Device Simulation of Ferroelectric Field-Effect Transistors Based on the Landau–Khalatnikov Equation

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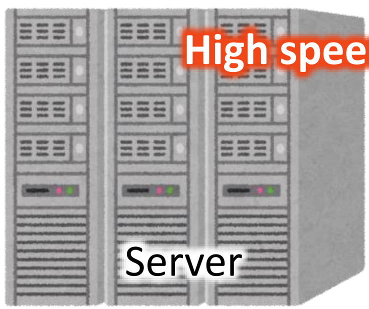
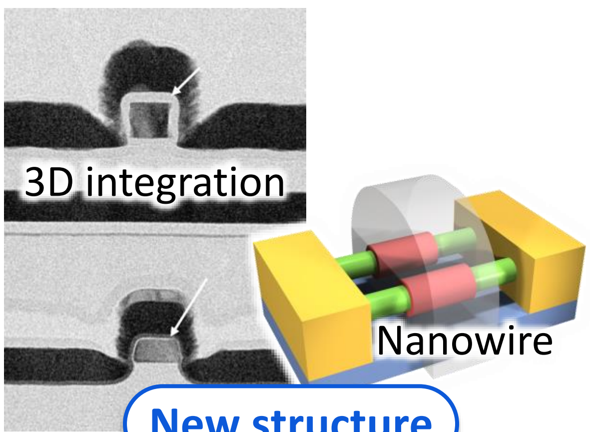
Introduction

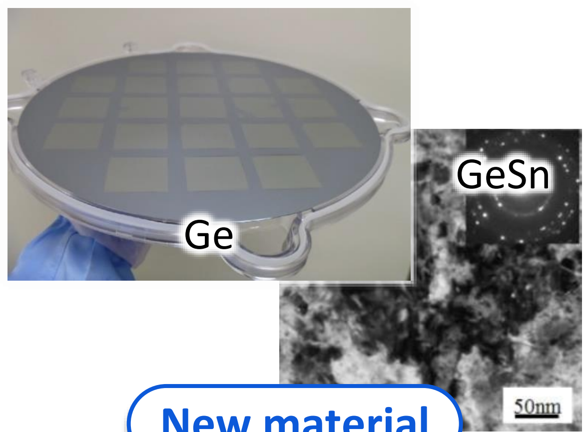
- The quality required of devices depends on the application



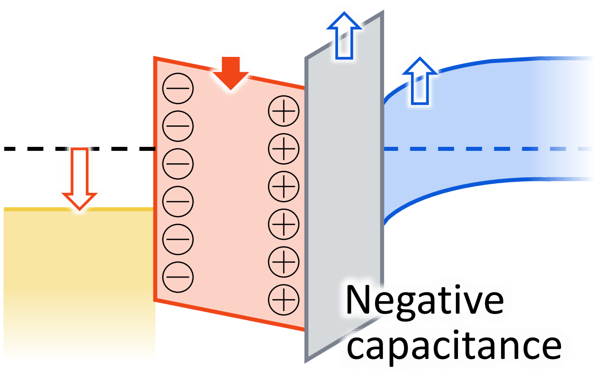
- There are various ways to meet that requirement



New structure



New material



New principle

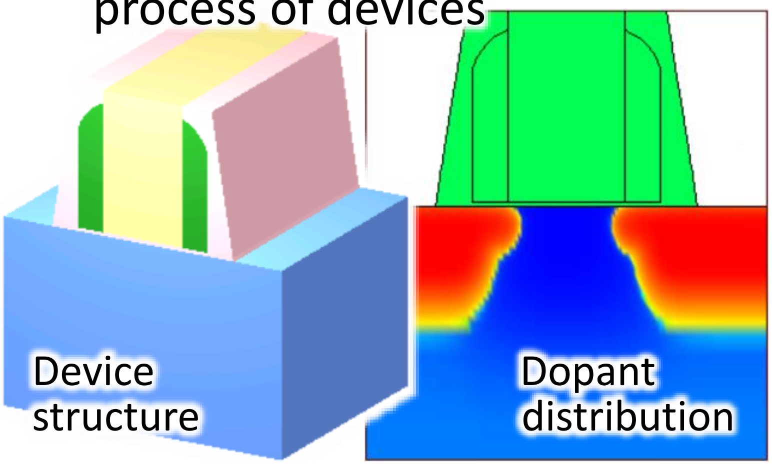
⇨ Every process from research to production is becoming complicated . . .

⇨ **Simulation is becoming increasingly important!**

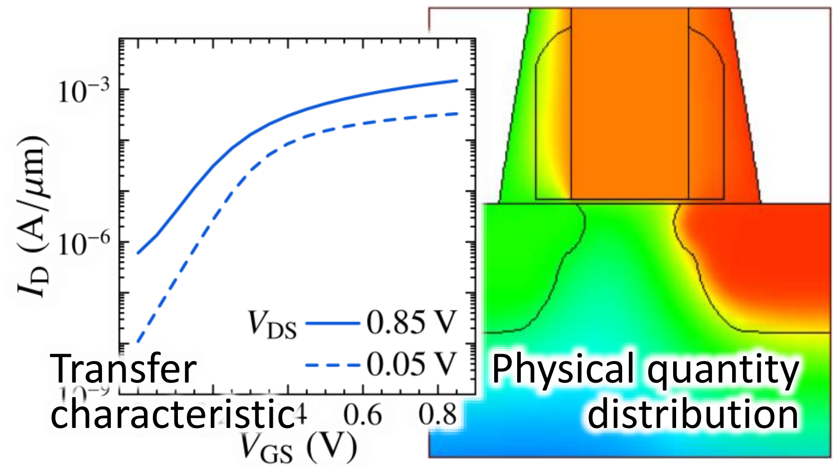
Introduction: TCAD

Technology Computer-Aided Design system

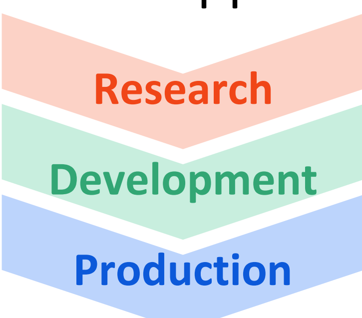
- Process simulation
  - reproduces the manufacturing process of devices



- Device simulation
  - reproduces the behavior of devices



- TCAD supports every step of devices from research to production



Developing a new device concept,

Narrowing down prototyping condition,

Maximizing device performance,

Analyzing the cause of defects, . . .

Introduction: Issues of TCAD

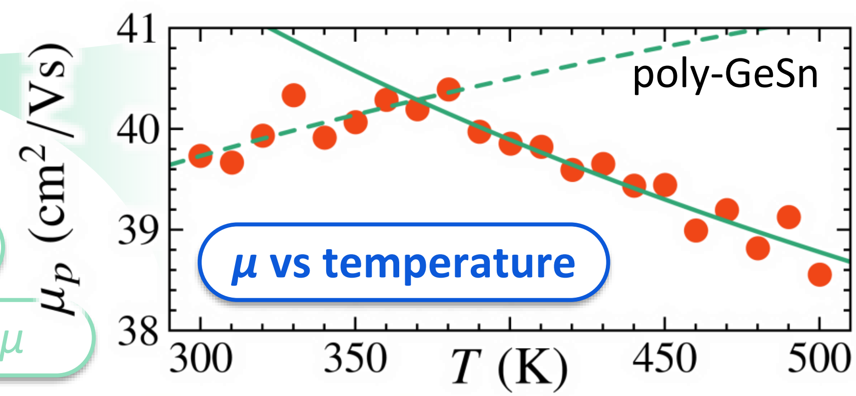
- Typical device simulator describes device states by the electric potential ψ and electron & hole concentrations n & p, and solves the equations governing them

$$\nabla \cdot (-\varepsilon \nabla \psi) - q(p - n + N_\mathrm{D}^+ - N_\mathrm{A}^-) = 0$$
$$\nabla \cdot (+\mu_n n \nabla \psi - \mu_n k_\mathrm{B} T \nabla n / q) - GR = 0$$
$$\nabla \cdot (-\mu_p p \nabla \psi - \mu_p k_\mathrm{B} T \nabla p / q) - GR = 0$$

Users cannot freely change variables & equations!

- Selecting suitable models and adjusting their parameters of the carrier mobility μ, generation-recombination rate GR, and so on, users can deal with various devices

Temperature dependent μ
↳ Impurity dependent μ
↳ Transverse-field dependent μ
↳ Lateral-field dependent μ



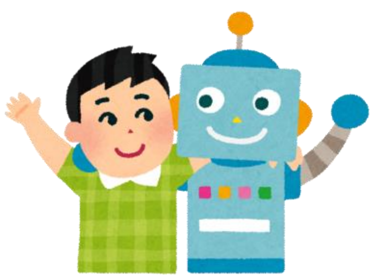
Provided models cannot cover all materials & phenomena!

Next generation of TCAD

- We, AIST TCAD team members, are developing a next-generation TCAD

⇨ **Impulse TCAD**

- Automatic differentiation
  - makes it possible and easy for users
    to change variables & equations and to incorporate original models in TCAD



$$GR_{\mathrm{user}} = \frac{n_{\mathrm{i}}^2 - pn}{\tau_p(n + n_{\mathrm{i}}) + \tau_n(p + n_{\mathrm{i}})}$$

Auto-generation

$$\frac{\partial}{\partial \psi} GR_{\mathrm{user}}, \frac{\partial}{\partial n} GR_{\mathrm{user}}, \frac{\partial}{\partial p} GR_{\mathrm{user}}, \ldots$$

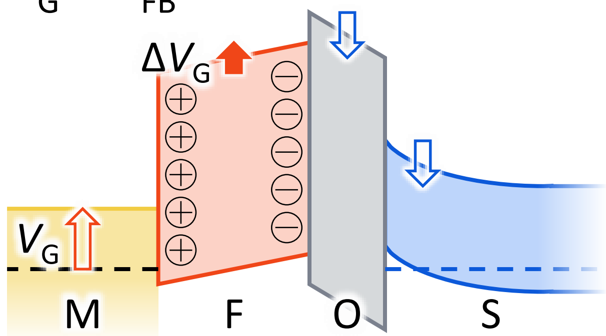
NC FET: Successful example of Impulse TCAD

Ferroelectric negative-capacitance (NC) field-effect transistor (FET)

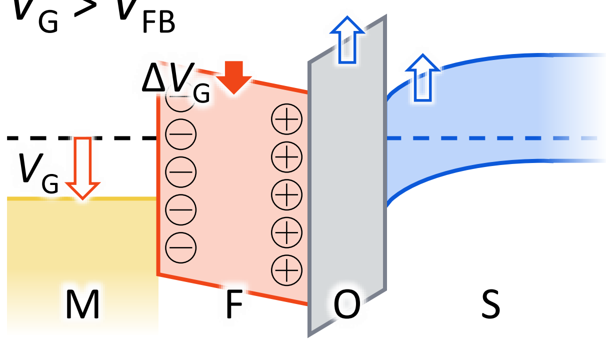
- Ferroelectric material is used as a gate insulator

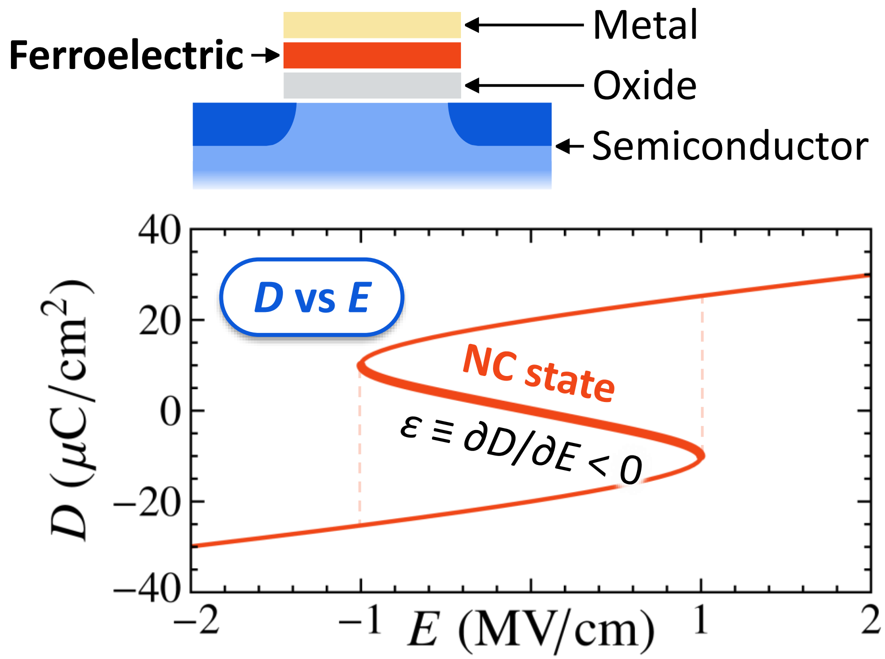
⇨ It enhances the gate voltage V_G when in NC state

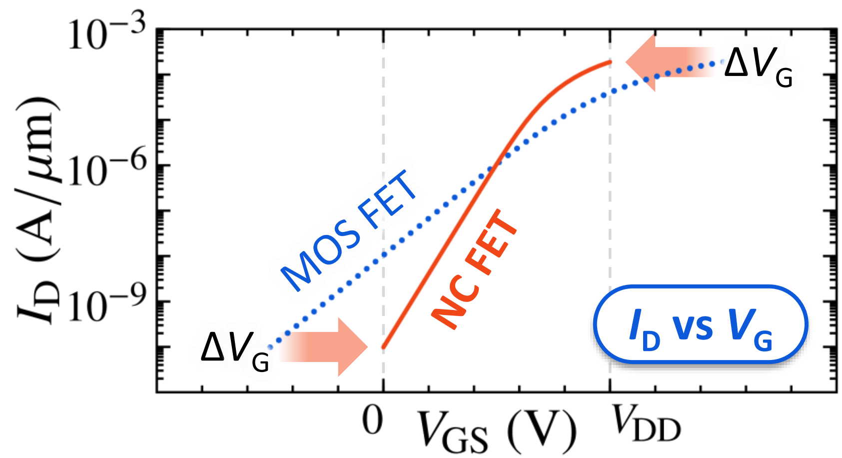
- $V_G < V_{FB}$



- $V_G > V_{FB}$







Equations governing ferroelectrics: LK eq.

- Time evolution of the polarization $\boldsymbol{P} = (P_X, P_Y, P_Z)$ in a ferroelectric is described in the Landau–Khalatnikov (LK) model by

$$\lambda \frac{\partial P_i}{\partial t} = -\frac{\partial G}{\partial P_i}$$

- Thermodynamic energy G can be written in the Landau–Devonshire model as

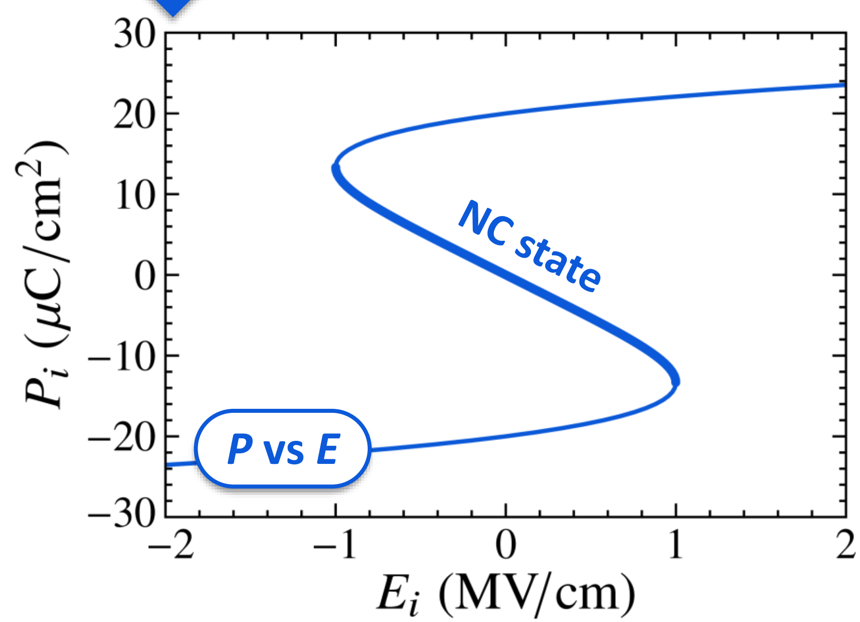
$$G = \int_V g \, dV$$

$$\begin{aligned} g = {} & \alpha\left(P_x^2 + P_y^2 + P_z^2\right) \\ & + \beta\left(P_x^4 + P_y^4 + P_z^4\right) \\ & + \gamma\left(P_x^6 + P_y^6 + P_z^6\right) \\ & - \boldsymbol{P} \cdot \boldsymbol{E} \end{aligned}$$

⇨ Relationship of $\boldsymbol{P}$ to the electric field $\boldsymbol{E}$ at steady state is given by

$$2\alpha P_i + 4\beta P_i^3 + 6\gamma P_i^5 - E_i = 0$$

- NC stems from negative α
  - $\alpha = -4.73 \times 10^9$ m/F
  - $\beta = 2.11 \times 10^9$ m^5/FC^2
  - $\gamma = 9.5 \times 10^{10}$ m^9/FC^4



Equations governing ferroelectrics: Poisson eq.

- Poisson's equation is another governing equation

$$\nabla \cdot \boldsymbol{D} = 0$$

- In a paraelectric,
  P is proportional to ***E*** and can be encapsulated into the permittivity *ε*

$$\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P} \approx \varepsilon_0 \boldsymbol{E} + \chi \varepsilon_0 \boldsymbol{E} = \varepsilon \boldsymbol{E}$$

⇨ $\nabla \cdot (\varepsilon \boldsymbol{E}) = 0$

- In a ferroelectric, however,
  P is not proportional to ***E***

⇨ ***P*** should be treated separately from ***E*** or ψ **New variable!**

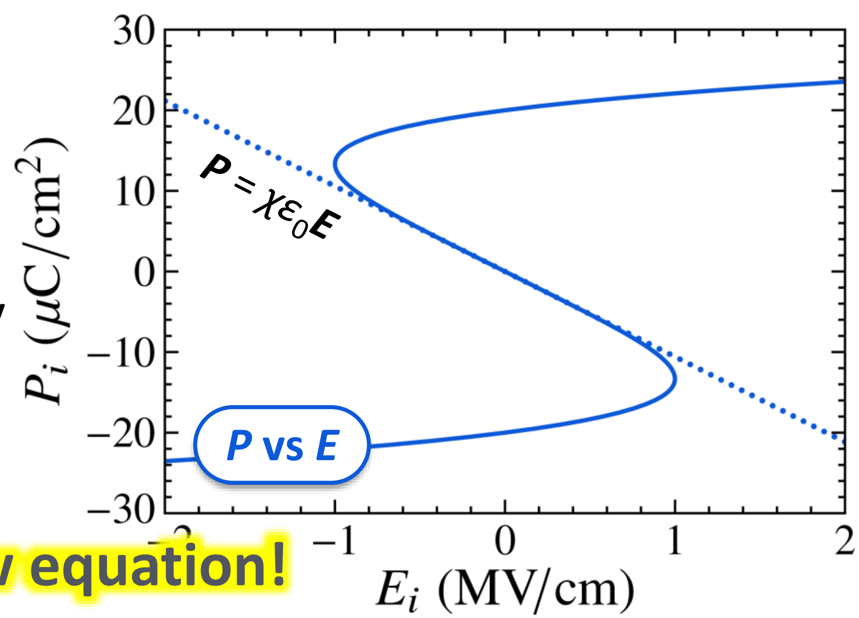
⇨ Ferroelectric's behavior is governed by

$$\nabla \cdot (\varepsilon \boldsymbol{E} + \boldsymbol{P}) = 0$$

Modified Poisson's equation!

$$2\alpha P_i + 4\beta P_i^3 + 6\gamma P_i^5 - E_i = 0$$

New equation!



Equations governing ferroelectrics: Implementation

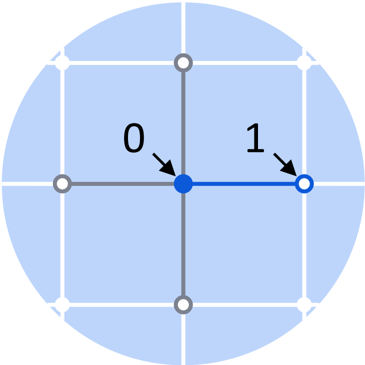
- Describe equations for a node & an adjacent node on computational mesh

```
def eqn_ferroelectric():
    E = -(ψ[1] - ψ[0]) / edge.len
    Pavg = (P[0] + P[1]) / 2

    ψflx = ε * E + dot(Pavg, edge / edge.len)
    ψsrc = 0

    Pflx = E * edge / 2
    Psrc = 2 * α * P[0] + 4 * β * P[0]**3 + 6 * γ * P[0]**5

    eqns = [(-ψflx, ψsrc), (-Pflx.x, Psrc.x),
            (-Pflx.y, Psrc.y), (-Pflx.z, Psrc.z)]
    vars = [ψ, P.x, P.y, P.z]

    return eqns, vars
```

Poisson eq. is modified

LK eq. is defined

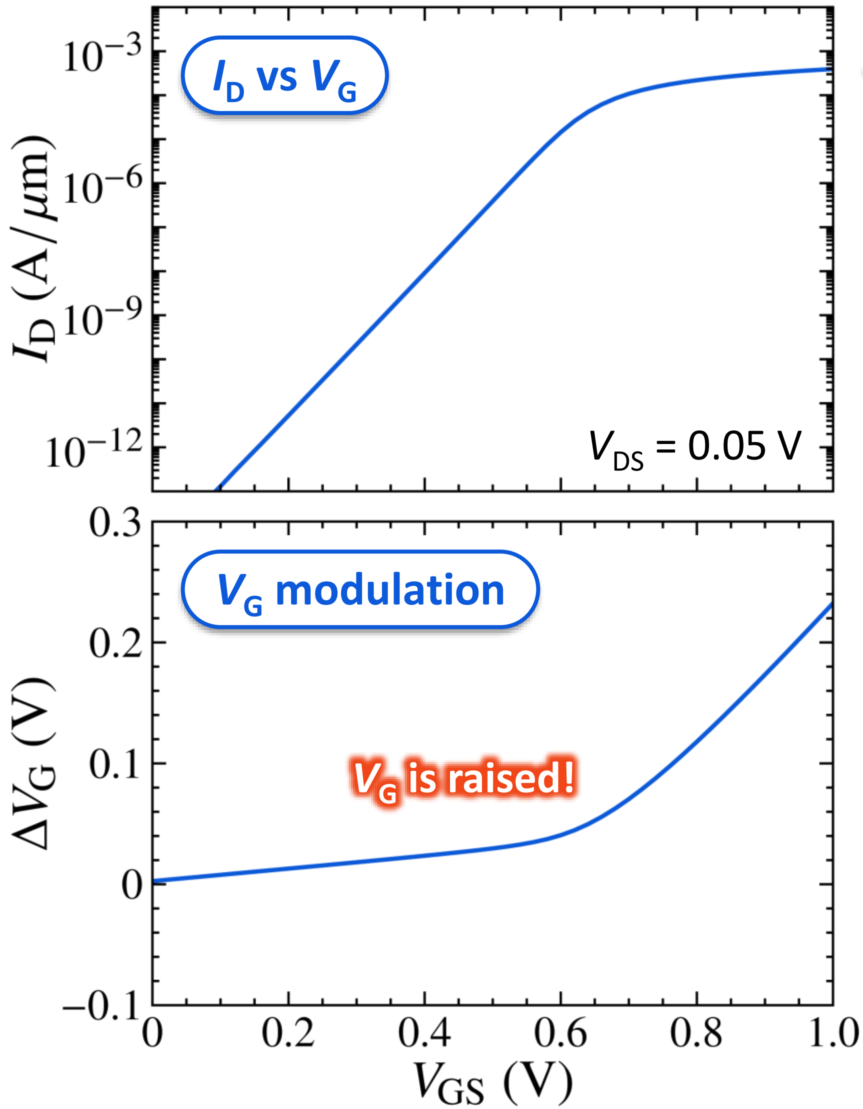
New variables & equations are added



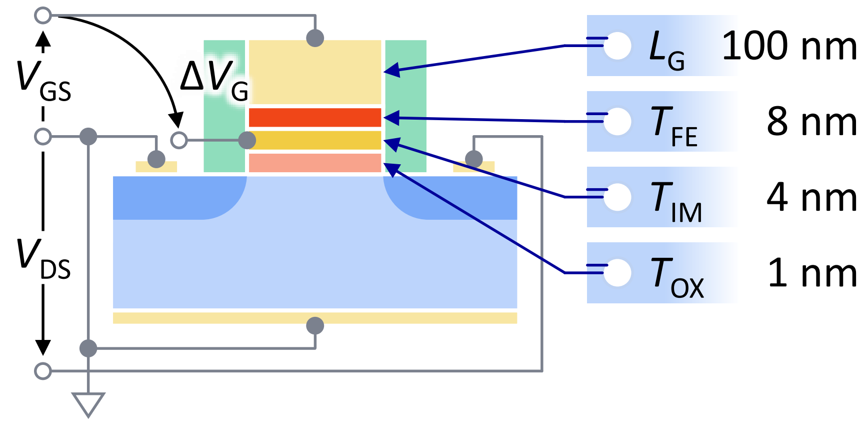
- For a given pair of inward flux & source terms (f, s), Impulse TCAD forms the following continuity equation

$$\int_{\partial V} f\, dS + \int_V s\, dV = 0$$

First simulation

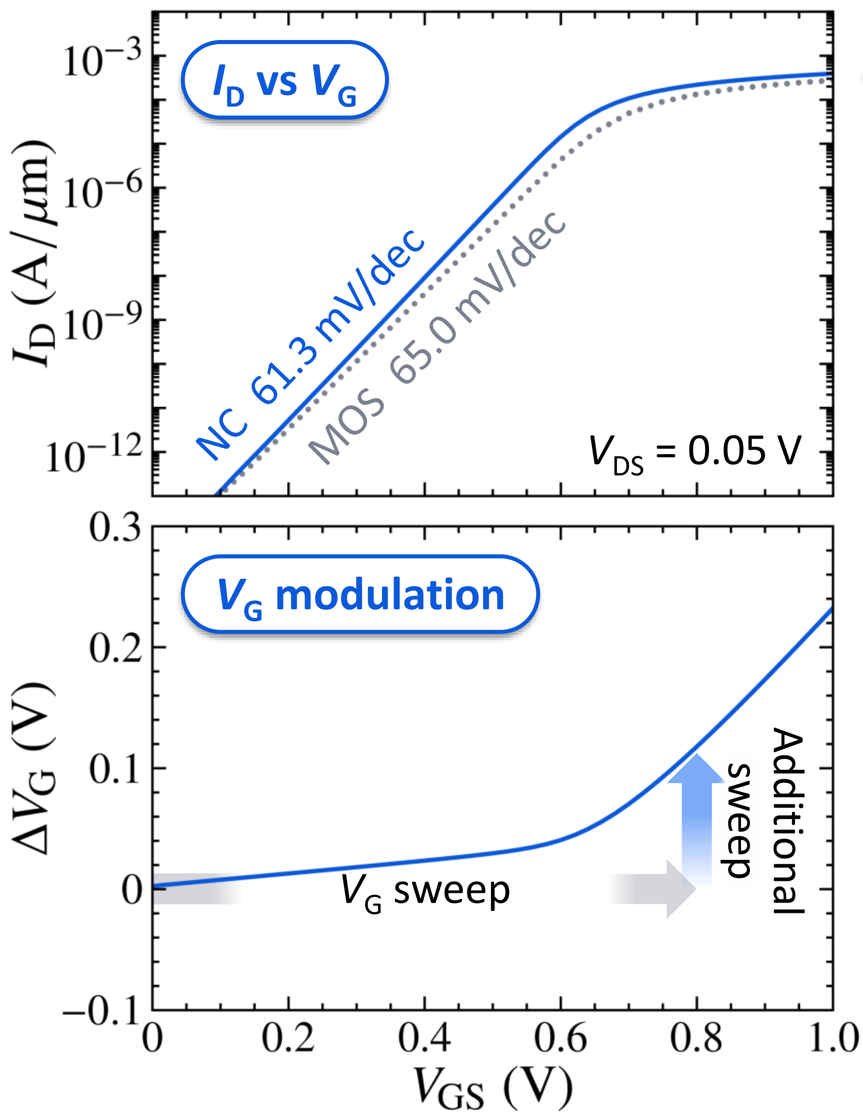


- Drain current I_D of an NC FET having an MFMOS structure was simulated

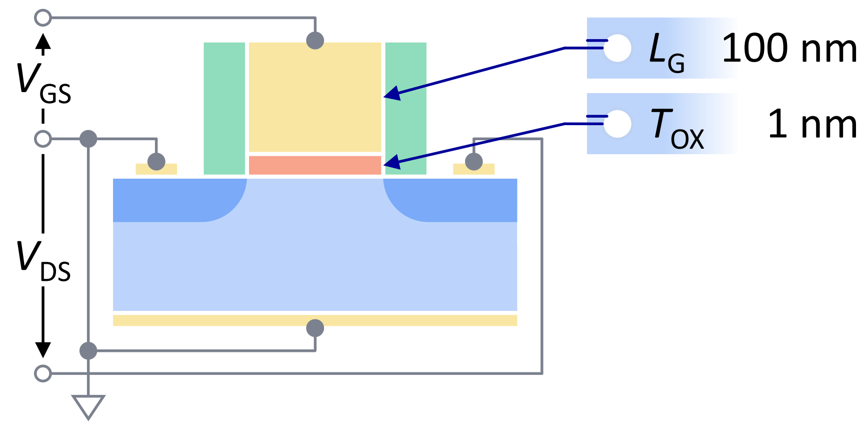


- Desired V_G enhancement by the ferroelectric film ΔV_G can be observed
  - MOS structure is subject to $V_G + \Delta V_G$

Steep switching

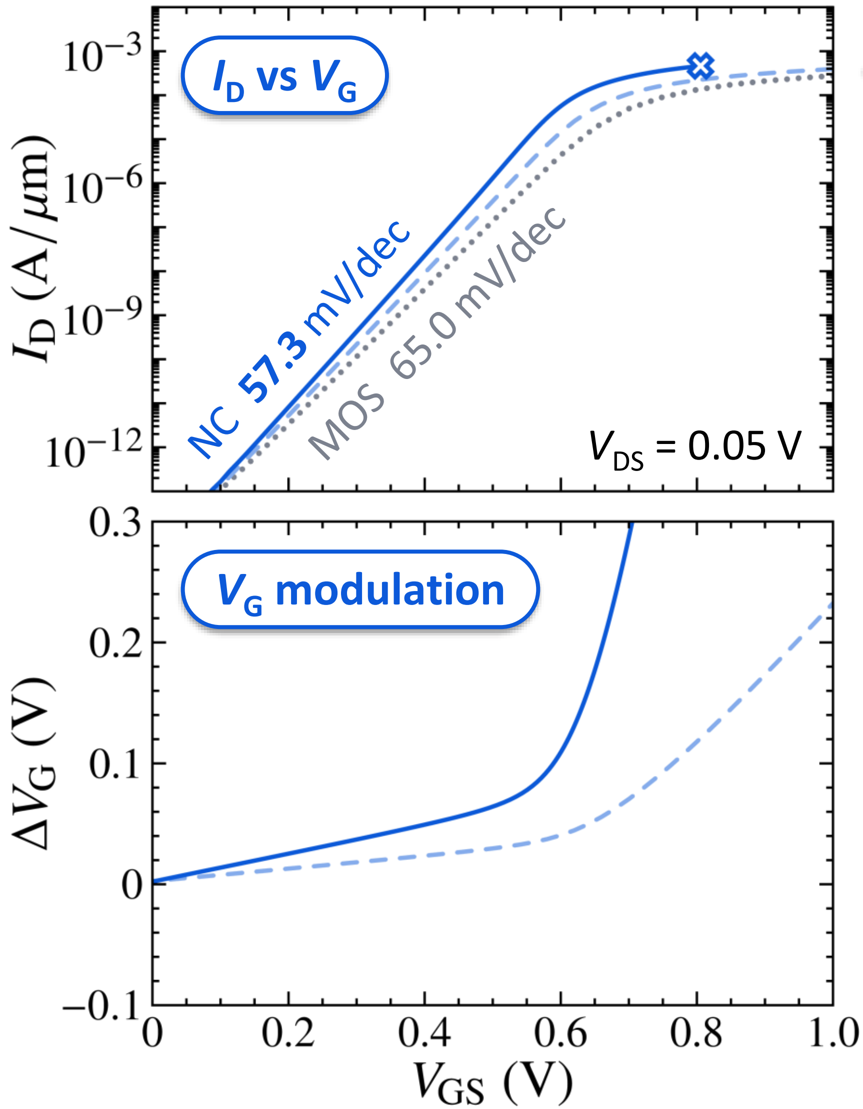


- MOS FET was also simulated

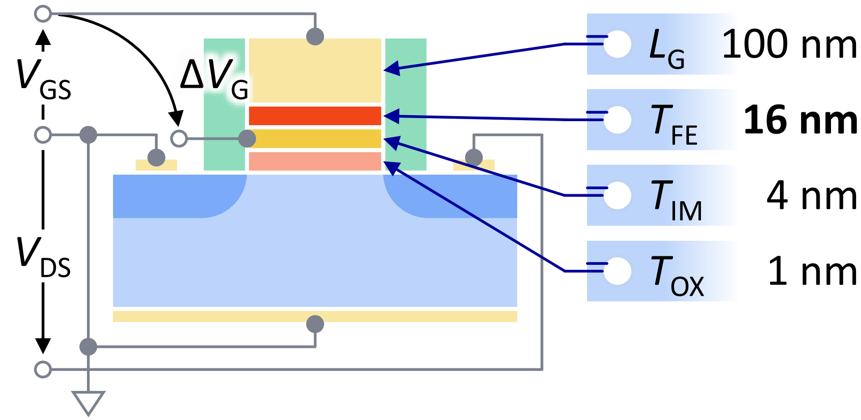


- NC FET's I_D increases with a steeper slope
  - Subthreshold swing is still worse than MOS FET's physical limit of 60 mV/dec

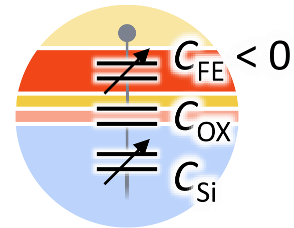
Steep switching: Beyond the limit



- Thicker ferroelectric film was used

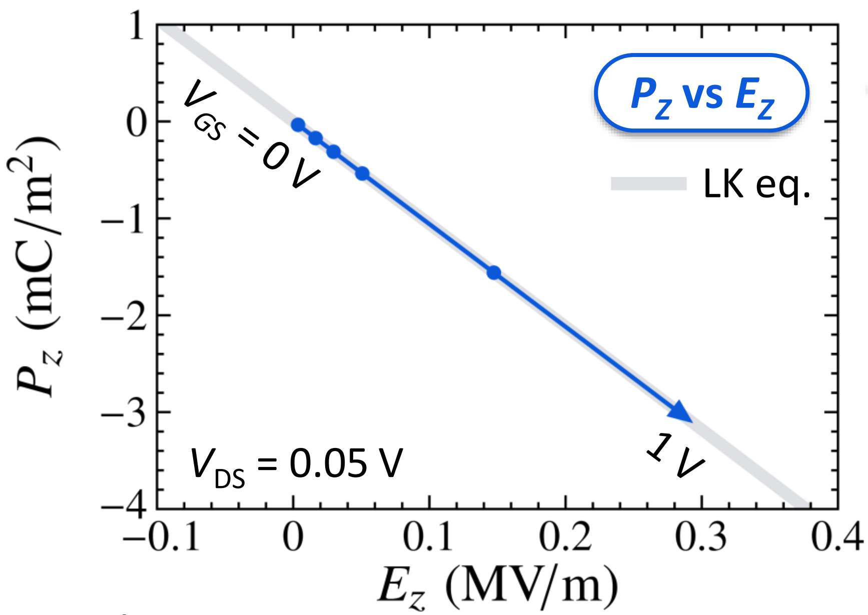


- NC FET's I_D increases with a steeper slope
  - Subthreshold swing can exceed MOS FET's physical limit of 60 mV/dec
  - Capacitance matching is severe

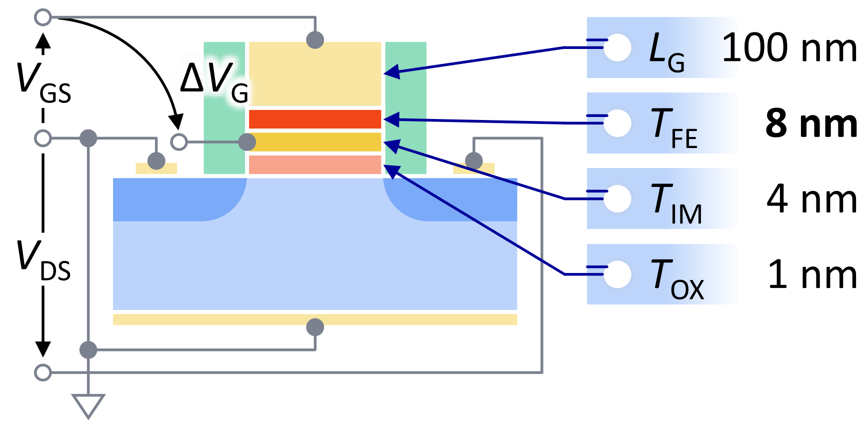


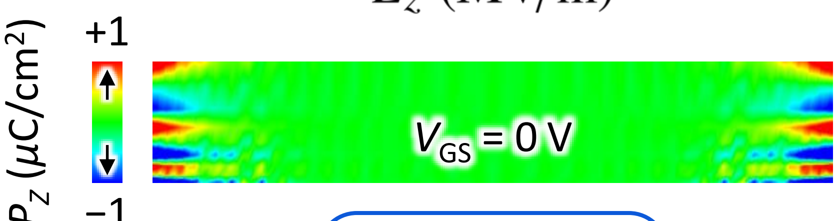
$$\frac{1}{C_G} \approx \frac{1}{C_{FE}} + \frac{1}{C_{OX}} + \frac{1}{C_{Si}}$$

Polarization field

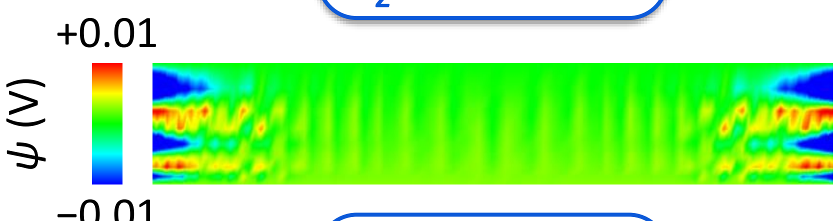


- Average ***P*–*E*** relationship in the ferroelectric film





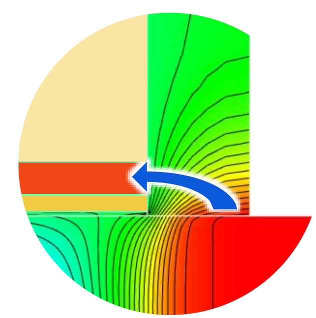
P_z distribution



ψ distribution

- ***P*** field near both edges is disturbed by the electric field entering from the gate side walls

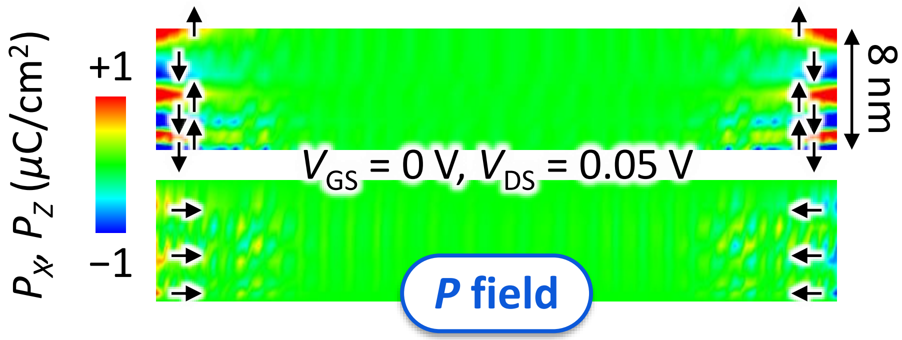
⇨ This disturbance leads to unnatural variation in ψ



Revisit to ferroelectric models

- Does this ***P*** field seem to be ferroelectric?

⇨ ***P*** vectors tend to align with each other . . .



- Such tendency is described in Ginzburg–Landau model as the energy penalty for the spatial variation in ***P***

$$g_{\mathrm{GL}} = (\delta_{11}/2)[(\partial_x P_x)^2 + (\partial_y P_y)^2 + (\partial_z P_z)^2] + \delta_{12}[(\partial_x P_x)(\partial_y P_y) + (\partial_y P_y)(\partial_z P_z) + (\partial_z P_z)(\partial_x P_x)] + (\delta_{44}/2)[(\partial_y P_x + \partial_x P_y)^2 + (\partial_z P_y + \partial_y P_z)^2 + (\partial_x P_z + \partial_z P_x)^2]$$

- By introducing g_{GL} and assuming $\delta_{11} = -\delta_{12} = \delta_{44} = \delta$ the LK equation can be rewritten as

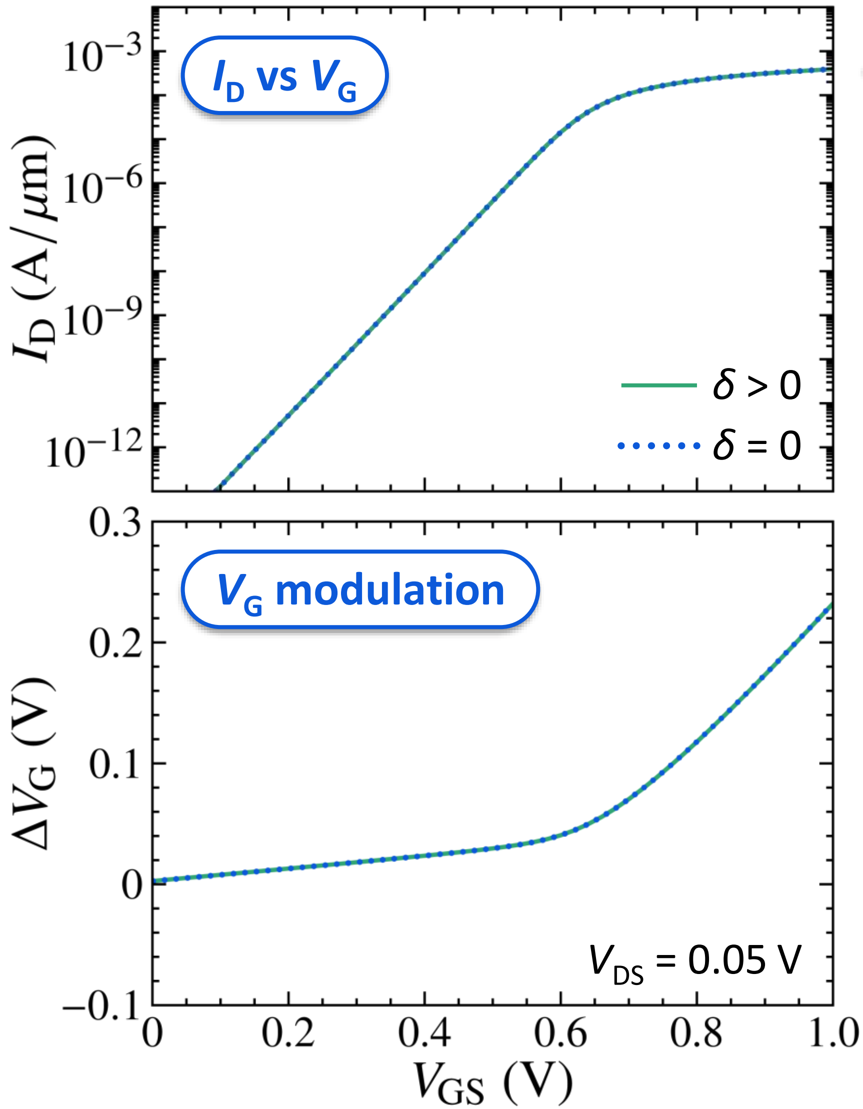
GL term

$$2\alpha P_i + 4\beta P_i^3 + 6\gamma P_i^5 - E_i - \delta\nabla\cdot(\nabla P_i) = 0$$

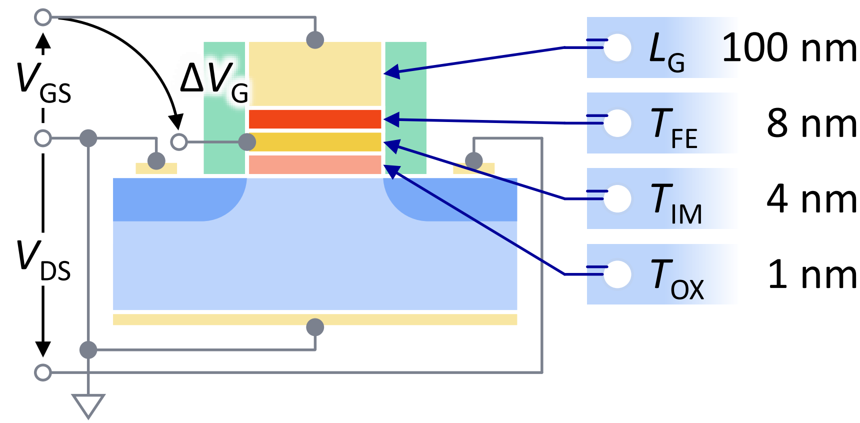
  - Implementation can be done by adding only one line in the code

```
Pflx += δ * (P[1] - P[0]) / edge.len
```

GL term's effects: Device performance

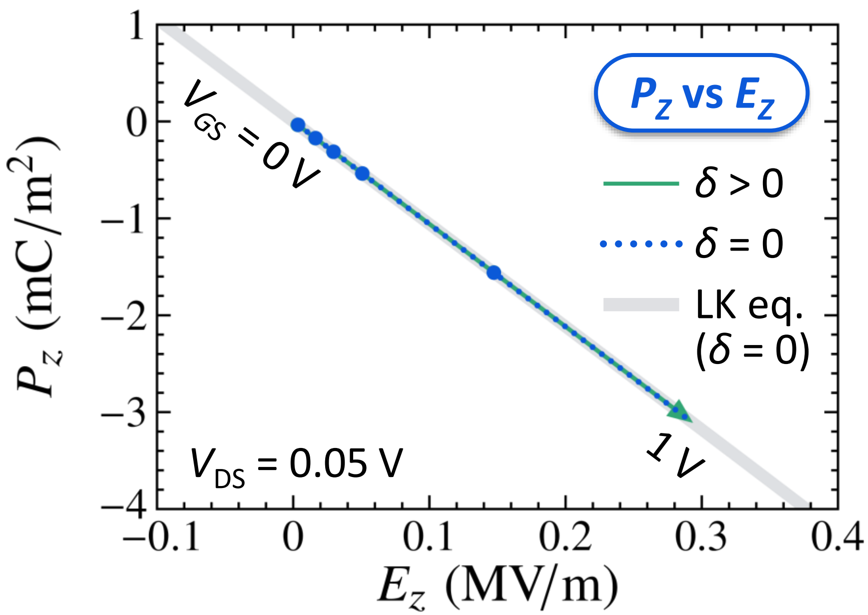


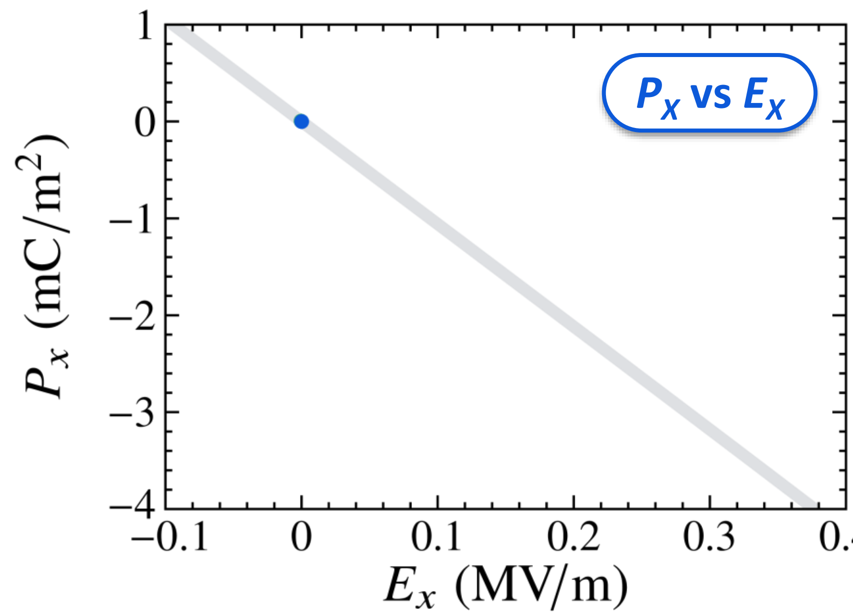
- When the GL term is taken into account . . .

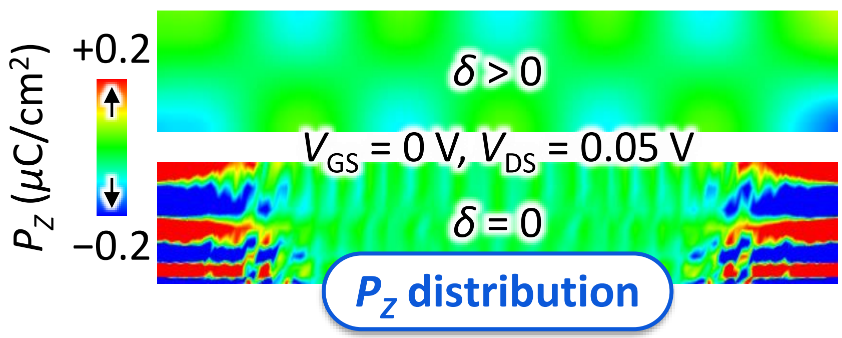


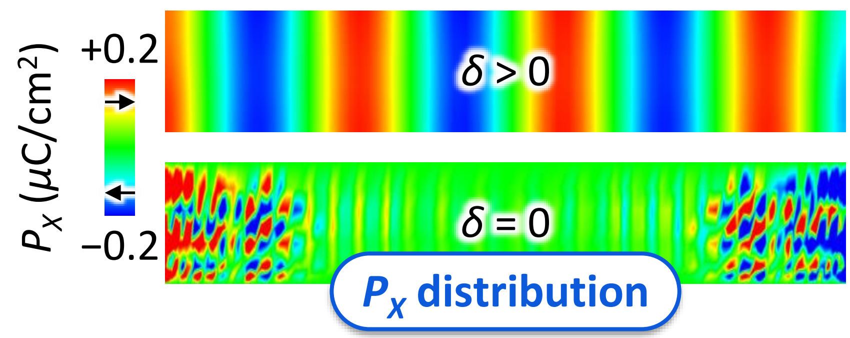
- GL term has little effect on the device performance

GL term's effects: Polarization field

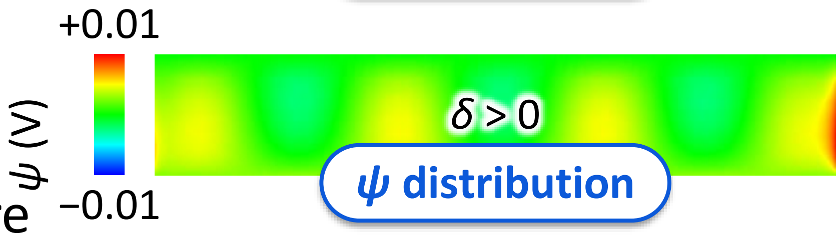




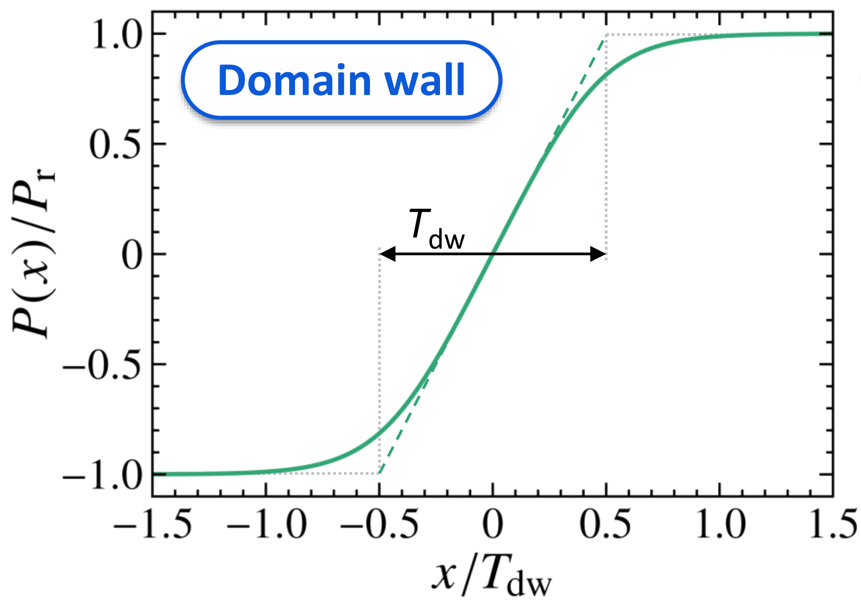




- GL term drastically changes the ***P*** field and relaxes its unnatural variation by forming quasi-multidomain structure



GL term's effects: Dependence on δ



- ***P*** profile in 1D ferroelectrics having two domains with opposite ***P***'s

$$2\alpha P + 4\beta P^3 + 6\gamma P^5 - \delta(\partial^2 P/\partial x^2) = 0$$

$$P(+\infty) = P(-\infty) = P_r$$

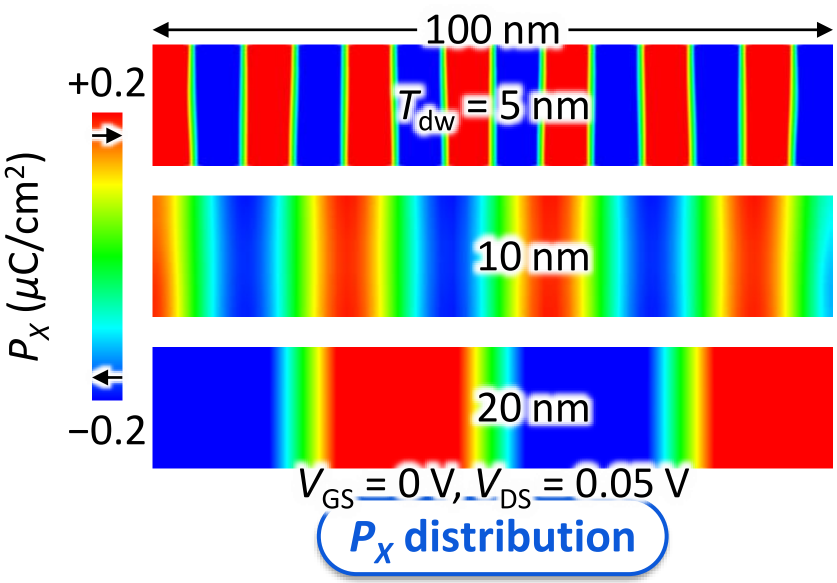
- δ determines the thickness of domain walls T_{dw}

$$T_{dw} = \sqrt{6\delta/-(2\alpha + \beta P_r^2)}$$

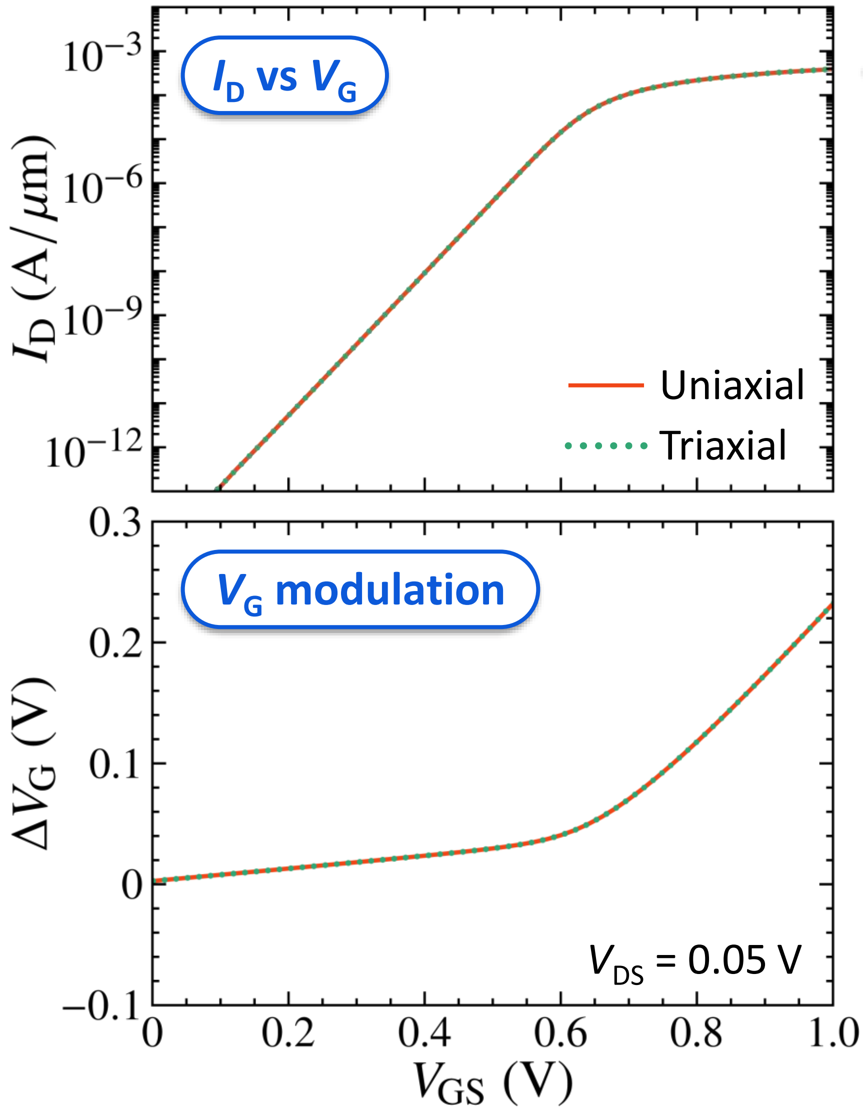
$$P_r = \left(-\beta + \sqrt{\beta^2 - 3\alpha\gamma}\right)/3\gamma$$

⇨ ***P*** field depends strongly on δ

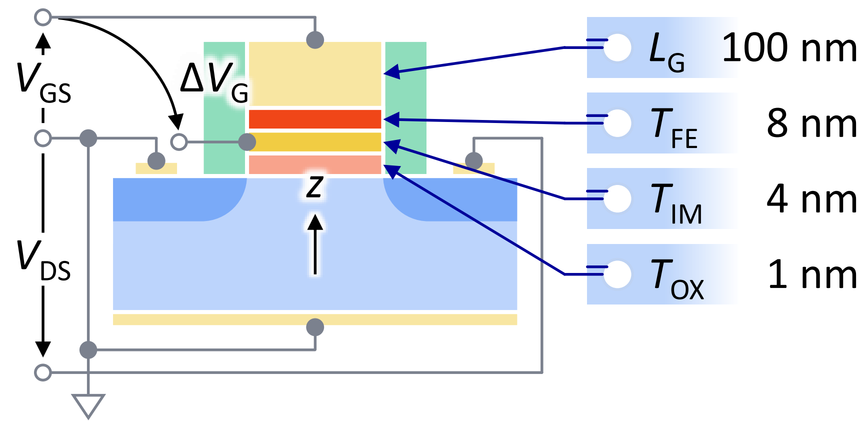
- Average ***P–E*** relationship is, however, almost independent of δ



Uniaxial ferroelectricity: *z*-oriented



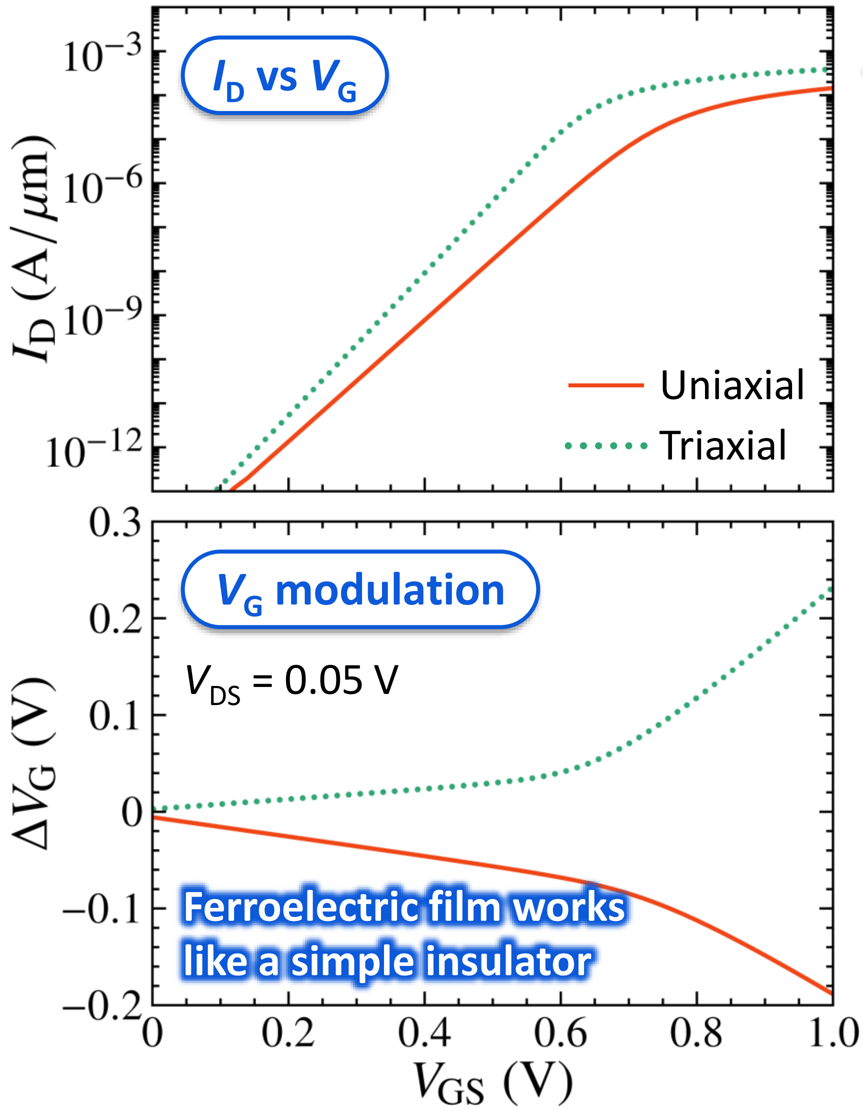
- When the ferroelectricity is uniaxial and along the *z*-axis



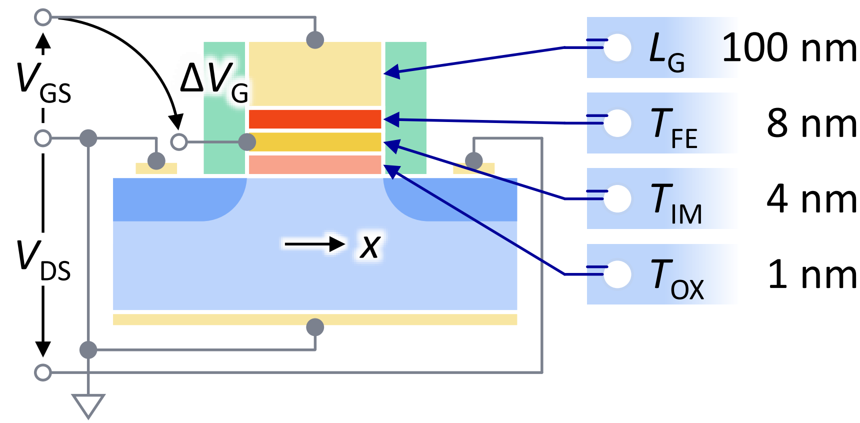
- Easy implementation:
  omit P_X's & P_Y's equations & variables

`eqns = [(-ψflx, ψsrc),`
`~~(-Pflx.x, Psrc.x),~~`
`~~(-Pflx.y, Psrc.y),~~`
`(-Pflx.z, Psrc.z)]`
`vars = [ψ, ~~P.x , P.y,~~ P.z]`

Uniaxial ferroelectricity: *x*-oriented



- When the ferroelectricity is uniaxial and along the ***x***-axis

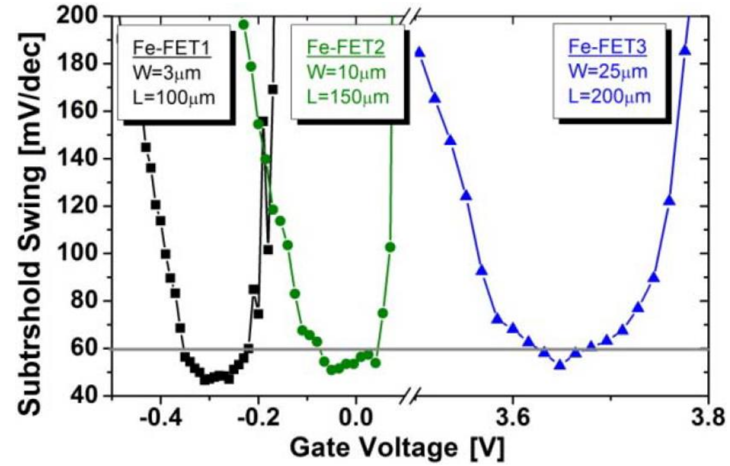


- General implementation: introduce ***P***'s direction

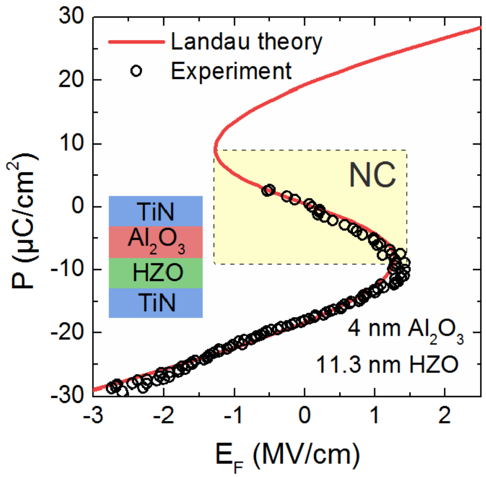
```
ψflx = ε * E + dot(P * pdir,
            edge / edge.len)
Pflx = dot(E * edge / 2, pdir)
eqns = [(−ψflx, ψsrc),
        (−Pflx, Psrc)]
vars = [ψ, P]
```

Need for transient simulation

- NC should happen at steady state . . .
  - Many research groups have demonstrated steep switching of NC FETs with a subthreshold swing $S < 60$ mV/dec, but such an ideal S was achieved only temporarily when V_G was swept



[A. Rusu *et al*., IEDM Tech. Dig., 395 (2010)]



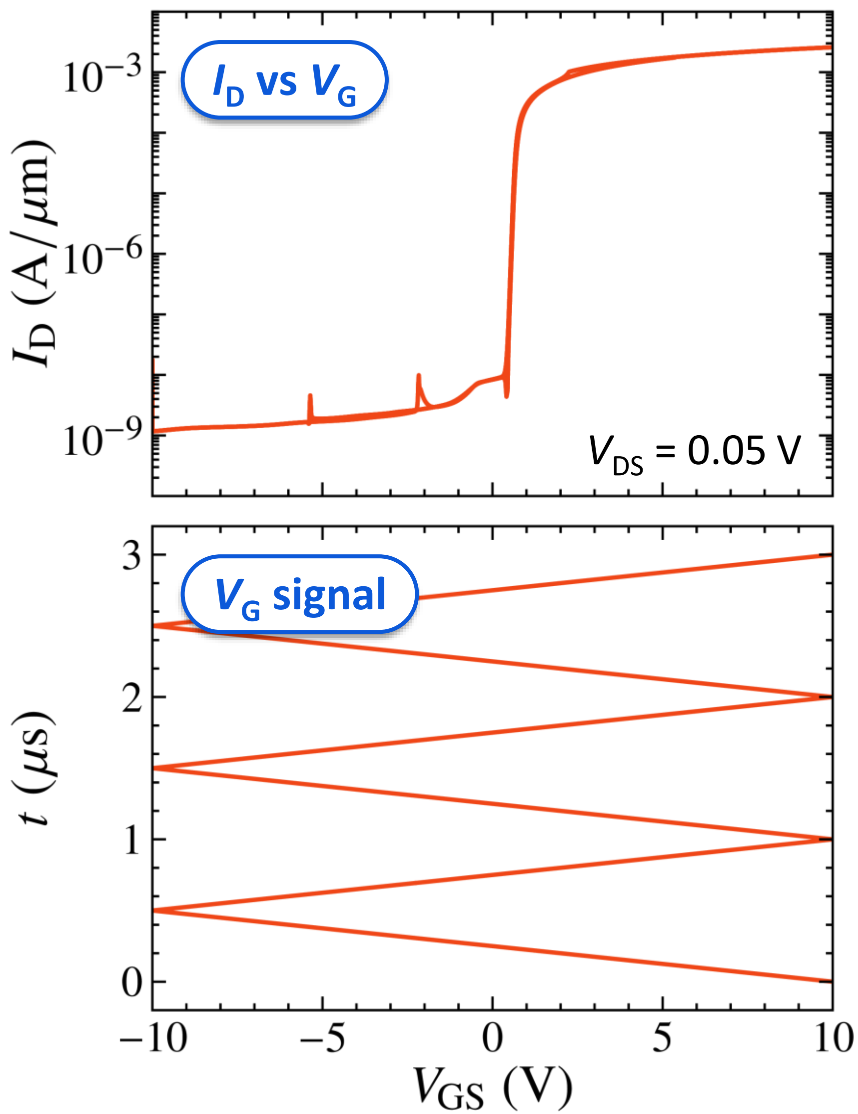
  - S-shape ***P*–*E*** relationship was recently observed experimentally. Though, that experiment was conducted with pulsed voltage

[M. Hoffmann *et al*., IEDM Tech. Dig., 727 (2018)]

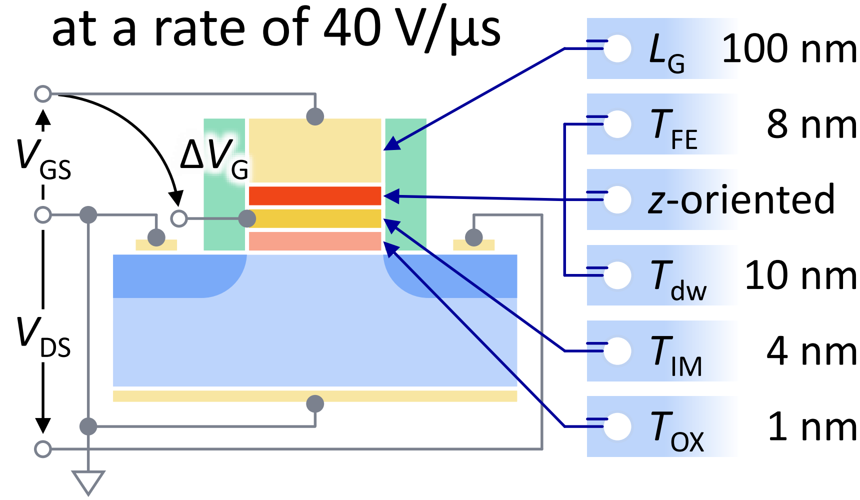
⇨ NC may be a transient phenomenon . . .

⇨ Transient simulation is needed!

Transient simulation: Device performance



- Triangular V_G signal from −10 to 10 V was applied at a rate of 40 V/μs



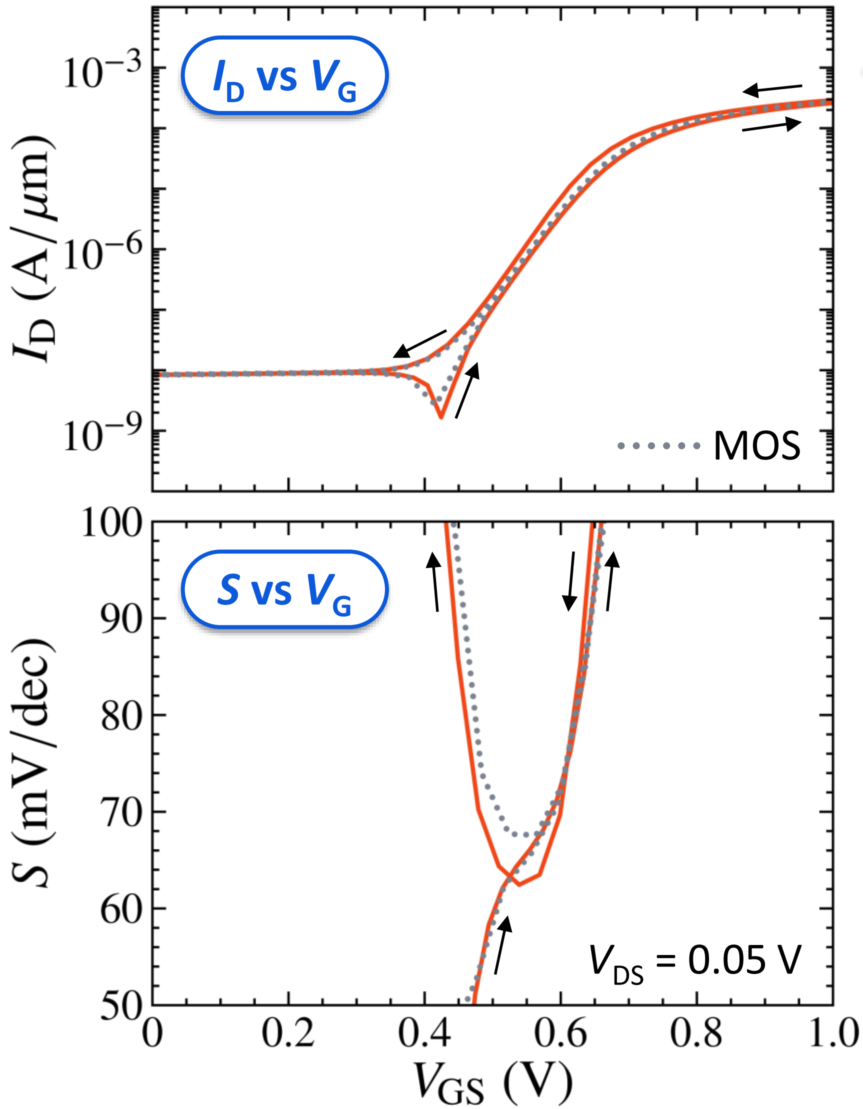
- Time-dependent LK eq.

$$2\alpha P_i + 4\beta P_i^3 + 6\gamma P_i^5 - E_i - \delta\nabla\cdot(\nabla P_i) + \lambda(dP_i/dt) = 0$$

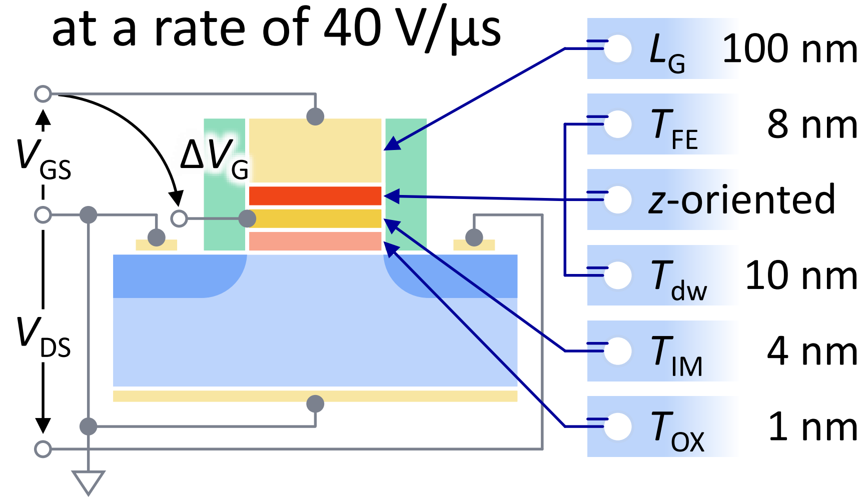
  - Simple implementation: use the backward Euler method

```
Psrc += λ*(P[0]-P0[0])/tstep
```

Transient simulation: Subthreshold swing

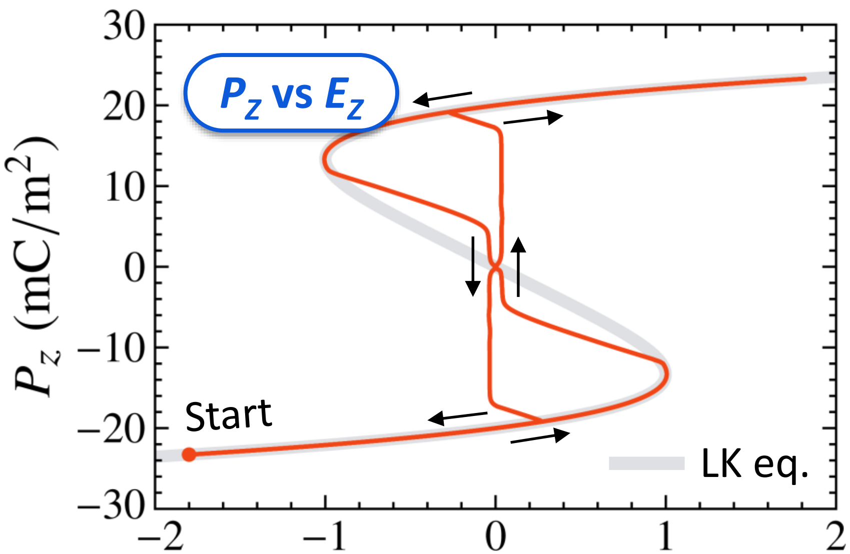


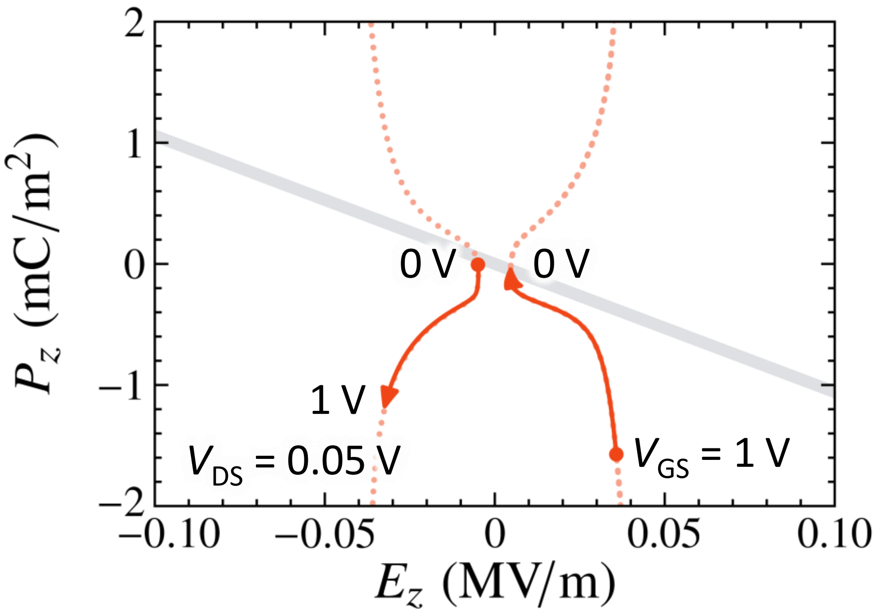
- Triangular V_G signal from −10 to 10 V was applied at a rate of 40 V/µs



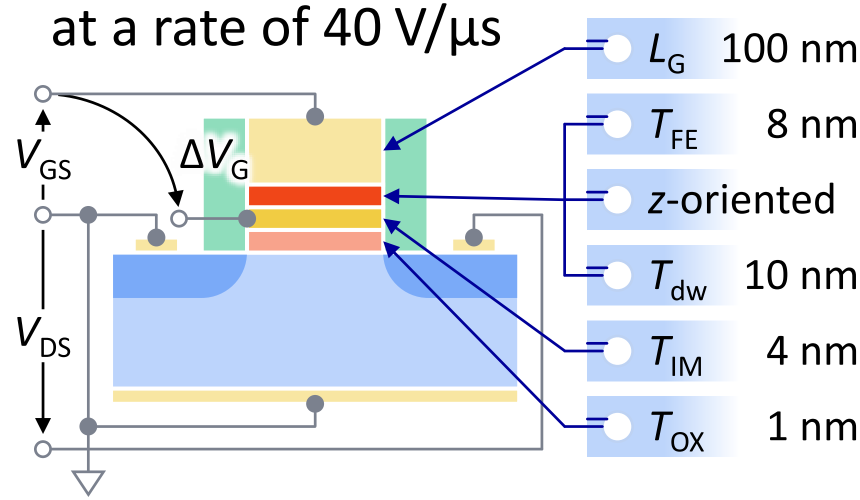
- Small hysteresis appears
- Subthreshold swing S improves only in backward sweep

Transient simulation: *P–E* relationship



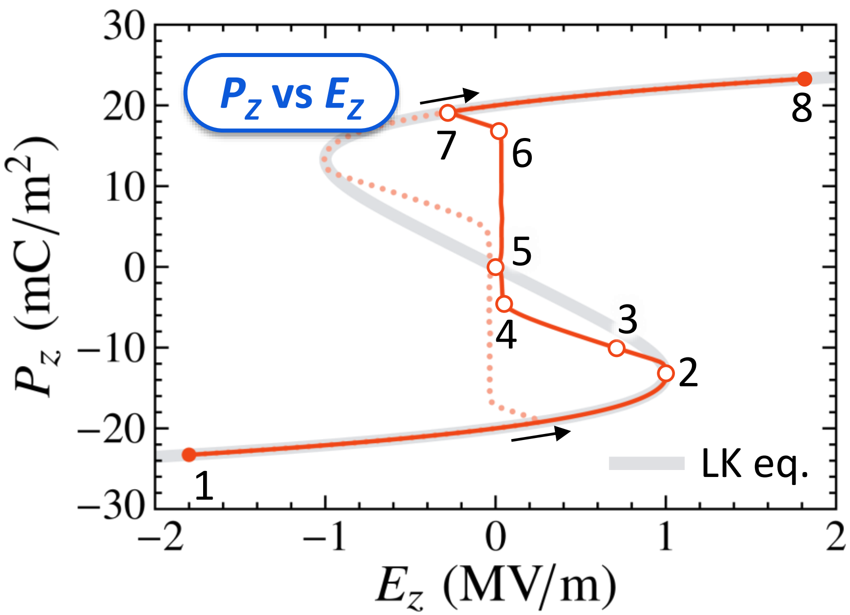


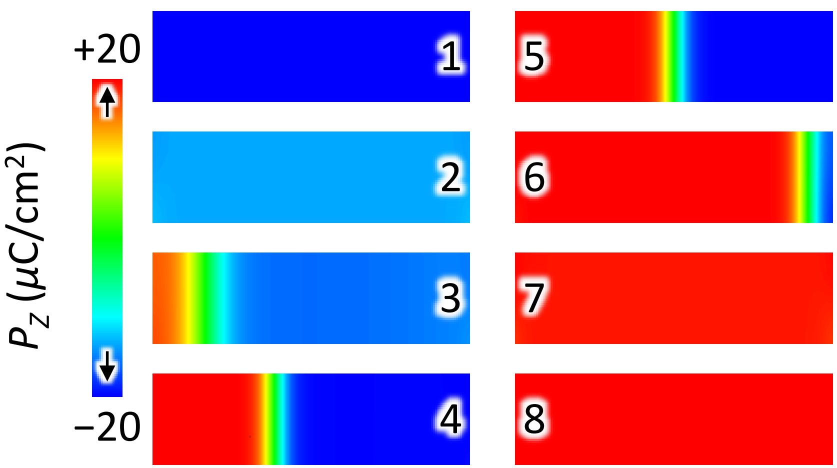
- Triangular V_G signal from −10 to 10 V was applied at a rate of 40 V/µs



- When V_G decreases from 1 to 0 V, the ferroelectric film is in NC state
  - while in forward sweep it is in non-NC state

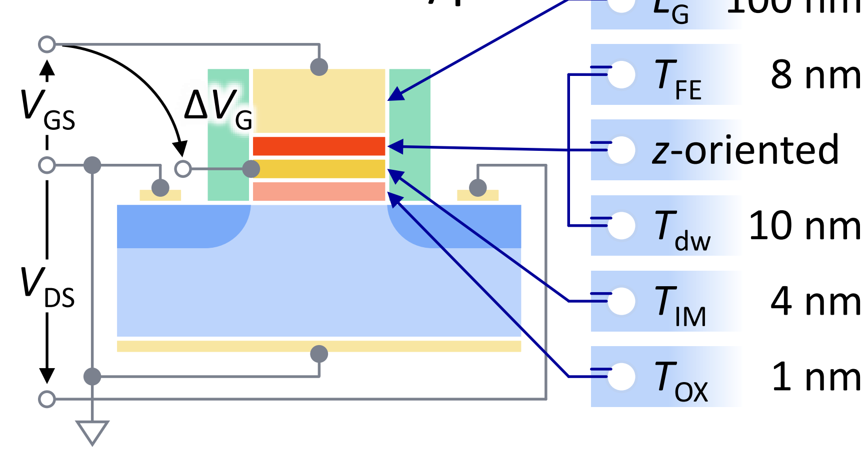
Transient simulation: Polarization field



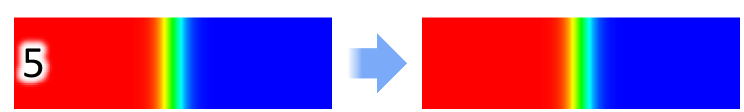


P_z distribution

- Triangular V_G signal from −10 to 10 V was applied at a rate of 40 V/μs

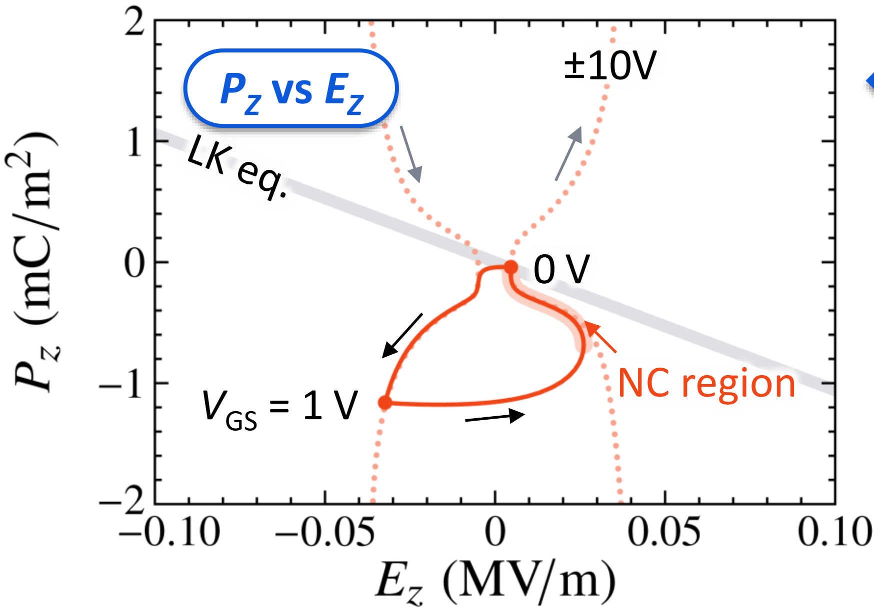


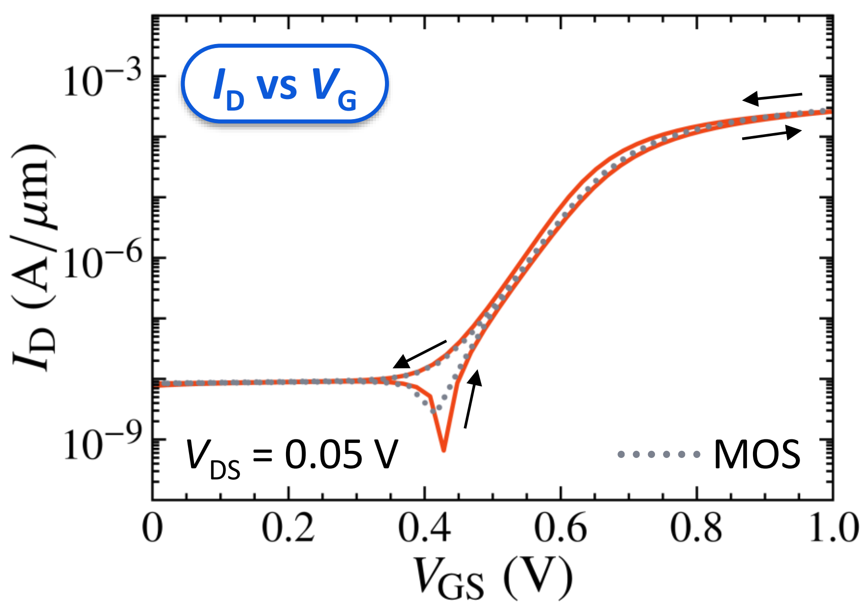
- Ferroelectric state deviates from the time-independent LK eq. when a multi-domain structure forms
  - Such a structure is stable



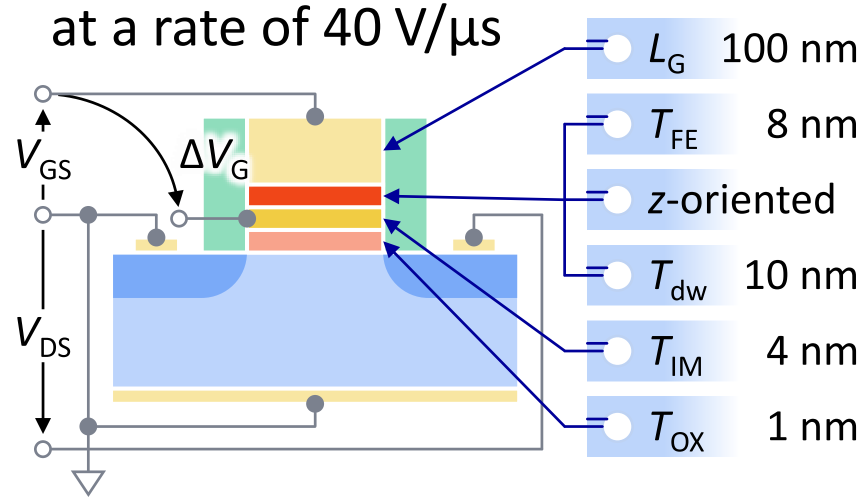
Steady-state simulation

Transistor operation



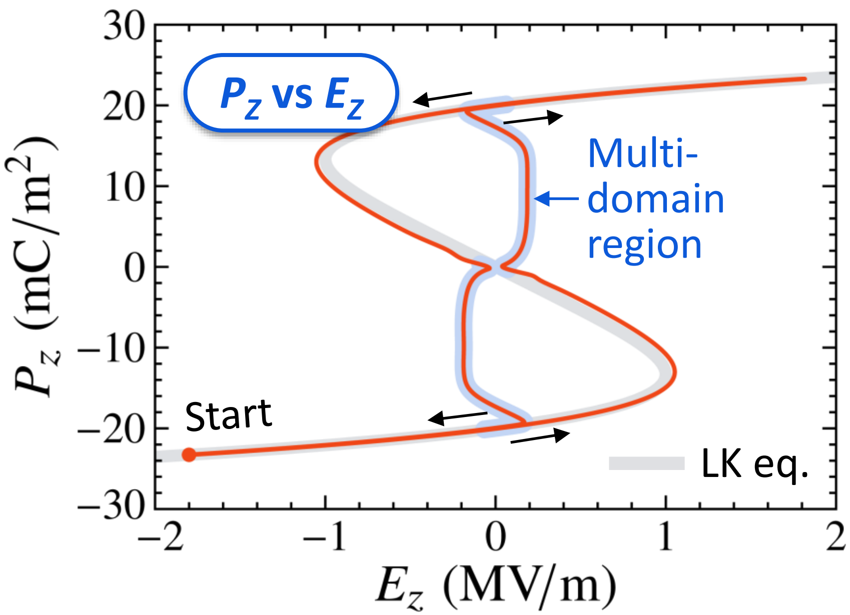


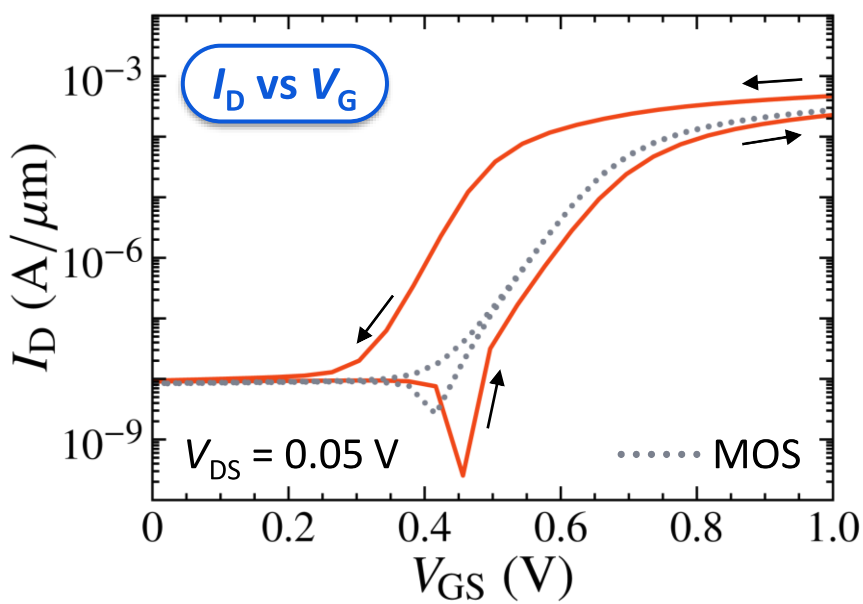
- Triangular V_G signal from **−1** to **1 V** was applied at a rate of 40 V/μs



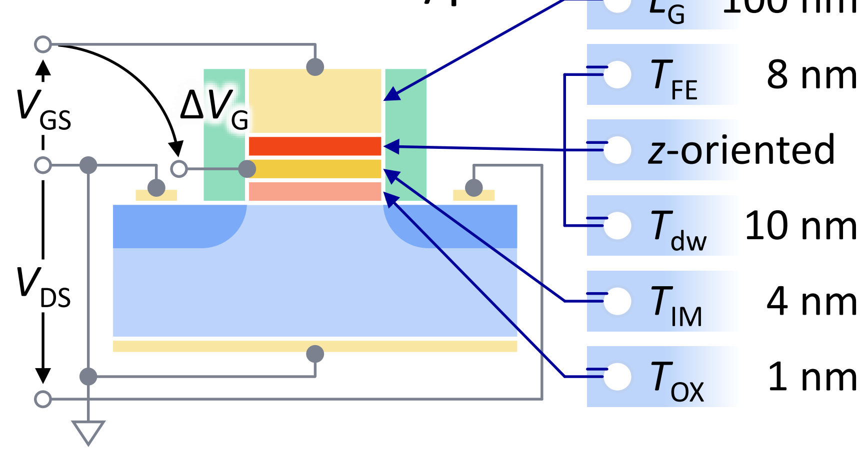
- Ferroelectric state tries to trace the two paths passed in the previous large backward & forward V_G sweeps
  - Hysteresis remains
  - NC region is limited

Viscosity of polarization





- Triangular V_G signal from **−10 to 10 V** was applied at a rate of 40 V/μs

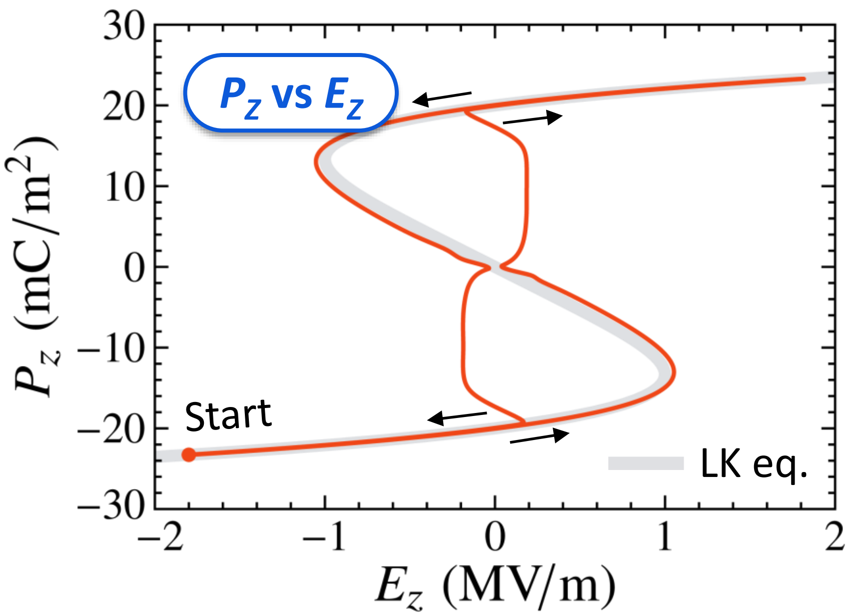


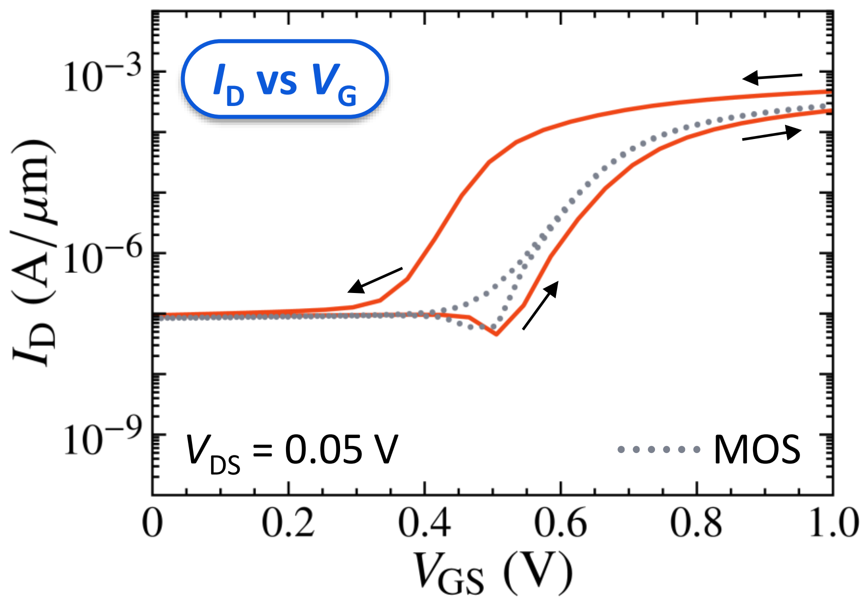
- When ***P*** is perturbed from the remanent polarization state P_r, it relaxes to P_r with a time constant

$$\tau_P = \lambda / -8(\alpha + \beta P_r^2)$$

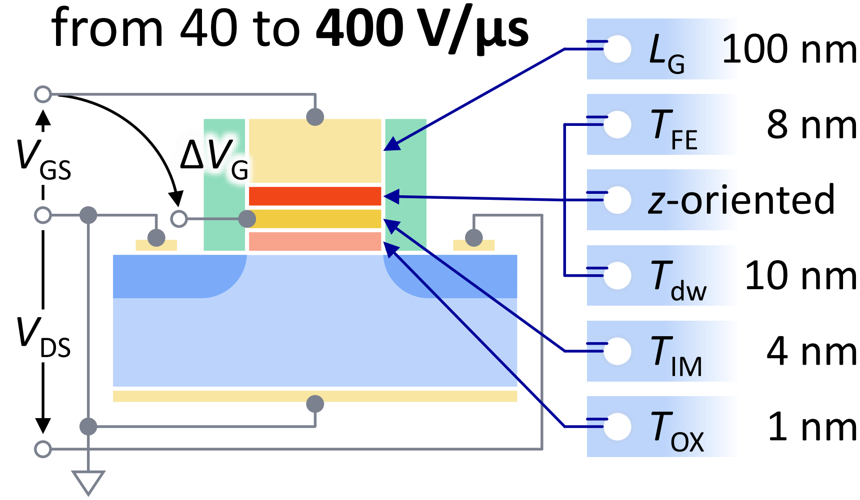
  - Here ***P***'s viscosity λ was set so that τ_P was changed from 0.1 to **1 ns**

Viscosity of polarization: Relationship to signal frequency



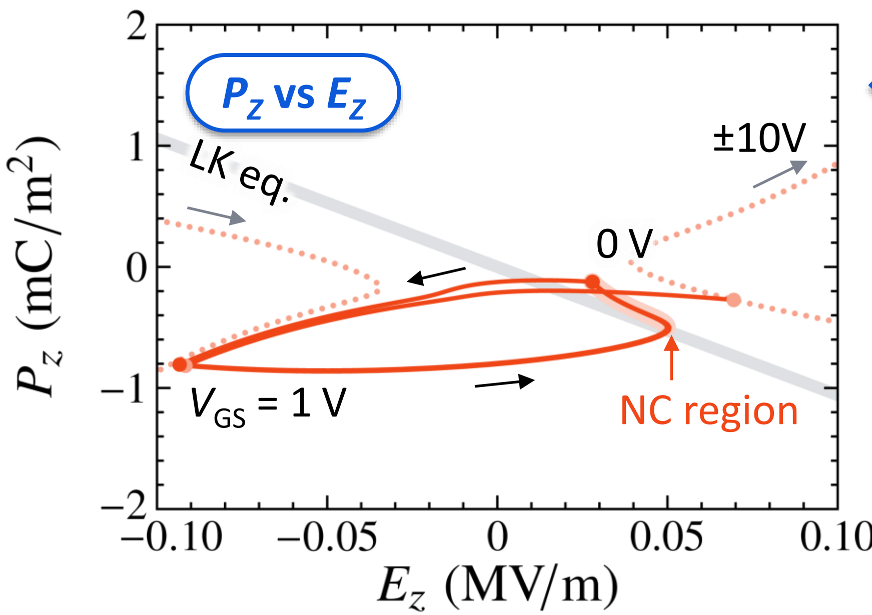


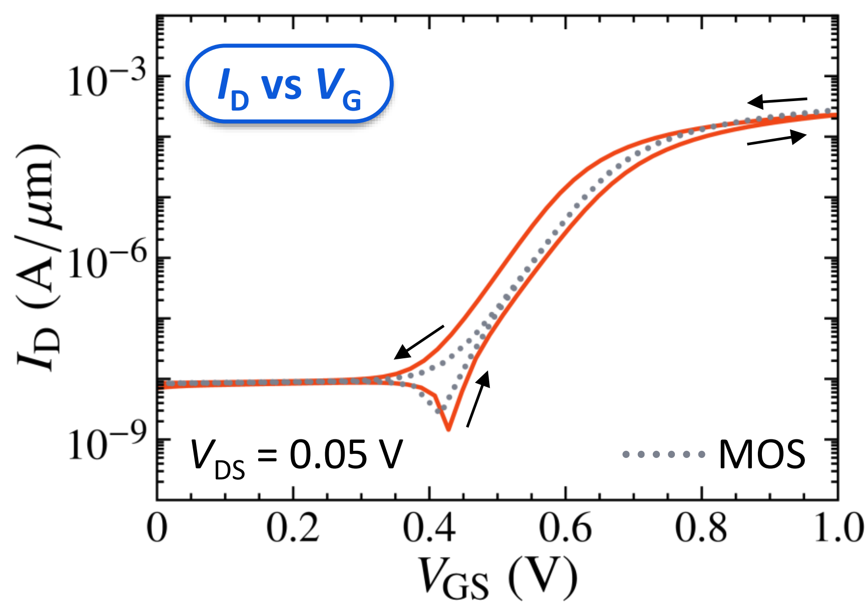
- τ_P was changed back to **0.1 ns** while V_G sweep rate was changed from 40 to **400 V/μs**



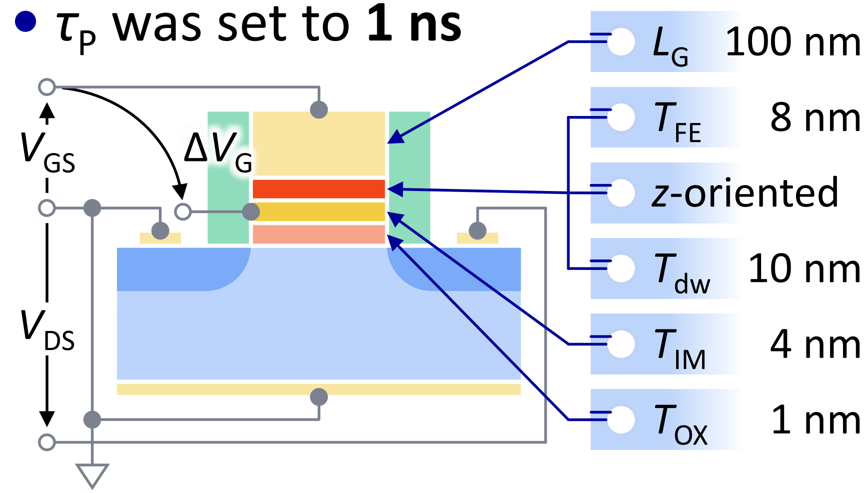
- Increasing τ_P or λ equals increasing the sweep rate of the applied voltage

Transistor operation with sticky ferroelectrics





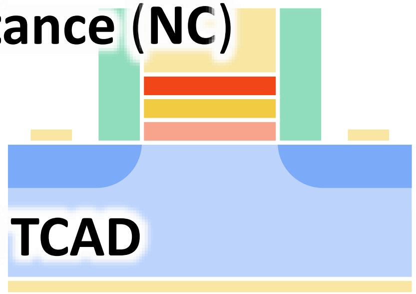
- Triangular V_G signal from **−1** to **1 V** was applied at the original rate of **40 V/μs**
- τ_P was set to **1 ns**



- Ferroelectric state still tries to trace the two paths passed in the large backward & forward V_G sweeps
  - Hysteresis shrinks but remains
  - NC region is limited

Conclusion

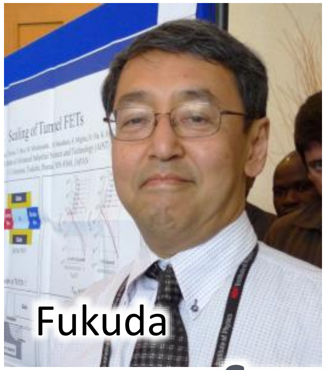
We studied the behavior of ferroelectric negative-capacitance (NC) field-effect transistors (FETs) on the basis of the Landau-Khalatnikov equation using our newly developed device simulator, Impulse TCAD



- Thanks to high flexibility of Impulse TCAD, we successfully simulated NC FETs with taking into account various aspects of ferroelectrics
  - Tendency of the polarization vectors to align with each other
  - Time dependence of the polarization field
  - Uniaxiality

⇨ **Design of NC FETs is a very tough work!**

- If you are interested in Impulse TCAD, . . .
  - see the website **Impulse TCAD**
  - join SISPAD 2019 at the Univ. of Udine, Italy
  - contact us at ImpulseTCAD@aist.go.jp



See you at SISPAD!