Device Simulation for Carbon Nanotube Electronics

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1. Introduction
2. NEGF formalism
3. Simulation Approach
4. Device Analysis
5. Summary
Acknowledgements

Theory: Mark Lundstrom, Supriyo Datta (Purdue)
Experiment: Hongjie Dai, Ali Javey (Stanford)
Carbon nanotubes


Top-down and bottom-up view

**Top-down view**

- **Gate**
- **S**
- **D**
- **E**
- **mobility**
- **k**

**Semiclassical approach**

applicable only when quantum effects not important

**Bottom-up view**

- **Gate**
- **atomistic p_2 orbitals**

**Quantum approach**

- tunneling at M/CNT contacts
- tunneling and interference in the CNT
Quantum simulation for Nanoelectronics

Challenges in nanoscale device simulation:

1) description at an atomistic level
2) quantum description of open systems under bias
3) treatment of inelastic scattering

Our approach: the Green’s function formalism
Outline

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One contact

in-flow: \( \frac{\gamma}{\hbar} D(E-U)f_0 \)

current:

out-flow: \( \frac{\gamma}{\hbar} N_E \)

\[
\frac{dN_E}{dt} = \frac{\gamma}{\hbar} \left[ D(E-U)f_0(E-E_F) - N_E \right]
\]

\[
N = \int dE D(E-U)f_0(E-E_F)
\]

Datta, *Quantum Transport Atom to Transistor*, Cambridge Univ. Press, 2005
Two contacts

in-flow: \( \frac{\gamma_1}{\hbar} D(E-U) f_1 \)

out-flow:

\[ \frac{\gamma_1}{\hbar} N_E \]

\[ \frac{\gamma_2}{\hbar} N_E \]

\[ \frac{\gamma_2}{\hbar} [D(E)f_2 - N_E] \]

\[ \frac{dN_E}{dt} = \gamma_1 \left[ D(E)f_1 - N_E \right] + \gamma_2 \left[ D(E)f_2 - N_E \right] \]
Two contacts

\[ N = \int dE \ D(E-U) \left[ \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right] \]

\[ I = \frac{2q}{h} \int dE D(E-U) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} [f_1 - f_2] \]

\[ U = U_L + U_0(N - N_0) \]

Multiple levels

\[ \epsilon \rightarrow [H] \]
\[ \gamma \rightarrow [\Gamma] \]
\[ N \rightarrow [\rho] \]
\[ G = [ES - H - \Sigma]^{-1} \]
Non equilibrium Green’s Function (NEGF)

\[
G = \left[ EI - H - \Sigma_1 - \Sigma_2 - \Sigma_S \right]^{-1}
\]

Charge density (ballistic)
\[
[\rho] = \int \left[ A_1(E) f_1(E) + A_2(E) f_2(E) \right] \frac{dE}{2\pi}
\]

Current
\[
I_D = \frac{2q}{h} \int T(E) \left( f_1(E) - f_2(E) \right) dE
\]

\[
A_{1,2}(E) = G \Gamma_{1,2} G^+
\]

\[
T(E) = \text{Trace}[\Gamma_1 G \Gamma_2 G^+] \]

\[
\Gamma_{1,2} = i[\Sigma_{1,2} - \Sigma_{1,2}^+] \]
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Real-space basis (ballistic)

Recursive algorithm for $G^r$: $O(m^3N)$

Lake et al., JAP, 81, 7845, 1997
Real-space results

Gate

2nd subband
interference

band gap

Confined states

E [eV]

x [nm]
Mode-space approach (ballistic)

\[ k_q = \frac{2\pi q}{c} \]

The \( q \)th mode

\[ H_q = \begin{bmatrix} u_1 & b_q \\ b_q & u_2 & t \\ & t & u_3 & \ddots \\ & & \ddots & \ddots & b_q \\ & & & b_q & u_N \end{bmatrix} \]

- \( \Sigma_S (1,1) \) and \( \Sigma_D (N,N) \) analytically computed
- Computational cost: \( O(N) \)
  real space \( O(m^3N) \)
Mode-space results

Conduction band profile (ON)

2 modes
real space

2 modes
real space

Coaxial G

$V_D = 0.4V$

$E_1 [eV]$

$x [nm]$

$G_{ate}$

$p^{++}$ Si

SiO$_2$

8nm HfO$_2$

Pd

Pd

CNT
Treatment of M/CNT contacts

$E_F \quad \phi_{B0} \quad E_C \quad E_V$

$\sqrt{\alpha t}$

metallic tube band

$\phi_{B0}$ : band discontinuity

$\sum_m \approx \begin{bmatrix} -i\alpha & 0 \\ 0 & 0 \\ \vdots \end{bmatrix}$
Treatment of M/CNT contacts

Gate

Metal S

metal D

\[ V_D = V_G = 0.4 \text{V} \]

Charge transfer in unit cell: Leonard et al., APL, 81, 4835, 2002
3D Poisson solver

Method of moments:

\[ V(\vec{r}) = \int K(\vec{r} - \vec{r}') \rho(\vec{r}') d\vec{r}' \]

Electrostatic kernel:

\[ K(\vec{r} - \vec{r}') \]

\[ K(\vec{r} - \vec{r}') \] for 2 types of dielectrics available in Jackson, Classical Electrodynamics, 1962
Numerical techniques

- Non-linear Poisson

- Recursive algorithm for
  \[ G(E) = [EI - H - \sum_S - \sum_D]^{-1} \]

- Gaussian quadrature for doing integral

- Parallel different bias points

- ~20min for full I-V of a 50-nm CNTFET
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Device issues

nanotube diameter ~1.7 nm
L_{ch} ~50 nm

Javey et al, Nano Lett., 2004

1) Can we model and understand I-V?
2) How close to the ballistic limit?
3) What is the role of scattering?
4) How to optimize I_{ON}?
5) How to reduce I_{off}?
6) How to compare to Si MOSFETs?
Modeling $I_D-V_G$

SB height: $\phi_{BP}=0$, $d_{CNT}\sim1.7\text{nm}$ $R_S=R_D\sim1.7\text{K}\Omega$

![Graph showing the relationship between $I_D$ and $V_G$ with experimental and theoretical curves.]

- $V_D=-0.3\text{V}$
- $-0.2\text{V}$
- $-0.1\text{V}$

- $-I_D$ [\mu\text{A}]
- $V_G$ [V]
Two kinds of transistors

MOSFET

SBFET

Carbon nanotubes as Schottky barrier transistors
Heinze et al, PRL, 89, 106801, 2002
Ambipolar conduction (thin oxide)

$\log I_D$ vs $V_G$

- Hole conduction at low $V_G$
- Electron conduction at high $V_G$

Barrier thickness set by $t_{ins}$ (geometric screening)
Thick oxide

opaque barrier for electron tunneling

barrier thickness set by $t_{\text{ins}}$ (geometric screening)

How close to ballistic limit?

SB height: $\phi_{Bp}=0$, $d_{CNT}\sim 1.7\text{nm}$, $R_S=R_D\sim 1.7\text{K}\Omega$

$\Rightarrow$ Deliver near-ballistic DC on-current
No surface roughness scattering in CNTs

phonon scattering dominates in CNTs

Phonon scattering in CNTs

AP: long mfp \( (\lambda_{1}^{\text{high}} \sim 1\mu\text{m}) \)
OP: short mfp \( (\lambda_{2}^{\text{high}} \sim 10\text{nm}) \)

Park, Rosenblatt, Yaish et al., Nano Lett., 4, 517
Small effect of OP scattering

\[ \omega \sim 0.16eV \]

OP/ZBP emission

\[ E_{FS} \]

\[ E_{FD} \]

\[ E \]

Position, \( x \)

\[ \Rightarrow \]

Deliver near-ballistic DC on-current

confirmed by a separate Monte-Carlo simulation
How close to the ballistic limit?

\[ \phi_{Bp} = 0 \]

\[ \text{zero SB still limits } I_D \]

Guo and Lundstrom, *IEEE TED*, 49, 1897, 2002 (silicon)
Improving $I_{ON}$: Scaling $t_{ins}$

Barrier thickness set by $t_{ins}$ (geometric screening)
Reduce $I_{\text{off}}$ for thin $t_{\text{ins}}$

$$\Delta_n \sim \Delta_p \sim \frac{E_g - eV_D}{2}$$

$E_g \sim 0.8 \text{eV/d(nm)}$

small $d_{\text{CNT}}$ reduces $I_{\text{min}}$
Reduce $I_{off}$ using MOSFET-like structure

**chemical S/D doping**
Chen et al., IEDM Tech Dig, 2004
Javey et al., Nano Lett., 2005

**electrical S/D doping**
Appenzeller et al, PRL, 2004
Reduce $I_{\text{off}}$ using MOSFET-like structure

SB CNTFET

- Electron leakage
- Hole leakage

MOSFET-like CNTFET

- Electron leakage negligible

Ambipolar $\Delta_n \sim \Delta_p \sim \frac{E_g - eV_D}{2}$

Unipolar $\Delta_p \sim E_g$

Suppressed ambipolar conduction
How to compare to Si MOSFET?

Si MOSFETs vs CNT array FETs

Si Channel

$W$

Key device metrics:

$I_{ON}/I_{OFF}$

$\tau = C_G V_{DD}/I_{ON}$
Control of $V_T$ shifts the window

$$\tau = C_G V_{DD} / I_{ON}$$
Compare to 90nm Si MOSFETs

90nm Si n-MOS data from Antoniadis and Nayfeh, MIT
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Summary: Simulation Approach

Quantum Transport (NEGF formalism)
  - Atomistic description
  - Non-equilibrium transport
  - Inelastic scattering

Three dimensional Electrostatics
  - Method of moments

Computational techniques
  - recursive algorithm
  - mode-space approach
  - parallel simulation
Summary

1) I-V can be modeled and explained.
2) The CNTFET delivers near-ballistic $I_{ON}$
3) Scaling $t_{\text{ins}}$ and using high-$\kappa$ improves $I_{ON}$
4) Thin $t_{\text{ins}}$ results in ambiploar conduction
5) Using small $d_{\text{CNT}}$ tube or MOSFET-like structure suppresses ambipolar conduction
6) The CNTFET performance is promising
Outlook:

**Transistors**
- 3D electrostatics
- phonon scattering
- Advanced transistor structures
- AC characteristics

**New devices**
- CNT optoelectronic devices
- CNT-based nanosensors