Lecture14

Sung-Min Hong (smhong@gist.ac.kr)

Semiconductor Device Simulation Lab.

School of Electrical Engineering and Computer Science

Gwangju Institute of Science and Technology

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Transport

- Central problem of the computational electronics
  - Calculation of terminal currents!
  - Example) Calculate the drain current, when $V_{GS} = V_{DS} = 0.7\ \mathrm{V}$.
- Quantum transport
  - Charge carriers (electrons and holes)
  - Most accurate method
- Semi-classical transport
  - Treat charge carriers as semi-classical particles
  - Still, it can be useful to many cases.

2DEG

- Our system of interest
  - Here, we mainly focus on the 2DEG.
  - Example) 2DEG in the MOS channel (Planar MOS or double-gate MOS)
  - Example) 2DEG in two-dimensional materials (such as graphene)
  - For 3DEG or 1DEG, we can apply similar approaches.

Governing equation

- Boltzmann transport equation
  - It reads

Velocity

Scattering

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \frac{1}{\hbar} \mathbf{F} \cdot \nabla_k f = \hat{S}$$

Force

  - Time-evolution of f is described.
  - Scattering can change f.
  - Motion of electrons
    - Non-zero velocity: Change its spatial position
    - Acceleration: Change its momentum

Force

- Electric force
  - It reads

$$\mathbf{F} = -q\mathbf{E} = q\nabla\phi$$

- Under the magnetic field,
  - Lorentz force can be considered.
  - (But it is not considered in this course.)

MATLAB example (1)

- Consider an one-dimensional system.
  - Your electrons have the free electron mass, m_0.
  - Since the magnitude of the electric field is E, their (constant) acceleration is given by $-\frac{qE}{m_0}$.

```
E = 1e6; % Electric field, V/m
q = 1.602192e-19; % Elementary charge, C
m0 = 9.109534e-31; % Electron rest mass, kg
acceleration = -q*E/m0; % Acceleration, m/s^2
```

MATLAB example (2)

- Set up the initial distribution.
  - At the initial time, the position and the velocity of your (several) electrons are randomly determined.

```
N = 1000; % Number of electrons
xmax = 10e-9; % Size of x range, m
vmax = 1e4; % Size of v range, m/s
x = (rand(N,1)-0.5)*xmax;
v = (rand(N,1)-0.5)*vmax;
```

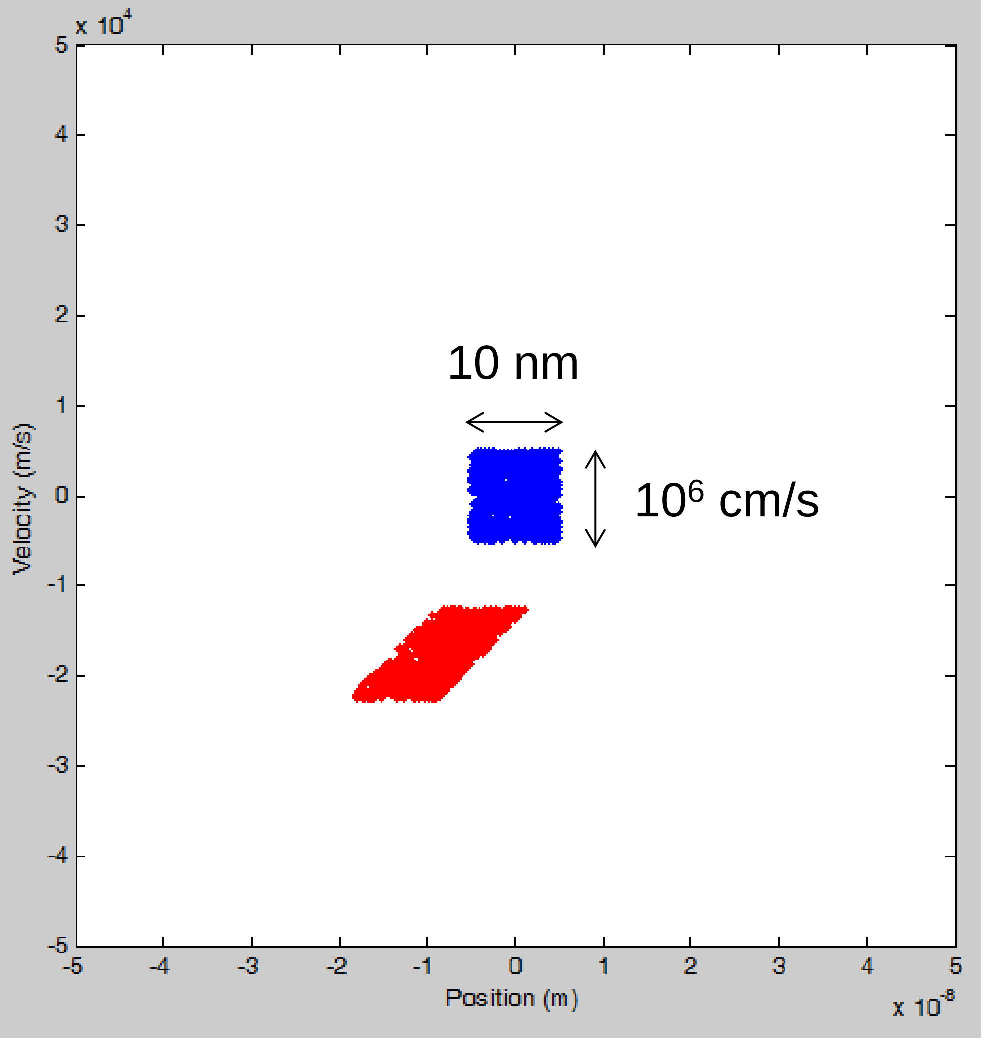
MATLAB example (3)

- Time evolution
  - Set up the time interval and the number of steps.

```
dt = 1e-15; % Time interval of each step, s
steps = 1000; % Number of steps
for ii=1:steps
   x = x + v.*dt;
   v = v + acceleration.*dt;
end
```

Result

- E = 1 kV/cm
  - Accel. ~ -1.759X10^{16} m/s^2
- Initial (Blue)
  - In average, zero velocity
- Final (Red)
  - After 1psec



BTE simulator (1)

- Derivation
  - Boltzmann equation

$$\frac{\partial f}{\partial t} + v\frac{\mathbf{k}}{k}\cdot\nabla_r f + \frac{1}{\hbar}\mathbf{F}\cdot\nabla_k f = \hat{S}$$

  - Explicitly,

$$\frac{\partial f(x,k,\phi)}{\partial t} + v\mathbf{a}_k\cdot\mathbf{a}_x\frac{\partial f(x,k,\phi)}{\partial x} + \frac{1}{\hbar}F\mathbf{a}_x \cdot\left(\mathbf{a}_k\frac{\partial f(x,k,\phi)}{\partial k} + \mathbf{a}_\phi\frac{1}{k}\frac{\partial f(x,k,\phi)}{\partial \phi}\right) = \hat{S}$$

  - Dot products are written as

$$\mathbf{a}_x\cdot\mathbf{a}_k = \cos\phi$$

$$\mathbf{a}_x\cdot\mathbf{a}_\phi = -\sin\phi$$

BTE simulator (2)

- Derivation
  - Using the previous relations,

$$\frac{\partial f(x,k,\phi)}{\partial t} + v\cos\phi \frac{\partial f(x,k,\phi)}{\partial x} + \frac{1}{\hbar}F\left(\cos\phi \frac{\partial f(x,k,\phi)}{\partial k} - \sin\phi \frac{1}{k}\frac{\partial f(x,k,\phi)}{\partial \phi}\right) = \hat{S}$$

  - Note that the above relation holds for arbitrary isotropic bnad structure. (Here, v is a function of k.)
  - In the energy space,

$$\frac{\partial f(x,\epsilon,\phi)}{\partial t} + v\cos\phi \frac{\partial f(x,\epsilon,\phi)}{\partial x} + F\left(v\cos\phi \frac{\partial f(x,\epsilon,\phi)}{\partial \epsilon} - \sin\phi \frac{1}{\hbar k}\frac{\partial f(x,\epsilon,\phi)}{\partial \phi}\right) = \hat{S}$$

BTE simulator (3)

- Derivation
  - We have the following relation:

$$kdkd\phi = \frac{\epsilon}{(\hbar v_F)^2} d\epsilon d\phi = \frac{k}{\hbar v} d\epsilon d\phi = (2\pi)^2 Z d\epsilon d\phi$$

  - For graphene, $Z = \frac{1}{(2\pi)^2} \frac{\epsilon}{(\hbar v_F)^2}$
  - For a parabolic band, $Z = \frac{1}{(2\pi)^2} \frac{m}{\hbar^2}$
  - Transformed Boltzmann equation reads:

$$\frac{\partial f}{\partial t} Z d\epsilon d\phi + v \cos\phi \frac{\partial f}{\partial x} Z d\epsilon d\phi + F \left(v \cos\phi \frac{\partial f}{\partial \epsilon} - \sin\phi \frac{1}{\hbar k} \frac{\partial f}{\partial \phi} \right) Z d\epsilon d\phi$$
$$= \hat{S} Z d\epsilon d\phi$$

BTE simulator (4)

- Derivation
  - Pham's Fourier harmonic, $Y_m(\phi)$, is defined as

$$Y_m(\phi) = c_m \cos(m\phi + \varphi_m)$$

$$c_m = \sqrt{\frac{1}{(1+\delta_{m,0})\pi}}$$

  - The phase, φ_m, is $\frac{\pi}{2}$ for negative m. Otherwise, it is zero.
  - Multiplying it,

$$Zd\epsilon\frac{\partial f}{\partial t}Y_m d\phi + vZd\epsilon\frac{\partial f}{\partial x}\cos\phi\, Y_m d\phi + vFZd\epsilon\frac{\partial f}{\partial \epsilon}\cos\phi\, Y_m d\phi$$
$$- F\frac{1}{\hbar k}Zd\epsilon\frac{\partial f}{\partial \phi}\sin\phi\, Y_m d\phi = Zd\epsilon\hat{S}Y_m d\phi$$

BTE simulator (5)

- Derivation
  - Note that $\cos\phi\, Y_m = \frac{1}{c_1} Y_1 Y_m$ and $\sin\phi\, Y_m = \frac{1}{c_{-1}} Y_{-1} Y_m$
  - By integration,

$$Zd\epsilon \frac{\partial}{\partial t} f_m(x,\epsilon,t) + vZd\epsilon \frac{\partial}{\partial x} \sum_{m'} \frac{1}{c_1} f_{m'}(x,\epsilon,t) \Upsilon_{m',m,1}$$
$$+ vFZd\epsilon \frac{\partial}{\partial \epsilon} \sum_{m'} \frac{1}{c_1} f_{m'}(x,\epsilon,t) \Upsilon_{m',m,1}$$
$$- F \frac{1}{\hbar k} Zd\epsilon \sum_{m'} \frac{-m'}{c_{-1}} f_{m'}(x,\epsilon,t) \Upsilon_{-m',m,-1} = Zd\epsilon \hat{S}_m$$

  - Here, $\Upsilon_{m,m',m''}$ is the integral of the triple product.