

# **Comparison of Non-Equilibrium Green's Function and Quantum-Corrected Monte Carlo Approaches in Nano MOS Simulation**

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# BACKGROUND

- Nano-scale MOSFETs with  $L_{ch} < 10\text{nm}$  have been realized in several research laboratories.
- A quantum mechanical modeling of nano-scale MOSFETs involving carrier's quasi-ballistic behaviors will be indispensable.
  - Non-equilibrium Green's function approach (NEGF)
  - Quantum-corrected Monte Carlo approach (QMC)



**We present a joint study on comparison between the NEGF and QMC approaches for a nano-scale MOSFET.**

# Quantum-Corrected MC Approach

- Transport equation with the lowest-order quantum correction

$$\frac{\partial f}{\partial t} + \sum_{i=x,y,z} \frac{\hbar k_i}{m_i^*} \frac{\partial f}{\partial r_i} - \frac{1}{\hbar} \nabla_{\mathbf{r}} U \cdot \nabla_{\mathbf{k}} f + \frac{1}{24\hbar} (\nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{k}})^3 U f = \left( \frac{\partial f}{\partial t} \right)_c$$

- Quantum-corrected Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \sum_{i=x,y,z} \frac{\hbar k_i}{m_i^*} \frac{\partial f}{\partial r_i} - \frac{1}{\hbar} \nabla_{\mathbf{r}} (U + U^{\text{QC}}) \cdot \nabla_{\mathbf{k}} f = \left( \frac{\partial f}{\partial t} \right)_c$$

- Quantum correction of potential

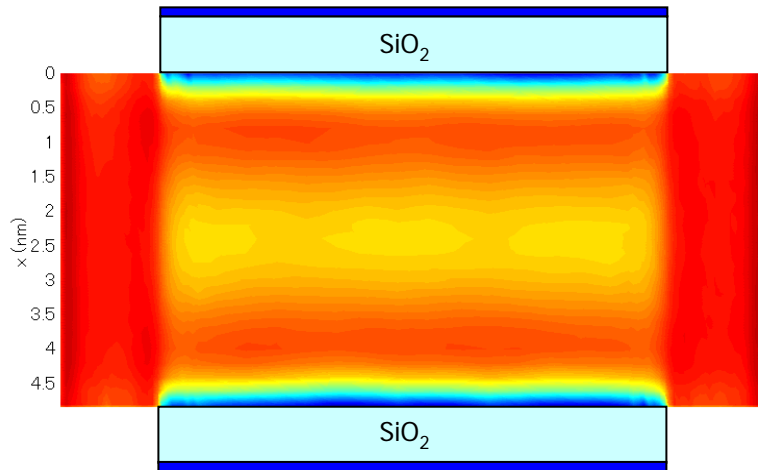
$$U^{\text{QC}}(\mathbf{r}) = -\frac{\hbar^2}{12m_x^*} \frac{\partial^2 \ln(n)}{\partial x^2} - \frac{\hbar^2}{12m_y^*} \frac{\partial^2 \ln(n)}{\partial y^2} - \frac{\hbar^2}{12m_z^*} \frac{\partial^2 \ln(n)}{\partial z^2}$$

- Quantum-corrected equations of motion

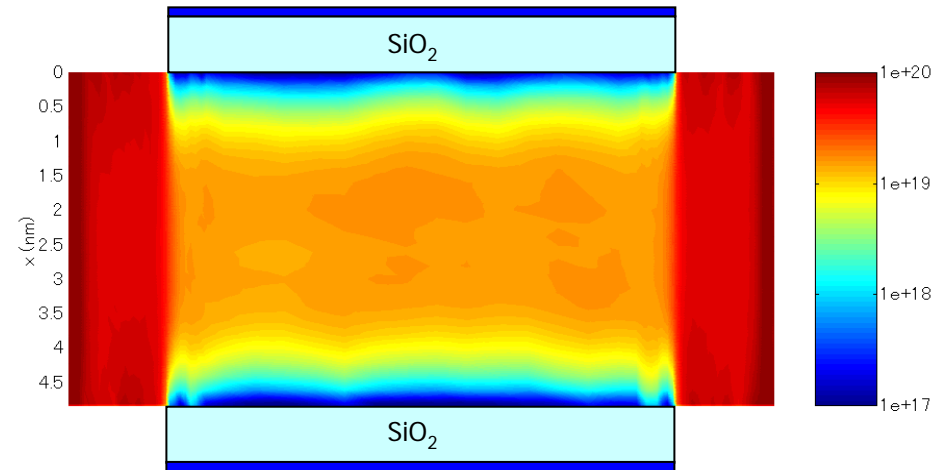
$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \quad , \quad \frac{d\mathbf{k}}{dt} = -\frac{1}{\hbar} \nabla_{\mathbf{r}} (U + U^{\text{QC}})$$

# Quantum-Corrected MC Simulation

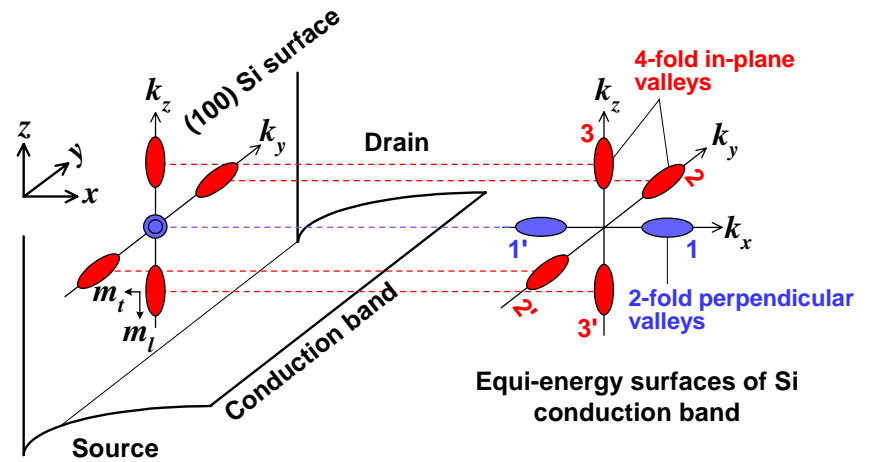
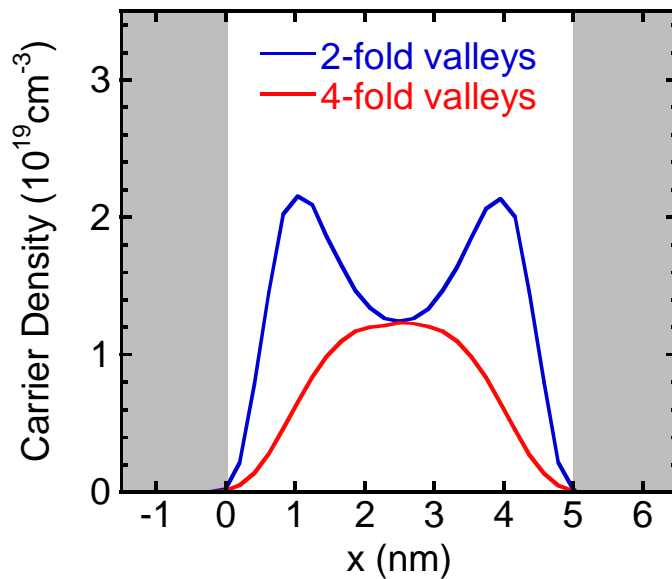
$T_{Si} = 5 \text{ nm}$



**2-fold valleys**



**4-fold valleys**



# Quasi-2D NEGF Approach

- 1D Schrödinger equation at each cross-section

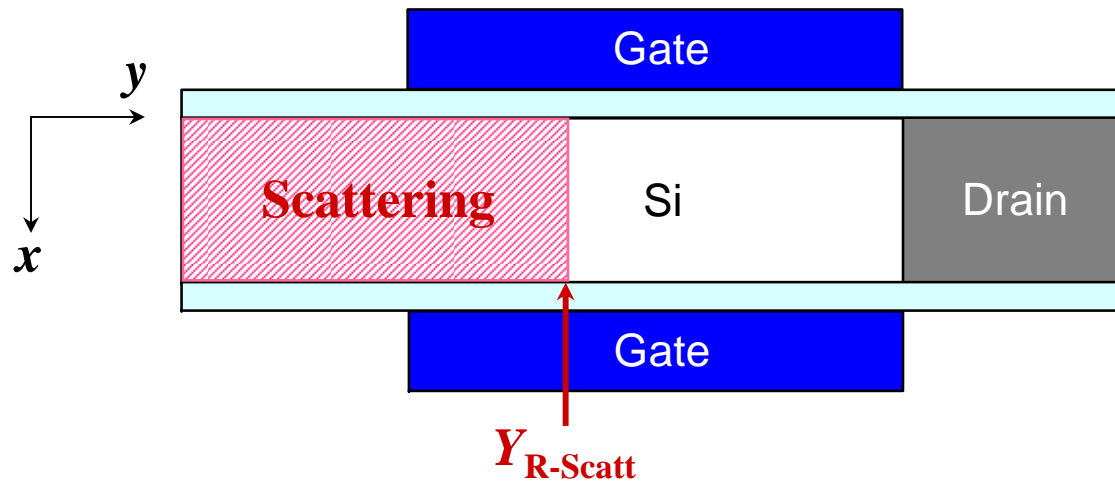
$$\left[ -\frac{\hbar^2}{2m_x^v} \frac{d}{dx} \left( \frac{1}{m_x^v} \frac{d}{dx} \right) + V(x, y) \right] \psi_n(x, y) = E_n(y) \psi_n(x, y)$$

- 1D Green's function equations along channel direction

$$\left[ E - \frac{\hbar^2 k_z^2}{2m_z^n} - \left( -\frac{\hbar^2}{2} \frac{d}{dy} \left( \frac{1}{m_y^n} \frac{d}{dy} \right) + E_n(y) \right) \right] G_n^r(y, y', k_z, E) - \int dy_1 \Sigma_n^r(y, y_1, k_z, E) G_n^r(y_1, y', k_z, E) = \delta(y - y')$$

$$\left[ E - \frac{\hbar^2 k_z^2}{2m_z^n} - \left( -\frac{\hbar^2}{2} \frac{d}{dy} \left( \frac{1}{m_y^n} \frac{d}{dy} \right) + E_n(y) \right) \right] G_n^{><}(y, y', k_z, E) - \int dy_1 \Sigma_n^r(y, y_1, k_z, E) G_n^{><}(y_1, y', k_z, E) = \int dy \Sigma_n^{><}(y, y_1, k_z, E) G_n^{><}(y_1, y', k_z, E)$$

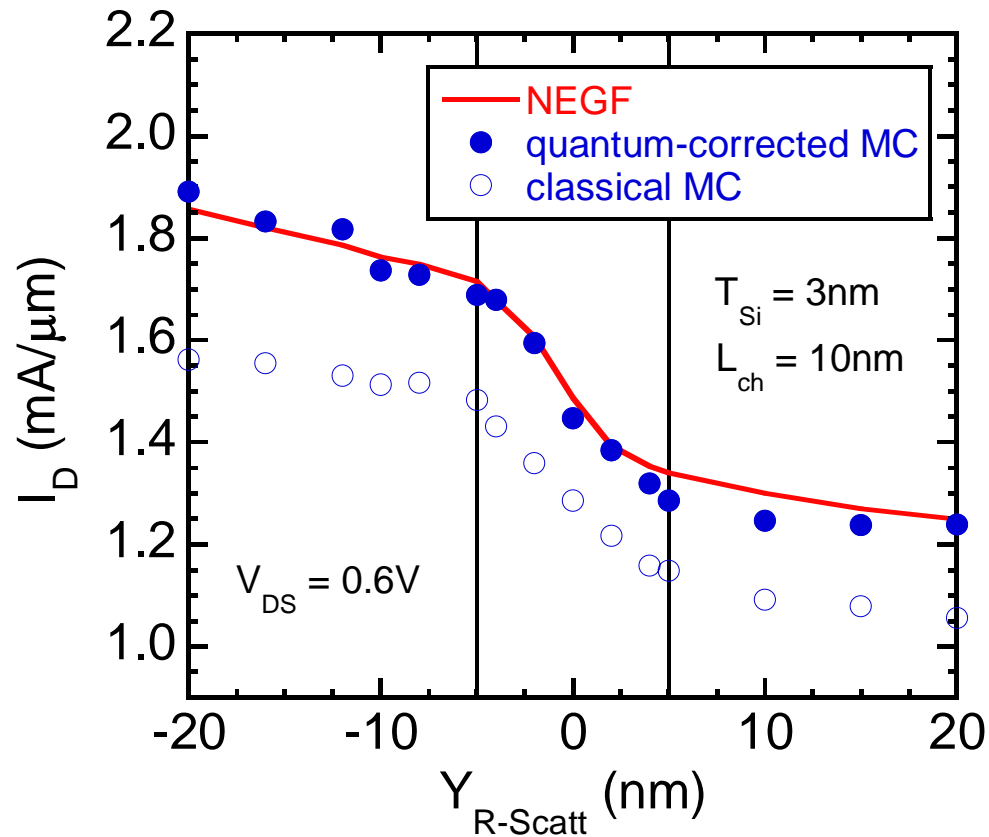
# Simulation Model



- $T_{\text{Si}} = 3\text{nm}$
- $L_{\text{ch}} = 10\text{nm}$
- $T_{\text{ox}} = 1.5\text{nm}$
- Channel: undoped
- $N_{\text{D}} = 10^{20}\text{cm}^{-3}$   
(source and drain)

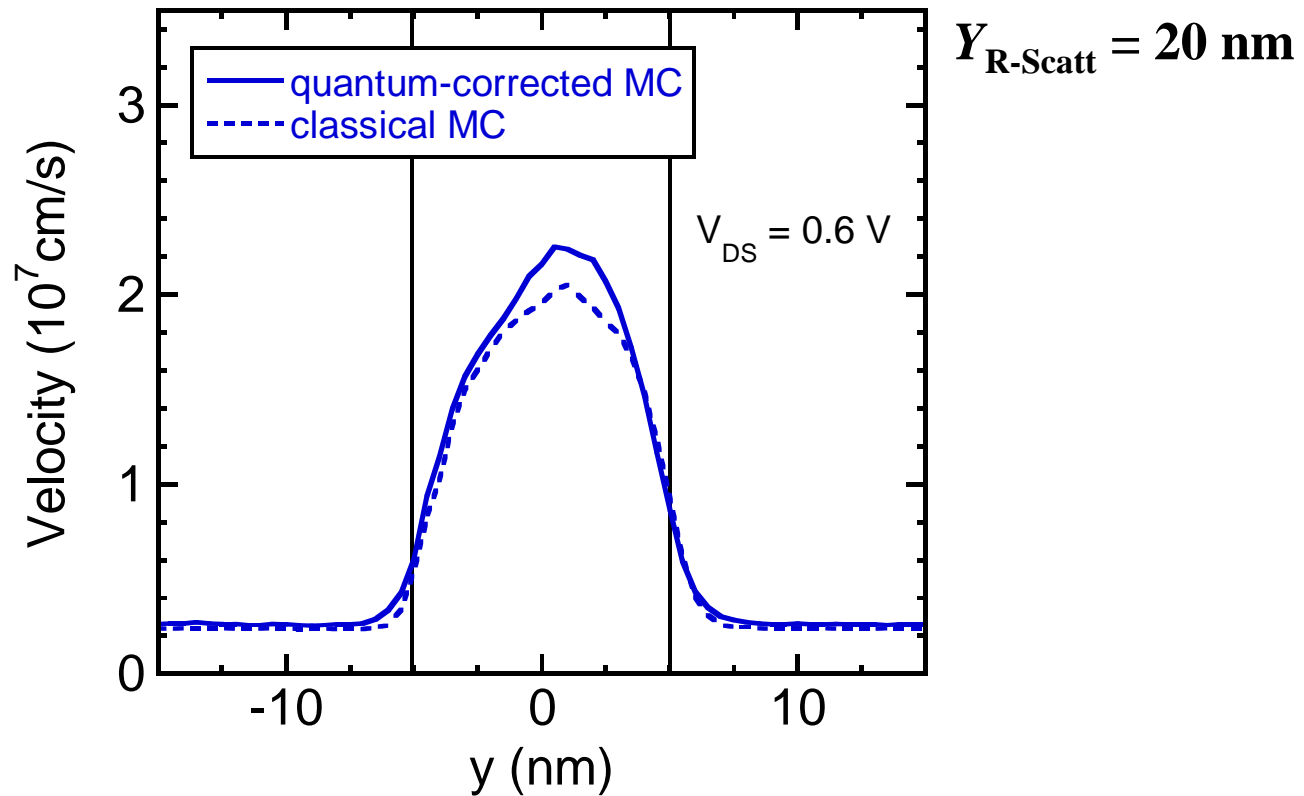
- ◆ Drain current as a function of right boundary of scattering,  $Y_{\text{R-Scatt}}$  is calculated.
- ◆ Only electron-phonon scattering is considered.
- ◆ Only the lowest quantized subbands for 2-fold and 4-fold valleys is considered in the NEGF method.
- ◆ Drain voltage is 0.6 V. Gate voltage is adjusted so that the injection electron density at the source edge of the channel becomes identical.

# Drain Current vs $Y_{R-Scatt}$



There is a good agreement between the NEGF and QMC results, while the classical model underestimates the drain current.

# Averaged Electron Velocity Profiles



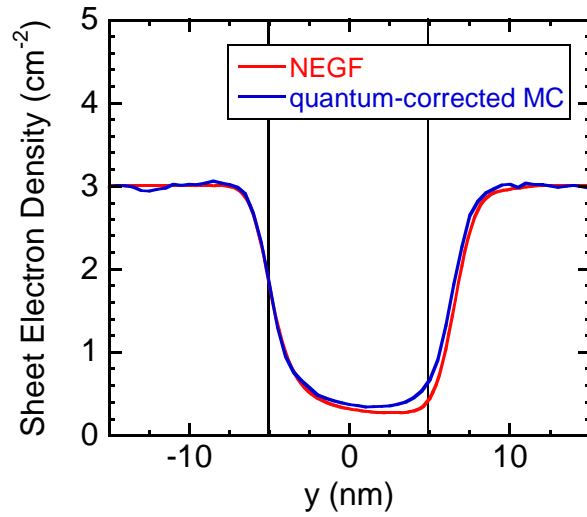
**Velocity (classical) < Velocity (quantum)**

because an increase in the occupancy of the 2-fold valleys due to the energy quantization is not taken into account in the classical model.

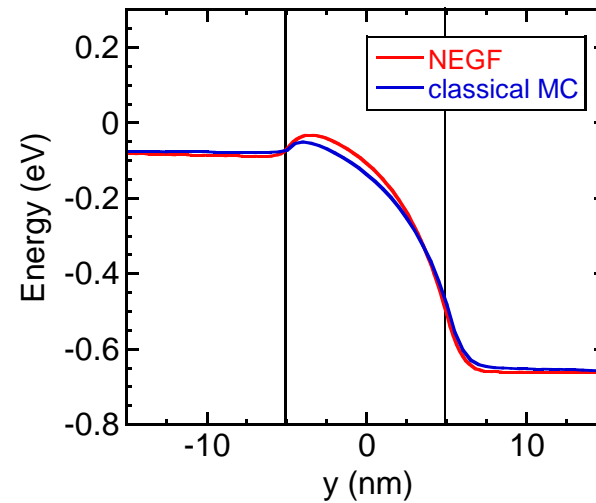
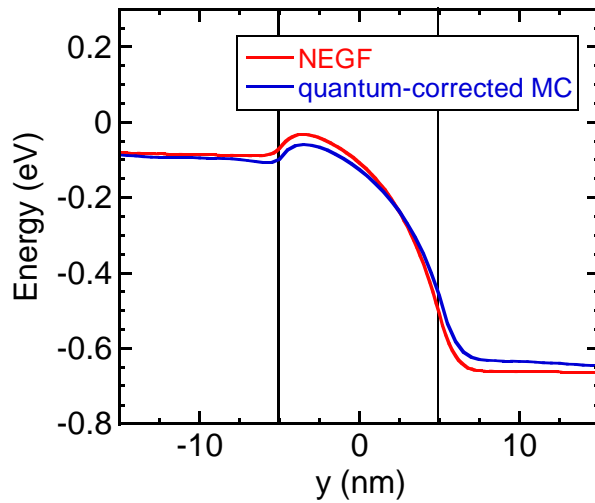
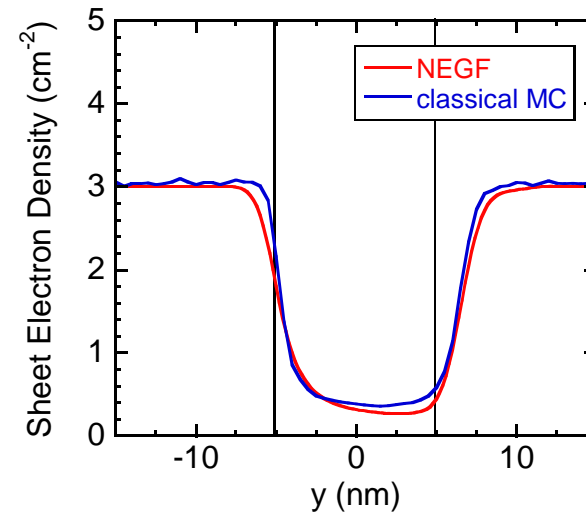
# Concentrations and Potentials

$$Y_{R-Scatt} = 20\text{nm}$$

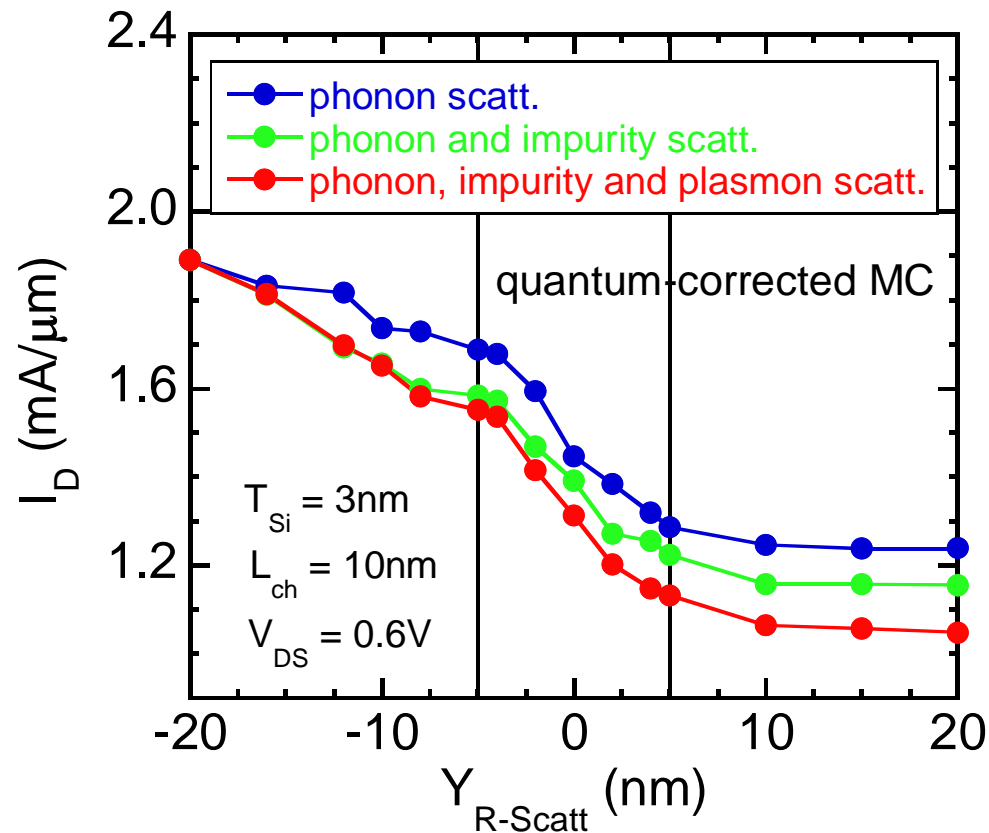
## NEGF vs QMC



## NEGF vs classical MC



# Influence of Impurity and Plasmon Scatterings



- Impurity scattering in source region
  - plasmon scattering at drain-end of channel
- are important to estimate drain current of MOSFET.

# SUMMARY

- **We have found that the non-equilibrium Green's function and quantum-corrected MC approaches are equivalent in the quantum transport simulation of nano-scale MOSFETs.**
  - **This result may be applicable to quantum correction models such as effective potential and Bohm potential, if the subband splitting is adequately incorporated.**
- **We have also demonstrated that the impurity scattering in the source region and the plasmon scattering at the drain-side of the channel are important to estimate the drain current accurately.**