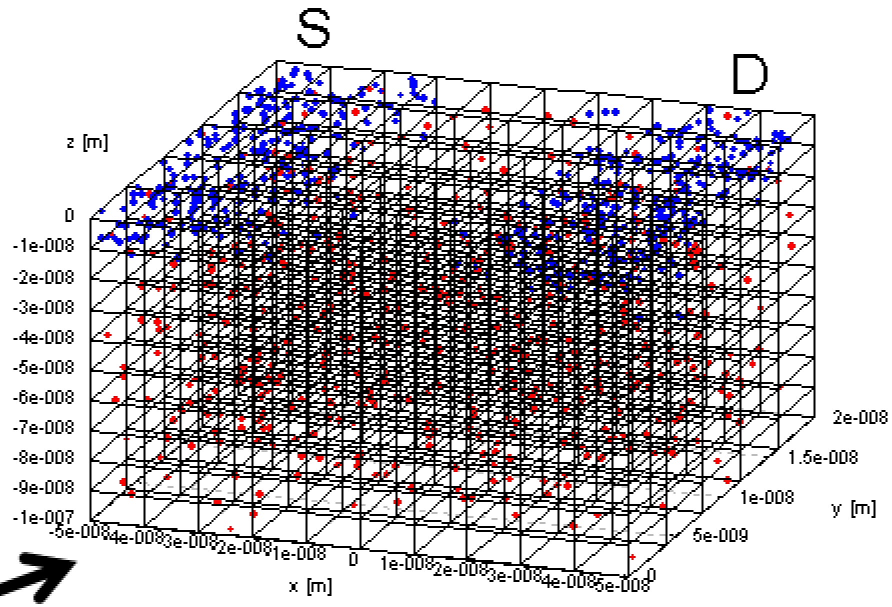
n_a Poisson random number

Stochastic variable: position r_i



Uniform random number

$$r_i \in \delta V$$



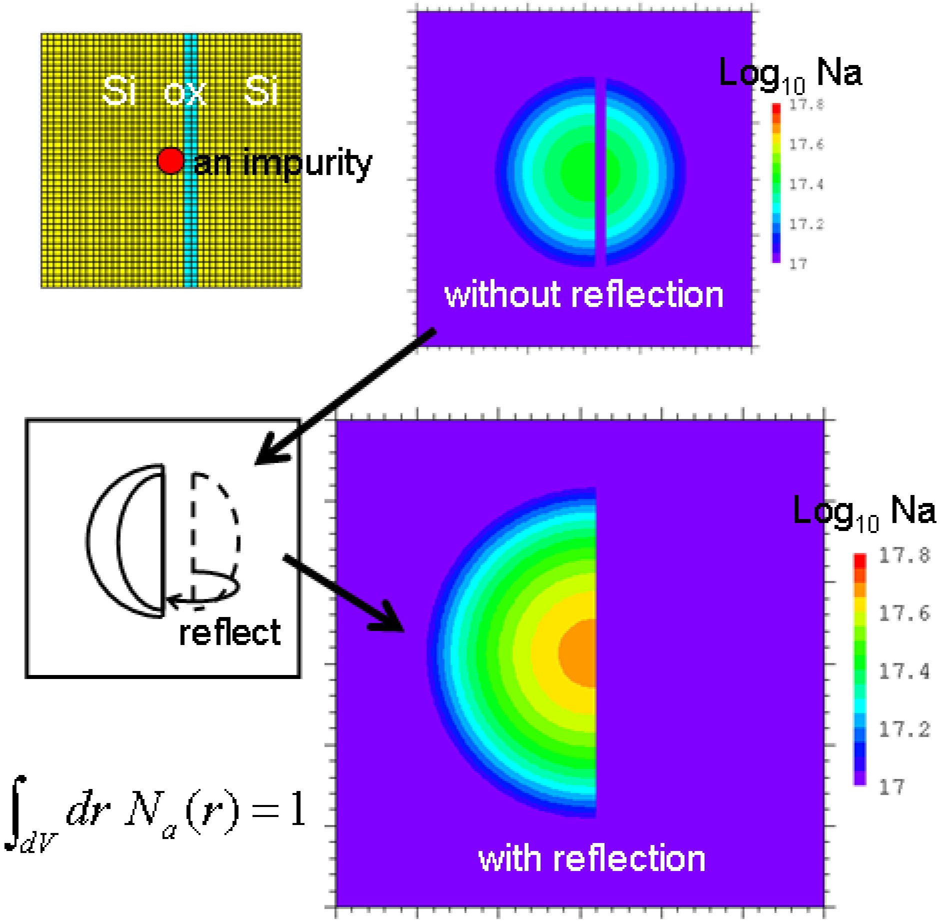
Repeated in all simulation domain...

: Assuming that nature favors randomness

↕

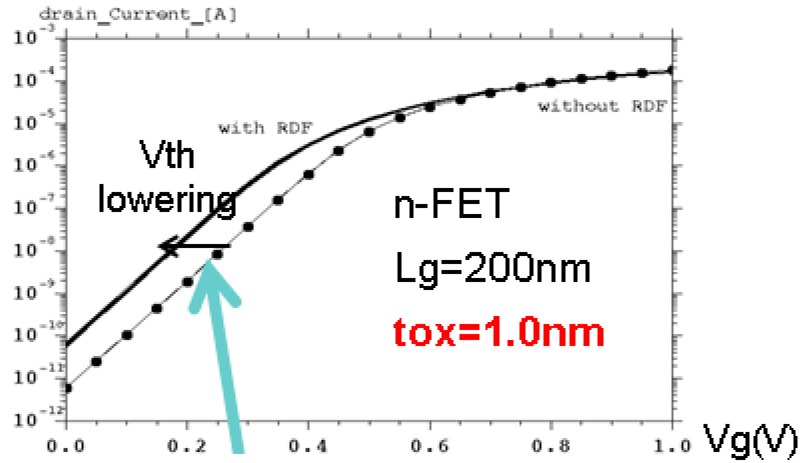
Correlated clusters

Necessity of Image Charge Reflection at the Interface



$$\int_{dV} dr\, N_a(r) = 1$$

The charge concentration from an impurity should be normalized to unity.



Without the reflection, donor concentration in the poly gate spreads beyond the thin gate oxide into the channel, resulting in artificial Vth lowering.