Analyzing Variability in Short-Channel Quantum Transport from Atomistic First Principles

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Outline

❖ Background for variability

❖ Methodology
  ▪ NEGF-DFT formalism
  ▪ Disorder average
  ▪ RDD induced variability

❖ Applications
  ▪ Variability in Si nano-FET
  ▪ Some other application

❖ Summary and Outlook
Background and Motivation

- Variability in MOSFET (<50nm)

  Source of device variability

  Random discrete dopant  Line edge roughness  Metal gate granularity

  Random telegraph noise
Background and Motivation

- RDD induced variability in nano devices

Fig. 1 Experimental saturation threshold voltage, $V_{ts}$, of NMOS transistors with $L_g$ down to 20nm for (a) width=200nm and (b) width=20nm at $V_d=1.0$V.

Existing Theory and Model

Classical drift-diffusion model

Continuum model

source channel drain

Poisson equation, Drift-diffusion equation
Existing Theory and Model

Classical drift-diffusion model

Continuum model

$I_1$

$I_2$

$I_3$

\( \bar{I}, \, dI \)
Existing Theory and Model

Classical drift-diffusion model

Comment:
✓ Fast in computation
✓ Accurate statistical information
✗ Physics less reliable

S. Markov, EDL, VOL. 33, NO. 3 (2012)
Existing Theory and Model

Quantum tight-binding model

Atomic model

source channel drain

Poisson equation + NEGF
Existing Theory and Model

Quantum tight-binding model

Comment:
- Physics more reliable
- Slow in computation
- Less accurate statistical information
- Many parameters needed

TED, VOL. 58, NO. 8, (2011)
Our solution to variability problem

Q: Quantum + Parameter free method to calculate RDD induced variability?
**NEGF-DFT**

- DFT, a solid way to determine $H$, parameter-free
- NEGF: Keldysh nonequilibrium Green’s function

\[ H = H[\rho(\vec{r})] \]

\[ \rho(\vec{r}) = \int G^< dE = \int G^R \Sigma^< G^A dE \]

\[ T(E) = \text{Tr} [G^R \Gamma_L G^A \Gamma_R] \]

DFT

\[ f_L \]

left electrode

scattering

right electrode

general model for electronic devices
Shortcomings

- Cannot handle realistic doping concentration
- Too many configurations

\[ A_x B_{1-x} \]


For any theoretical calculation, disorder averaging must be done.
Want: derive an analytical averaged NEGF-DFT

When there are impurities, translational symmetry is broken. Coherent Potential Approximation (CPA) is an effective medium theory that averages over the disorder and restores the translational symmetry. An atomic site has $x\%$ chance to be occupied by A, and $(1 - x)\%$ chance by B. This approximation recovers the translational symmetry.


Average over random disorder: $\overline{T(E)} = \text{Tr}[G_R^\Gamma L G^A \Gamma_R]$ 

Our solution: derive an analytical averaged NEGF-DFT

\[ \rho(\vec{r}) = \int G^< dE = \int G^R \Sigma^< G^A dE \]

Average over random disorder:

\[ \overline{\rho(\vec{r})} = \int \overline{G^<} dE = \int \overline{G^R \Sigma^< G^A} dE \]

\[ T(E) = \text{Tr} [\overline{G^R \Gamma_L G^A \Gamma_R}] \]

\[ \overline{G^R \Gamma_L G^A \Gamma_R} = \overline{G^R (\Gamma_L + \Omega_{NV} G^A) \Gamma_R} \]

specular  diffusive

Youqi Ke, Ke Xia and Hong Guo  PRL 100, 166805 (2008)
Some comments for the disorder average

- CPA has been proven to be accurate through the whole doping region, from 0 to 1

- It has a different, but more beautiful form, NECPA, by applying Langreth theorem and analytical continuation

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Quantum transport theory with nonequilibrium coherent potentials

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Variability, Green’s function method

- Standard deviation of $T$: $dT = \sqrt{T^2 - \bar{T}^2}$

- $\bar{T}^2 \sim G^r \Gamma_L G^a \Gamma_R G^r \Gamma_L G^a \Gamma_R$, average of four Green’s function can be calculated exactly (see ref.)
RDD induced variability in Si nanoFET

- Variability of off-state tunnel conductance of the Si n-p-n junction
- Uniform doping: dopants distributed uniformly within the whole channel
- Localized doping: same number of dopants as uniform doping, but distributed within a 1nm’s region
- MBJ XC functional, bandgap of 1.11eV for bulk Si

Uniform doping, $dG$ vs. channel length

Both $G$ and $dG$ decays in some exponential fashion with $L$, the dotted curves are fitted to WKB model

$$T \sim e^{-2\gamma}, \quad \gamma = \frac{1}{\hbar} \int \sqrt{2m^*|V(z)| - E_F} \, dz$$,

$$dG \propto \sqrt{\left| \frac{\partial G}{\partial l} \right|^2 + \left| \frac{\partial G}{\partial h} \right|^2 \hbar}$$

Not strictly $T \sim \exp(-L)$ because the channel potential is not a constant
Uniform doping, $dG$ vs. doping concentration

$5 \times 10^{18} cm^{-3}$ to $5 \times 10^{19} cm^{-3}$

- Potential profile gets higher and wider as concentration increases.
- Turning point, determines how many dopants to avoid short channel effects.
- $dG$ increases drastically as concentration decreases due to the barrier lowering.
- $dG/G$ decays as concentration decreases due to fewer random dopants.

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Localized doping, $dG$ vs. doping position

$5 \times 10^{18} \, cm^{-3}, L = 10.9 nm$
Localized doping, $dG$ vs. doping position

$5 \times 10^{18} cm^{-3}, L = 10.9 nm$

- One expects localized doping to reduce $dG$ – this is however NOT always true;
- If doping is away from the leads, $dG$ is drastically reduced; if doping is close to the leads, $dG$ gets even larger than uniform case
- Can be understood by studying the microscopic detail of the potential profile.
- The dotted curves are fit to a WKB;

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Localized doping, $dG$ vs. doping position

$5 \times 10^{18} \text{ cm}^{-3}$, $L$ varies from 6 to 15 nm

- If doping is away from the leads, $dG$ is drastically reduced
- Doping close to leads produces even larger variability, non-intuitive
Mini-summary

• In uniform doping, \( dG \) scales exponentially with 
\[ \exp\left(-L^{3/2}\right) \]

• \( dG \) increases significantly with decreasing doping concentration

• Doping close to source/drain may produce non-intuitive larger variability; doping close to the middle can drastically reduce variability
Spin devices

- Magnetic tunnel junction (MTJ)
- Oxygen vacancies at interface
- Variability on tunnel magnetoresistance (TMR)
Spin devices

TMR vs. oxygen vacancies (%)

STT vs. oxygen vacancies (%)

5 MgO layers

11 MgO layers

To be published
We introduce a newly invented first principle parameter-free method that can predict device to device variability by deriving an averaged-transport-formula.

Both the average transport and its variance can be solved by calculating the formula once.
Future work

- How to do CPA when spin-orbit coupling is included?
- How to implement CPA with TB basis?
  - simulation of real size devices
Thank you and Questions?