Implementation and Application of Gate Voltage in NEGF Calculations

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My 2nd Visit to South Korea This Month

Oct. 30 – Nov. 3
7th A3 Symposium on Emerging Materials
Buyeo, 2.5 h

Nov. 24 – 25
2nd OpenMX Developer's Meeting
Daejeon, 3 h
Outline

■ Introduction
  ■ Motivation and Significance for the Implementation of a Gate Function in NEGF Calculations

■ Implementation of a Gate Function
  ■ Symmetric Zigzag Graphene Nanoribbon Spin Filter

■ Application to All Two-Dimensional (2D) Tunneling Field Effect Transistors (TFETs)
  ■ P-doped GeSe/MoS$_2$/VS$_2$ TFETs

■ Summary
Introduction

MPU High-Performance Physical Gate Length

MPU
Micro processor unit

MOS (metal oxide semiconductor) transistor

GL$_{ph}$

Equivalent scaling
High mobility channel materials
High-$\kappa$ metal gate
Non-classical CMOS
Tunneling, Spin

Dimensional scaling

Physics-Based Simulation, OpenMX

Year of Production

2010 2015 2020 2025 2030
Toward Whole-Device Simulations

- O(N) Parallelization of NEGF calculations
- Implementation of Gate Voltage

Number of Atoms

- 10,000
- 3,000
- 1,000

Years

- 2011
- 2014
- 2016
- 2018

Publications:

Implementation of a Gate Function

Symmetric Zigzag Graphene Nanoribbon Spin Filter\(^1\)

\(^1\)T. Ozaki et al., PRB 81, 075422 (2010).

\(\sigma\): symmetric
\(\pi\): symmetric
\(\pi^*\): antisymmetric

Antiferromagnetic junction

\[ V_b = 0 \]

\[ V_b > 0 \]

\(E\)

Transmission

\(eV_b\)

\(I\)

\[ \text{up} \]

\[ \text{down} \]
Model for tests of the implementation

Symmetric Zigzag Graphene Nanoribbon

Ferromagnetic junction

$V_{SG} < 0$

Transmission

Double gate structure
3D Poisson equation

Boundary condition (BC)

\[
\left( \frac{\partial}{\partial x^2} - k_y^2 - k_z^2 \right) \varphi(x, k_y, k_z) = -\frac{4\pi}{\varepsilon_0} \rho(x, k_y, k_z)
\]

Parallelization in bc plane (63x125)

\[
\left( \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} - k_z^2 \right) \varphi(x, y, k_z) = -\frac{4\pi}{\varepsilon_0} \rho(x, y, k_z)
\]

Parallelization in only c line (125)
Modification of only 10 Files

- tran_variables.h
- openmx_common.h
- lapack_prototypes.h
- tran_prototypes.h
- Allocate_Arrays.c
- Free_Arrays.c
- init_alloc_first.c
- truncation.c: Preparation for transforming from AB to C partition
- TRAN_Input_std.c
- TRAN_Poisson.c — TRAN_Poisson_FDG

- FFT for the boundary conditions
- Transformation from AB to C partition
- 2D real space Poisson equation
- Transformation from C to AB partition
- FFT to real space
Hartree Potential (eV)

$V_{SD} = 0 \text{ V, } V_{SG} = 0 \text{ V}$

$V_{SD} = 0.3 \text{ V, } V_{SG} = -10 \text{ V}$
This provides another possible spin filter.
All 2D Material Tunneling FETs

- **Graphene**
  Discovery (2004)

- **hBN**
  B C N

- **Transition metal dichalcogenide (TMDC)**

- **Phosphorene**

- **Group-IV monochalcogenide**

Chemical Elements:
- Transition metal dichalcogenide (TMDC): Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W
- Group-IV monochalcogenide: P, S, Ge, Sn, Te, S, Se, Te

Graphene, hBN, Phosphorene, and Group-IV monochalcogenide are 2D materials used in tunneling field-effect transistors (FETs).
The lattices of these materials are matched with a relatively small unit cell.

The subthreshold swing (SS) in conventional FETs is limited to 60 mV/dec.
Computational Details

- DFT code: OpenMX
- Exchange-correlation potential: GGA-PBE with van der Waals correction
- Norm-conserving pseudopotential: Troullier-Martins
- Pseudo atomic orbitals (PAOs)
  - Geometry optimization:
    - Ge7.0-s3p3d3f2, Se7.0-s3p3d2f1, P7.0-s3p3d2f1, Mo7.0-s3p2d2f1, S7.0-s3p3d2f1, V6.0-s3p3d2
  - Transport: s2p2d1
- Temperature: $T = 300 \text{ K}$
Atomic Structure

Channel

Source

Drain

$V_2S_2$

$MoS_2$

$GeSe$

$L_{Ch}$

Number of atoms

$1.9 \text{ nm}$ $244$

$2.6 \text{ nm}$ $280$

Interlayer distance: 0.323 nm

Contact length: 0.6 nm
Partial density of states (PDOS) of Mo atom in the center of the channel ($L_{Ch}=1.9$ nm)

$V_{SD} = 0.1$ V

$V_{SG}$
- 0 V
- 10 V
- 20 V
- 30 V
- 50 V

Energy (eV)

PDOS (a.u.)
The subthreshold swing (SS) would be further improved by using a high-κ material as a gate dielectric that is a vacuum in the present model.
Computational Cost

Computer: Fujitsu PRIMERGY CX400

Information Technology Center, Nagoya University
568 nodes
28 cores (128 GB)/node

<table>
<thead>
<tr>
<th>$L_{Ch}$ (nm)</th>
<th>Number of atoms</th>
<th>Number of mpi</th>
<th>Number of threads</th>
<th>Time (day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.9</td>
<td>244</td>
<td>105</td>
<td>7</td>
<td>1.5</td>
</tr>
<tr>
<td>2.6</td>
<td>280</td>
<td>105</td>
<td>7</td>
<td>2.7</td>
</tr>
</tbody>
</table>

We need further parallelization of Poisson equation calculation.
Summary

- We implemented a gate function in OpenMX (DFT-based NEGF code), by applying open boundary conditions to the 3D Poisson equation.

- We designed GeSe/MoS$_2$/VS$_2$ TFETs and examined the device properties using the developed code.
  
  - $I_{on}/I_{off} > 10$, SS = 8.5 V/dec @ $L_{Ch} = 1.9$ nm
  
  - $I_{on}/I_{off} > 10^3$, SS = 3.6 V/dec @ $L_{Ch} = 2.6$ nm

- This could be a powerful tool for exploring novel nanoelectronic and spintronic devices.
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