

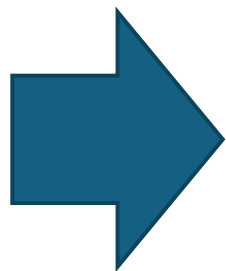
강유전체 기반 뉴로모픽 컴퓨팅을 위한
전도 변조 시뮬레이션
(분극 반전 동역학을 가미한)

한양대학교 ERICA 캠퍼스
첨단융합대학 국방지능정보융합공학부 지능정보양자공학전공
(구) 응용물리학과
강보수

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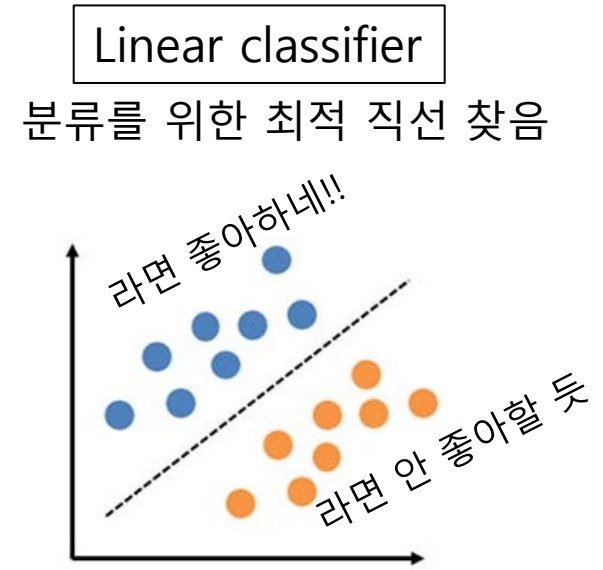
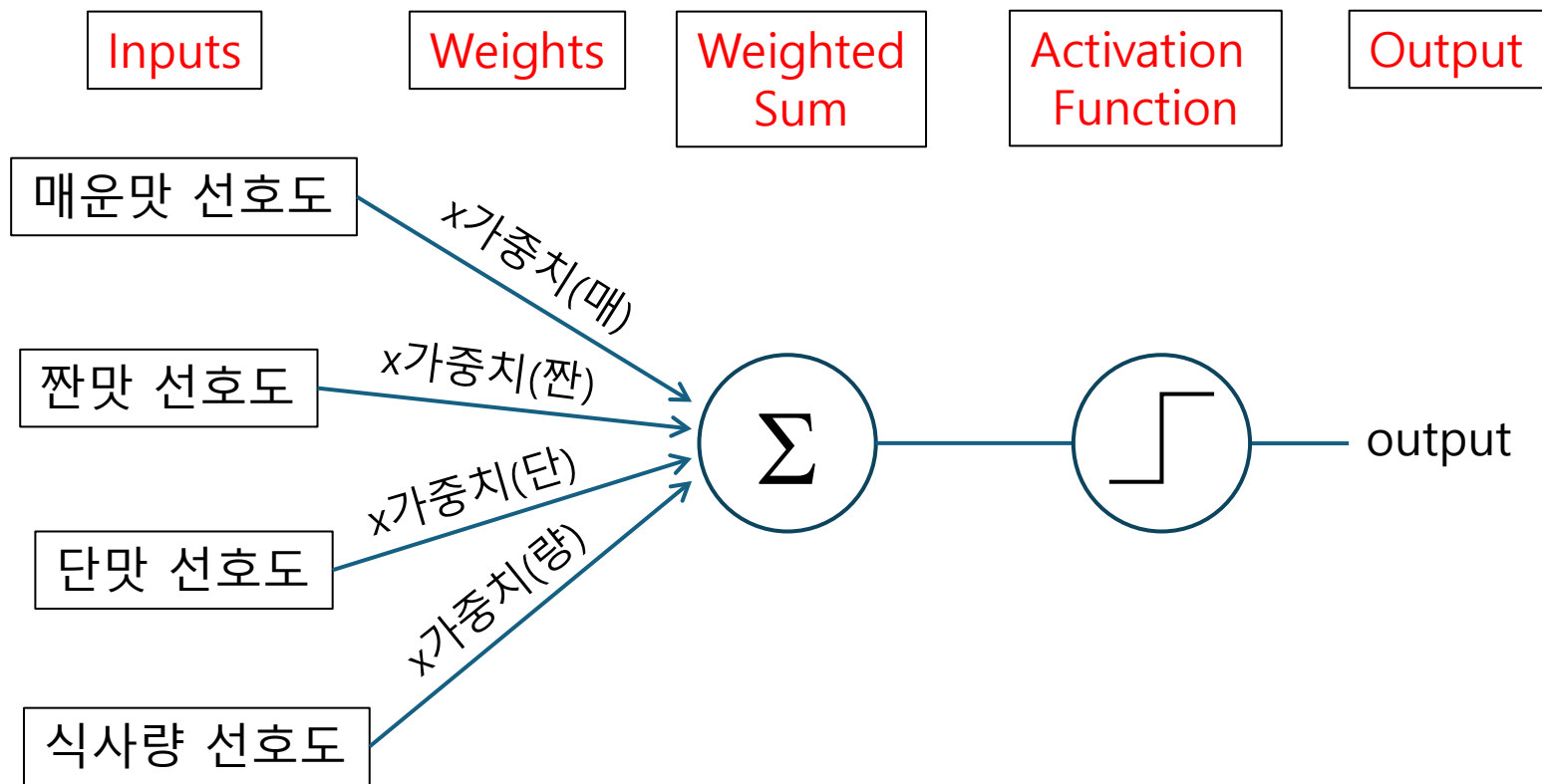
1. Introduction to Neuromorphic Computing
2. Ferroelectrics
3. Polarization Switching Dynamics Simulation
4. Conductance Modulation of Neuromorphic Computing
5. Conclusion

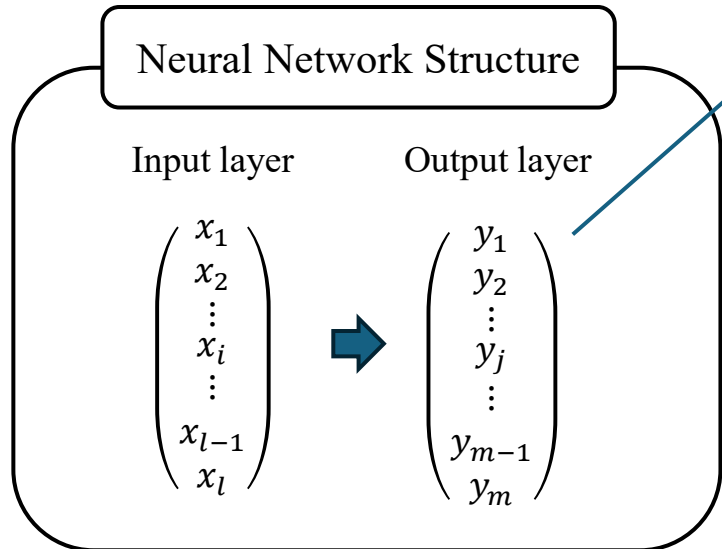
Input: 매운맛 선호도
짠맛 선호도
단맛 선호도
식사량 선호도



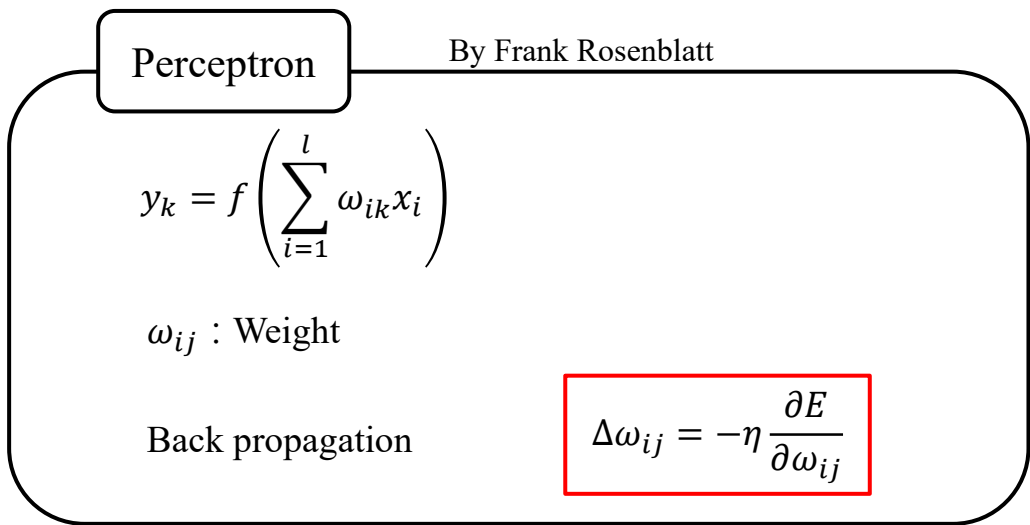
Output: 이 사람이 라면을 좋아할 것인가 여부

Perceptron – 인공신경망 기본 모델이자 선형 분류 알고리즘



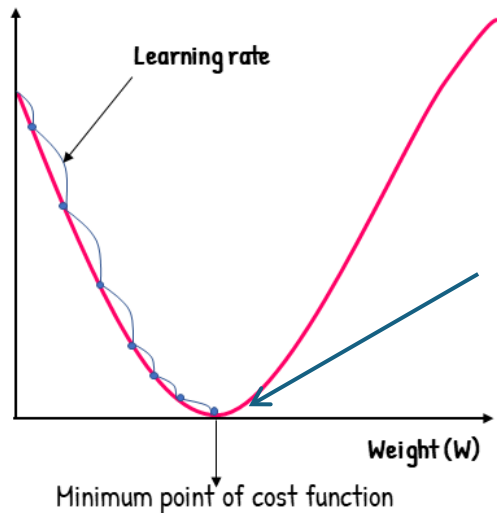
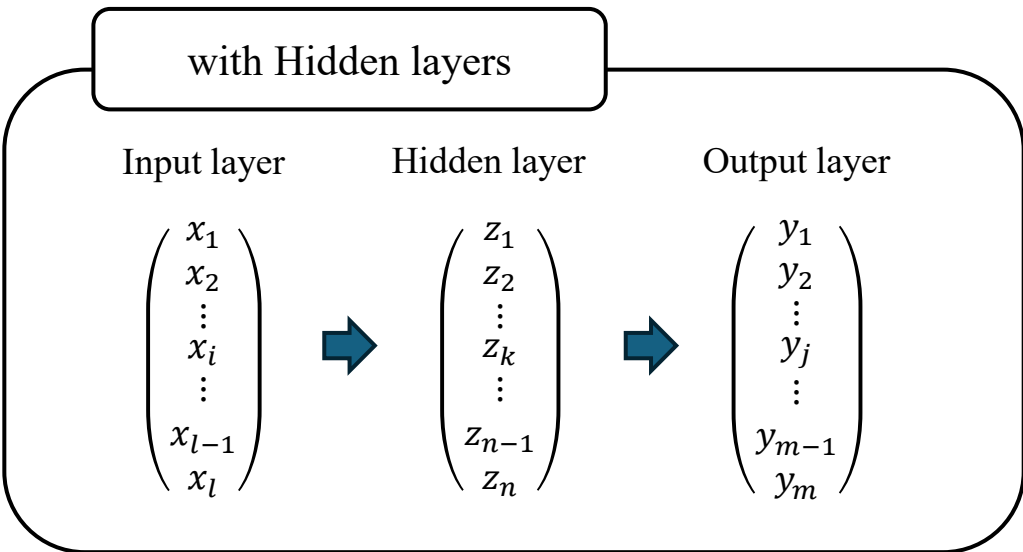


라면 좋아함?
치킨 좋아함?
맥주 좋아함?
...



E : cost function

Cost function이란, weights가 최적인지의 척도.
Minimize해야 함. 그 과정이 weight update



경사하강법
(gradient descent)

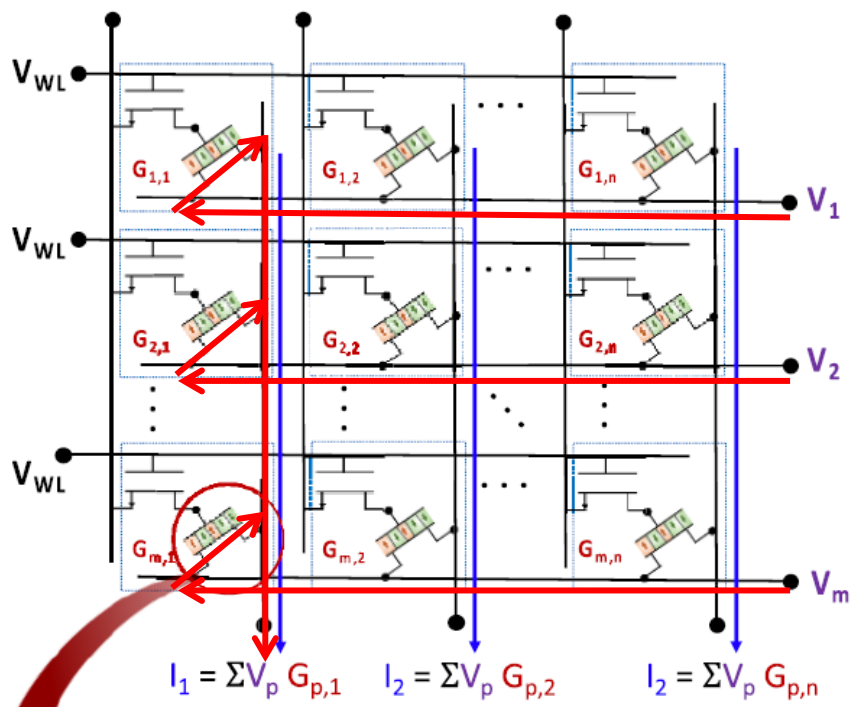
이 곳에
가고 싶다!!

$$\omega_{new} = \omega_{old} - \alpha \frac{\partial E}{\partial \omega}$$

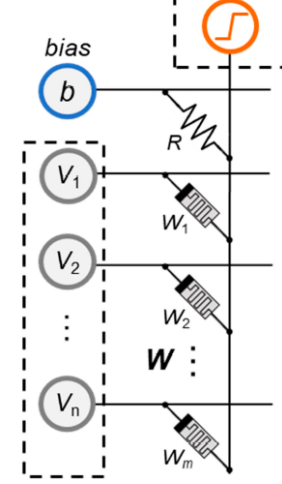
Introduction to Neuromorphic Computing: Crossbar array 구조로 perceptron 개념을 구현

$\omega \leftrightarrow G$

G : Conductance

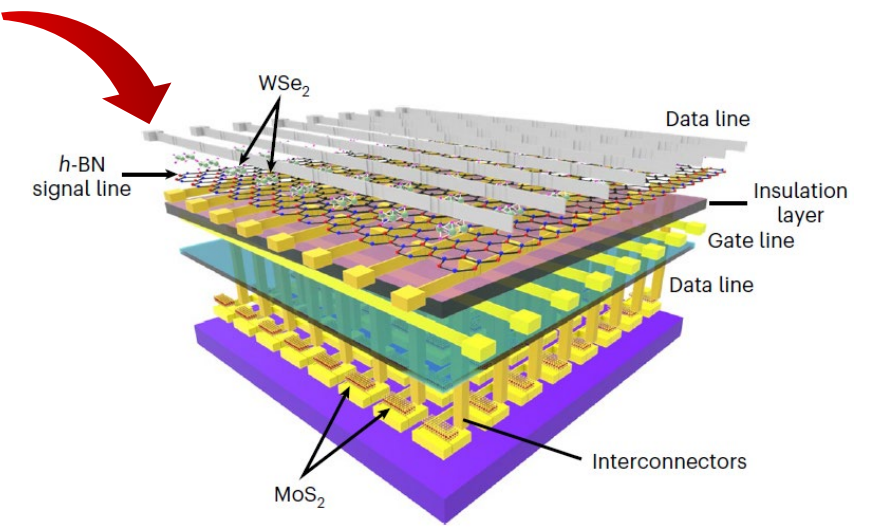


Output layer
 $y = f(\mathbf{V} \cdot \mathbf{W} + b)$



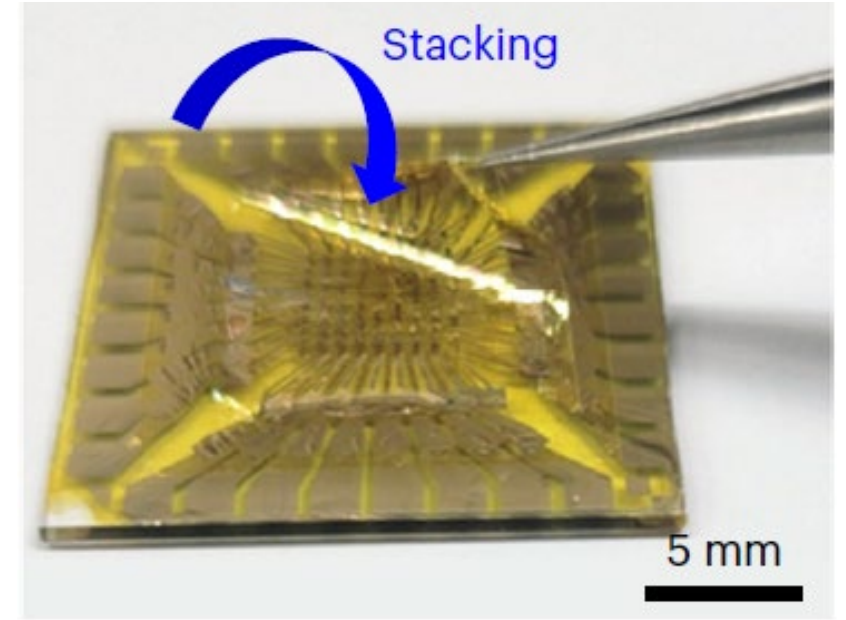
Input layer $N \times 1$ array
 $\mathbf{V} = [V_1 \ V_2 \ \dots \ V_n]$

Adv. Devices Instrum. 5, 0044 (2024)



Ferroelectric 10nm $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$

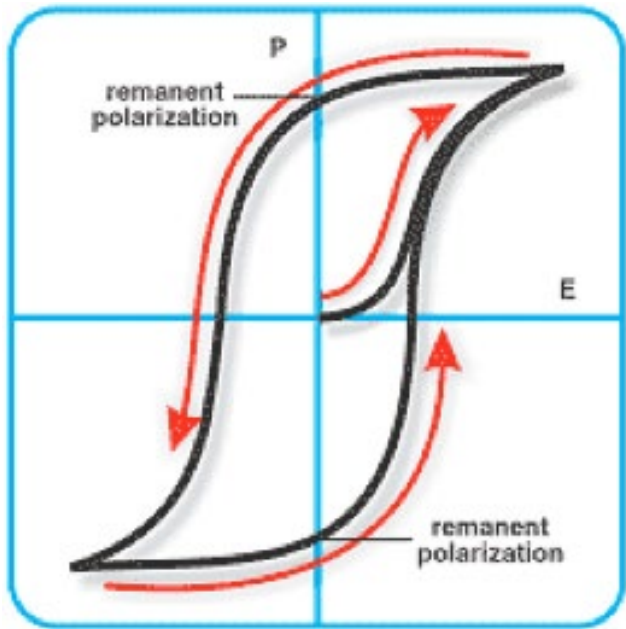
J. Phys. D: Appl. Phys. 51, 434001 (2018)



Nat. Mater. 22, 1470 (2023)

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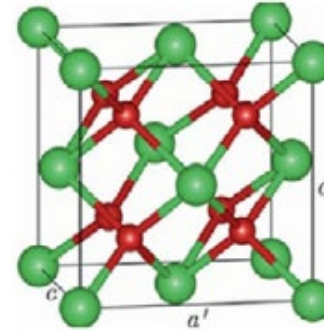
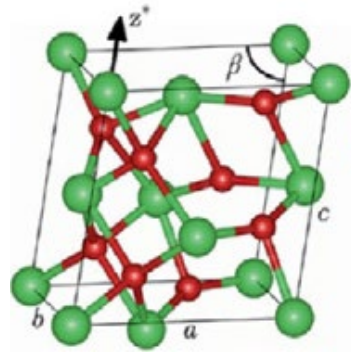
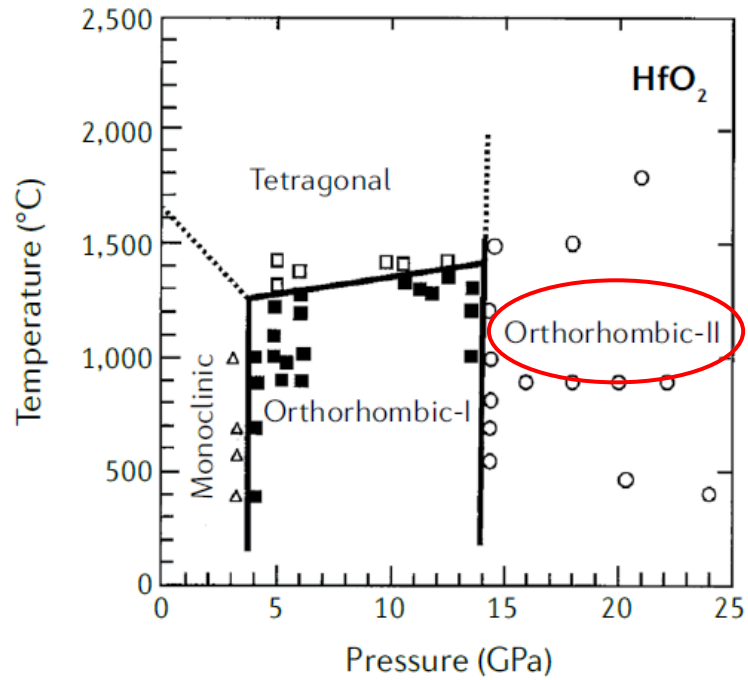
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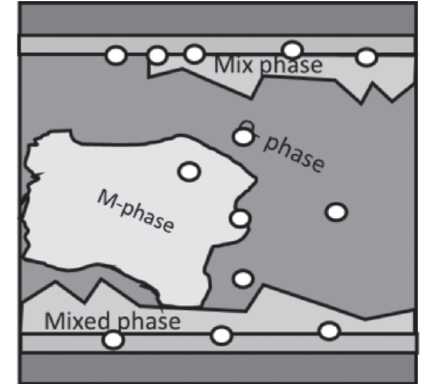
- IRDS (Int. Roadmap for Devices and Systems)에서 차세대 소자의 후보 물질로 매년 꼽힘
- 대표적으로 세 가지 구조로 연구되고 있음.
Capacitor, Ferroelectric-gated FET, Ferroelectric Tunnel Junction

유형	1T-1C type (FeRAM)	1T type (FeFET)	1R type (FTJ)
모식도			
셀 크기	15-34F ²	4-8 F ²	4-8 F ²
읽기	파괴적	비파괴적	비파괴적
Endurance	-10 ¹² 이상 -HfO ₂ 계열은 최대 10 ¹¹ 회	-10 ¹² 회 이상 -HfO ₂ 계열은 10 ⁵ 회 정도 -최근 10 ¹⁰ 회 결과 보고.	-HfO ₂ 계열은 최대 10 ⁷ 정도 보고
Retention	-10 년 -상대적으로 retention 우수	-10 년 (extrapolation) -Depolarization field 로 retention이 이슈	-10 년(extrapolation) -매우 얇은 두께로 retention 이슈 있음.

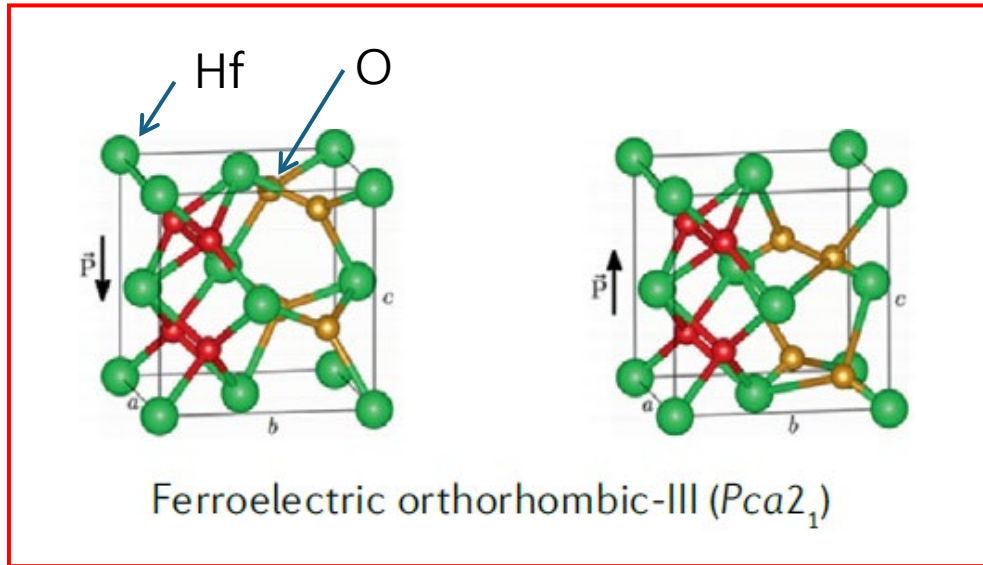
Ferroelectric hafnium oxide thin films는 흔히 polycrystalline structure로 만들어 진다.



<side view>

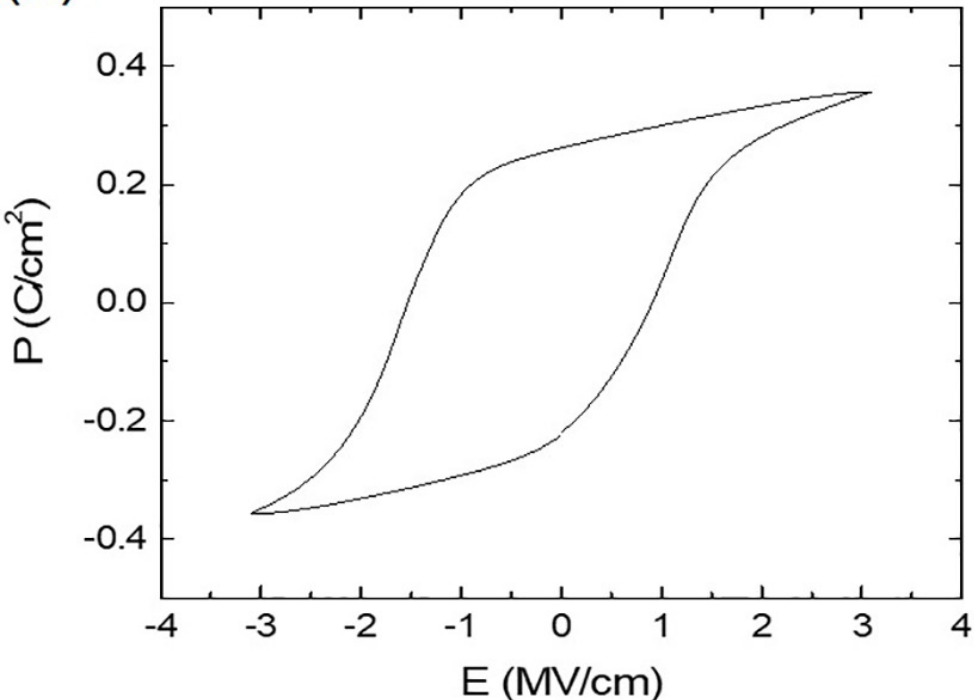


Adv. Funct. Mater. 26, 4601 (2016)



FE HfO₂는 본디 고압 phase인 O phase를 상압에서 구현한 것

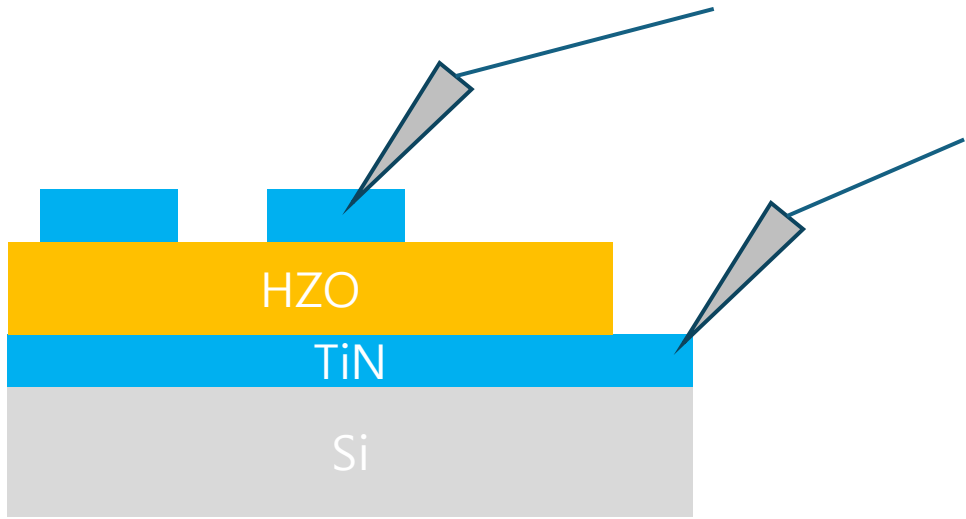
Ferroelectrics



TiN / Hf_{0.6}Zr_{0.4}O₂ / TiN thin film capacitor

Atomic Layer Deposition

두께 9.7 nm



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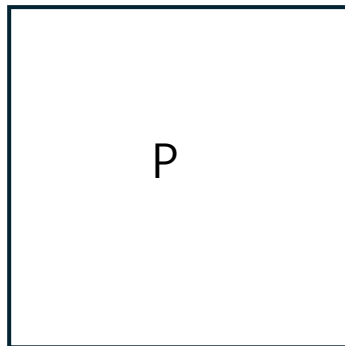
Landau theory

상전이 근처에서 free energy는 적절한 order parameter(여기선 polarization P)의 다항식으로 표현 가능하며, 그것을 통해 상전이와 임계현상을 탐구할 수 있다.

Ferroelectric free energy density

$$u = \alpha P^2 + \beta P^4 - E_{\text{eff}}P$$

<top view>



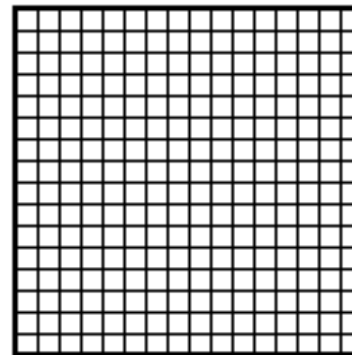
Landau-Ginzburg-Devonshire (LGD) theory

Local free energy density

$$u_l = \alpha P^2 + \beta P^4 - E_{\text{eff}}P + k(\vec{\nabla}P)^2$$

$$u = \int u_l(P, \vec{\nabla}P; \vec{r}) d^3r$$

<top view>



Ginzburg term.

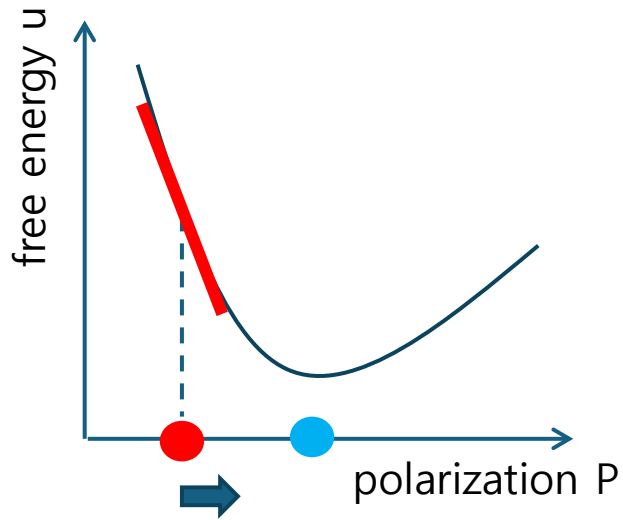
polarization의 spatial variation에 대한 energy penalty.
polarization이 up, down 들쭉날쭉한 상태를 싫어하게 됨.
어느 한 쪽으로 정렬된 polarization 상태가 안정적.

$u = \int u_l(P, \vec{\nabla}P; \vec{r}) d^3r$ 를 minimize하는 것은

역학에서 action $J = \int L(x_j, \dot{x}_j, t) dt$ 을 minimize하는 것과 비슷함.

Dynamics의 식, Landau-Khalatnikov 방정식

$$-\frac{\partial u}{\partial P} = \rho \frac{\partial P}{\partial t}$$



현재 ● \Rightarrow 최종적으로 ● 로 가면 equilibrium

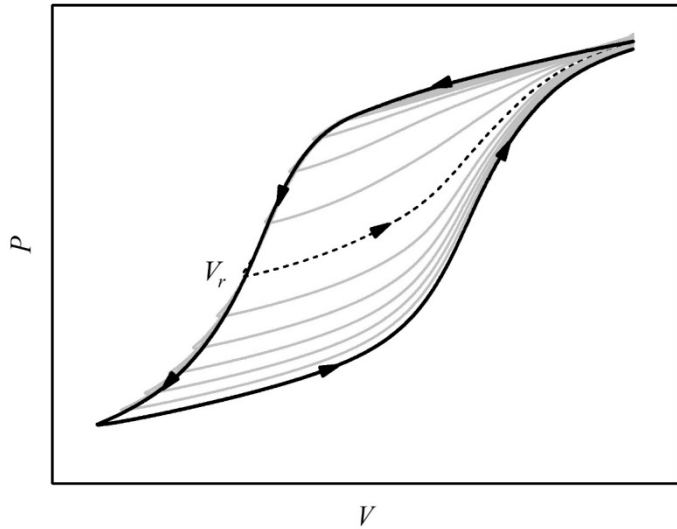
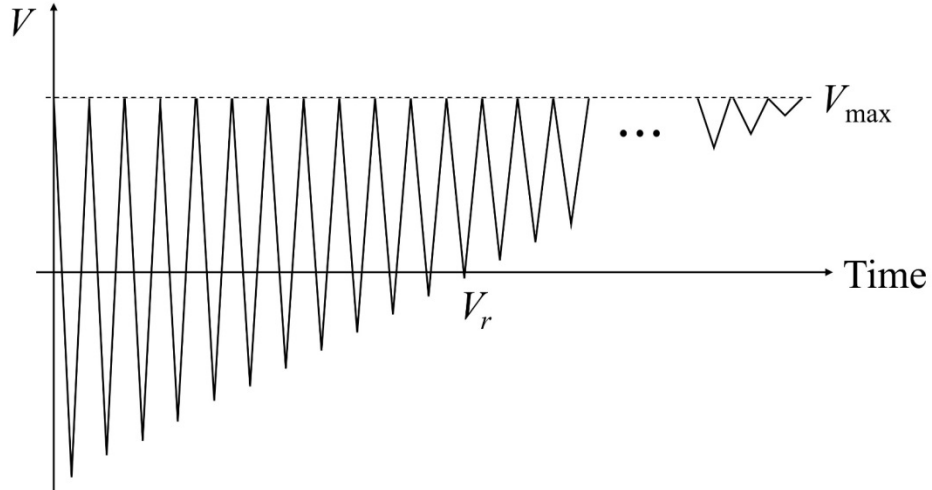
기울기 $\frac{\partial u}{\partial P} < 0$ 인 상황.

그러면 시간에 따라 P 는 어떻게 변해야 하는가?

$\Rightarrow -\frac{\partial u}{\partial P} = \rho \frac{\partial P}{\partial t}$ 에 따라 $\frac{\partial P}{\partial t} > 0$ 가 되도록 한다.

기울기가 클 때는 빨리빨리 변하고,
 종착점에 가까워져서 기울기가 작아지면 천천히 변한다.

First order reversal curves method



Switching density

$$\rho_{sw} = -\frac{1}{2} \frac{\partial^2 P(V, V_r)}{\partial V \partial V_r}$$

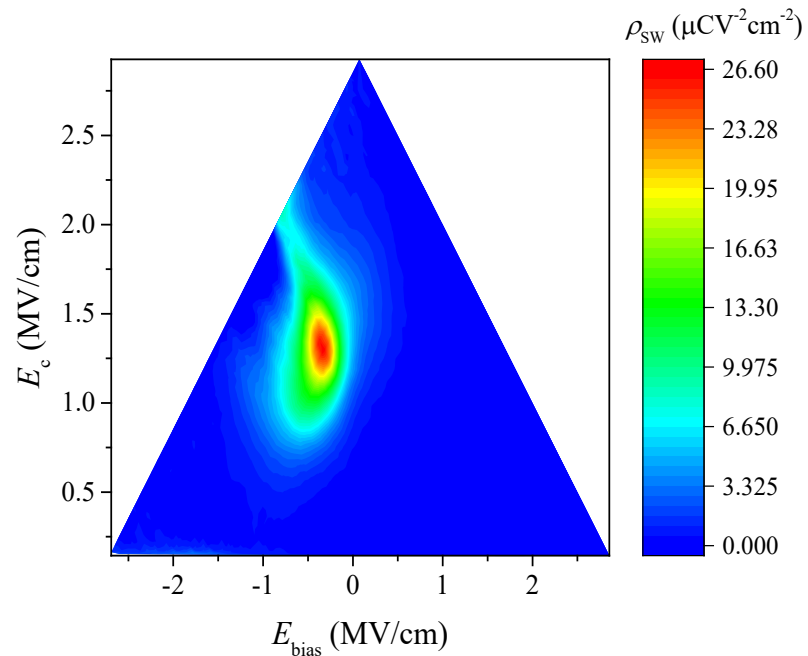
Coordinate transformation

$$E_{bias} = \frac{V + V_r}{2t_F}$$

(bias field)

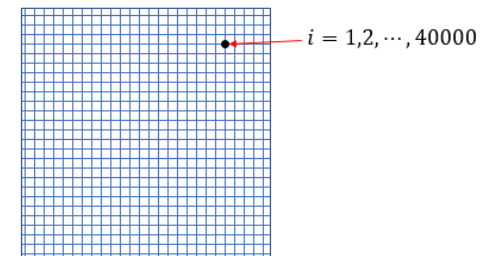
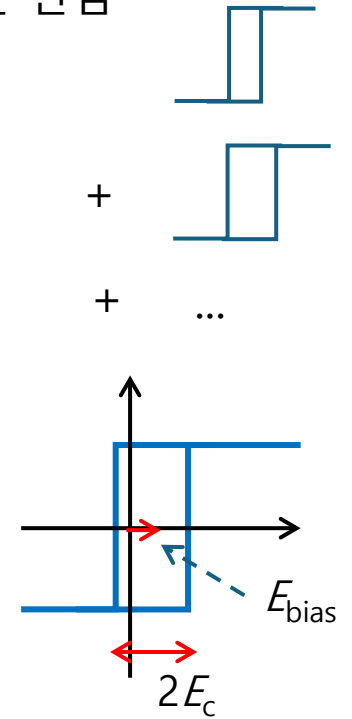
$$E_c = \frac{V - V_r}{2t_F}$$

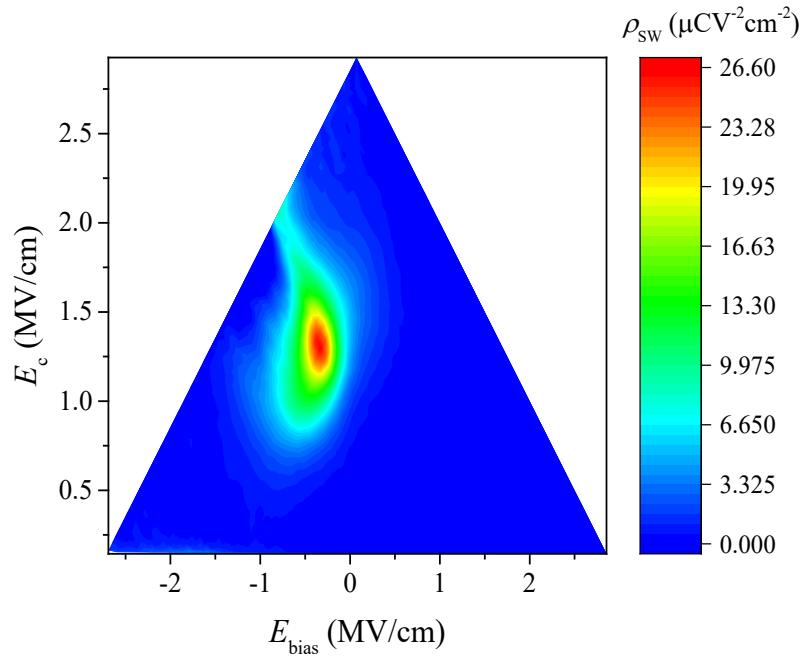
(coercive field)



Ferromagnetic의 Preisach model 응용.

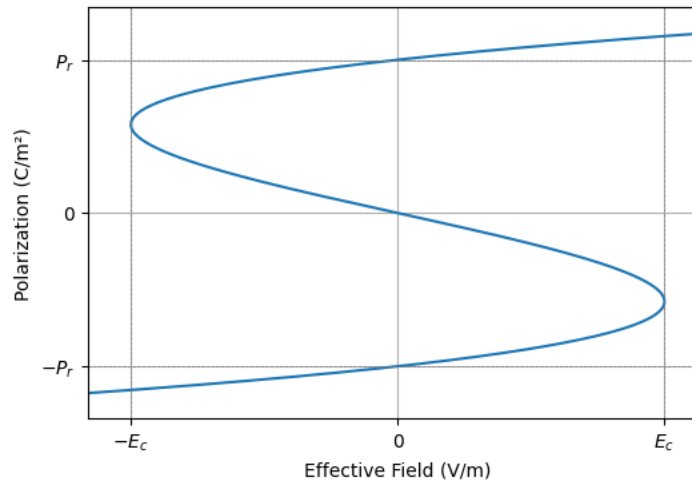
다양한 E_c , E_{bias} 를 가진 작은 hysteresis loop들의 총합으로 보는 관점





$$\frac{\partial u}{\partial P} = 2\alpha P + 4\beta P^3 - E_{\text{eff}} = 0$$

$$E_{\text{eff}} = 2\alpha P + 4\beta P^3$$



$$(0, P_r) \quad (0, 0) \quad (0, -P_r)$$

$$\frac{\partial E_{\text{eff}}}{\partial P} = 0 \quad (\text{when } E_{\text{eff}} = \pm E_c)$$

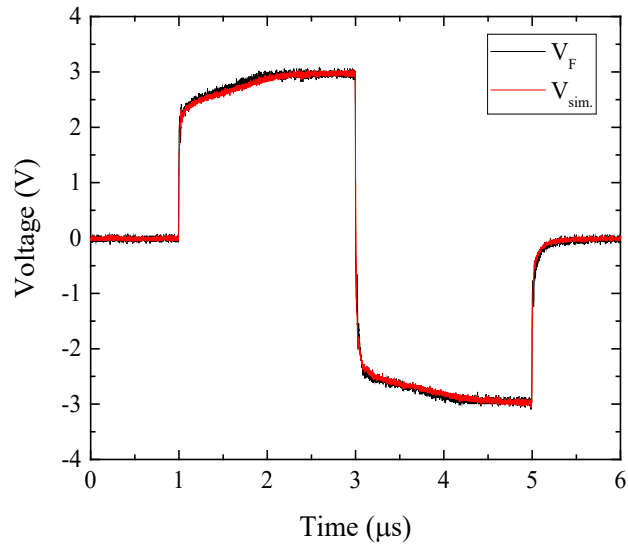
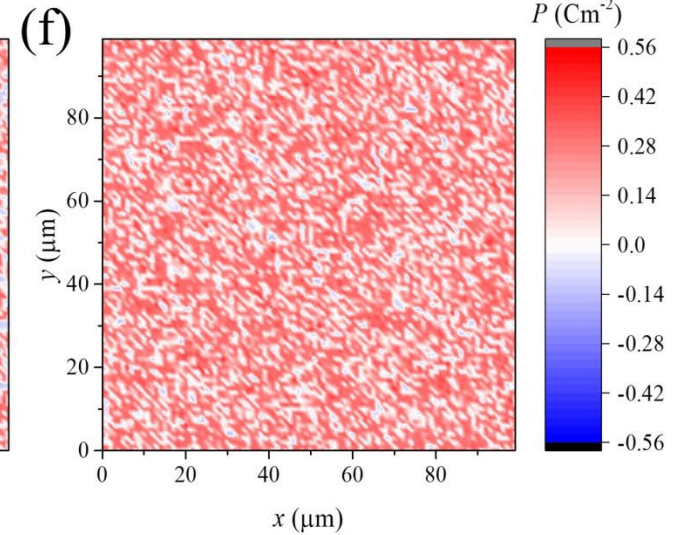
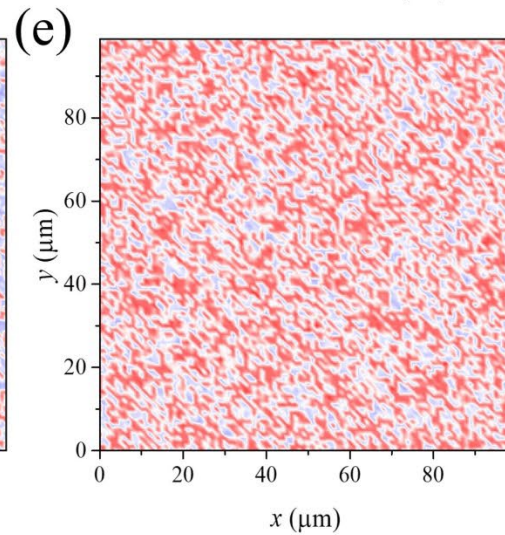
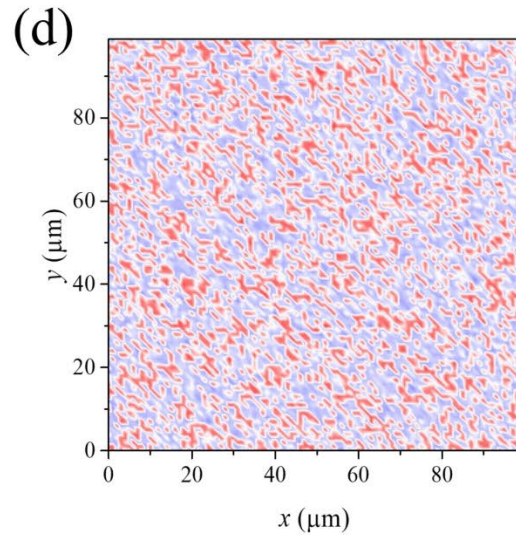
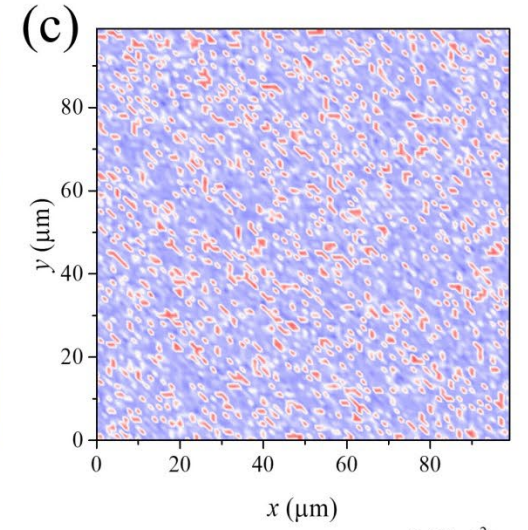
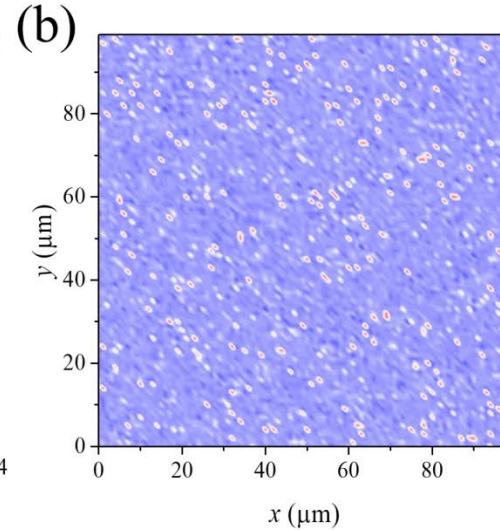
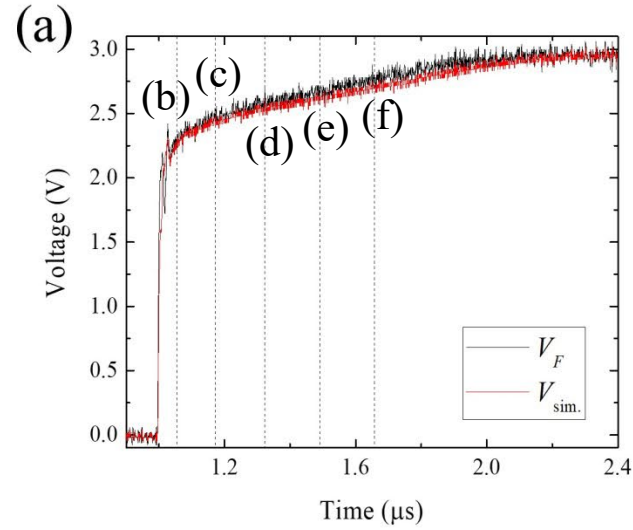
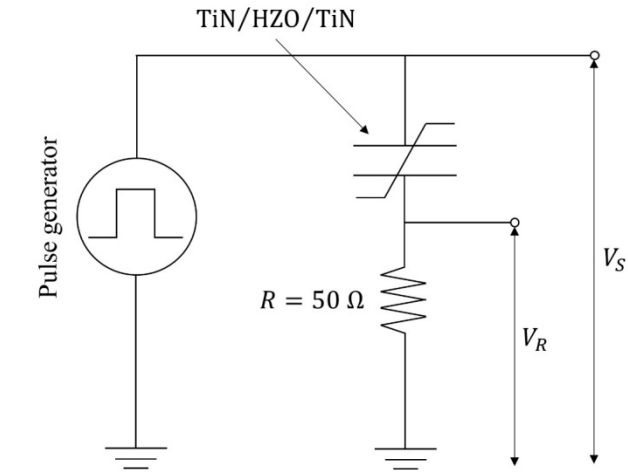
$$u_i = \alpha_i P_i^2 + \beta_i P_i^4 - E_{\text{eff},i} P + k(\nabla P_i)^2$$

$$E_{\text{eff},i} = \frac{V_F}{t_F} - E_{\text{bias},i}$$

$$\alpha_i = -\frac{3\sqrt{3}E_{c,i}}{4P_r} \quad \beta_i = \frac{3\sqrt{3}E_{c,i}}{8P_r^3}$$

Polarization Switching Dynamics Simulation

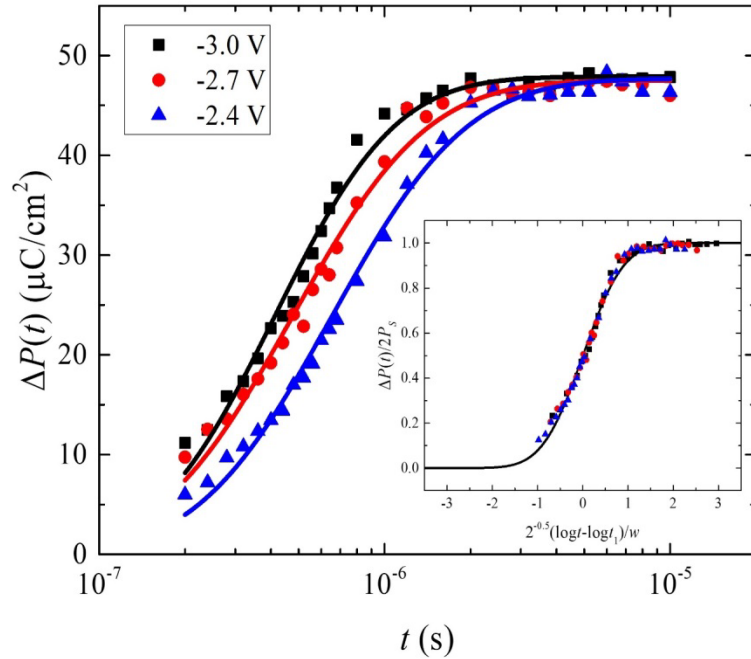
(1) b,c,d,e,f의 simulation을 하고, (2) 그로부터 a를 얻음.



Nucleation-limited-switching model

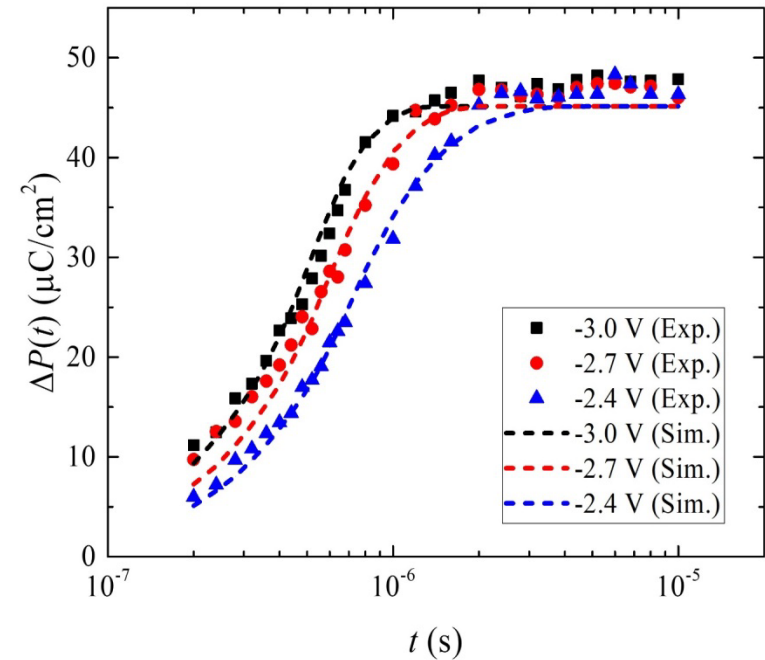
$$\Delta P(t) = 2P_S \int_{-\infty}^{\infty} [1 - \exp\{-(t/t_0)^n\}] F(\log t_0) d(\log t_0)$$

$$= P_S \left(1 + \operatorname{erf} \frac{\log t_0 - \log t_1}{w\sqrt{2}} \right)$$

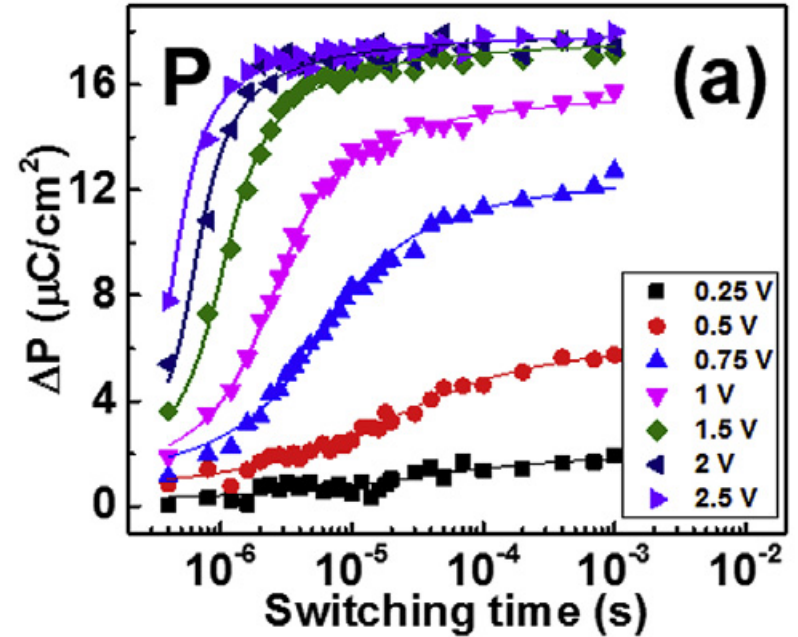
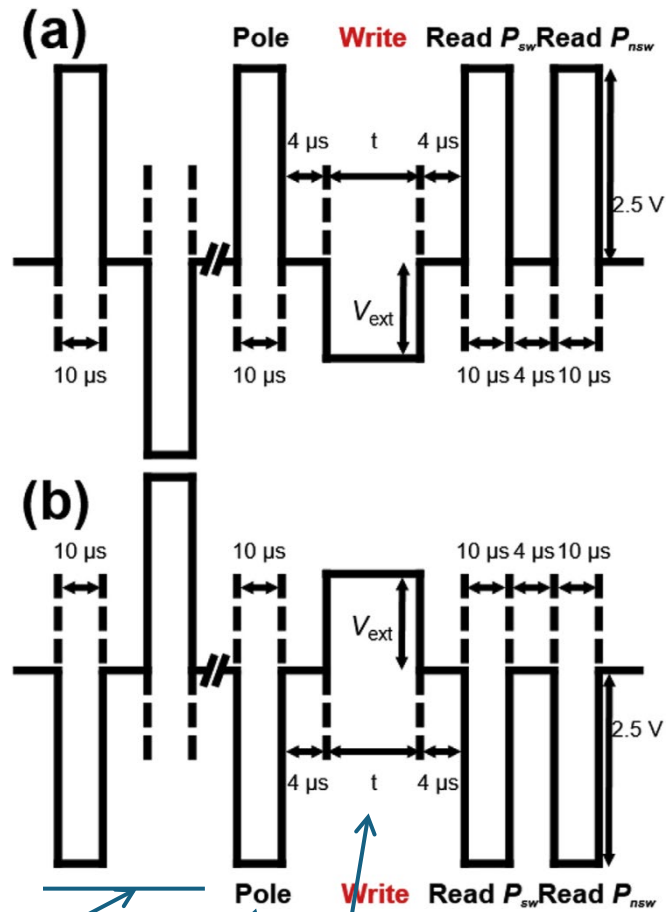
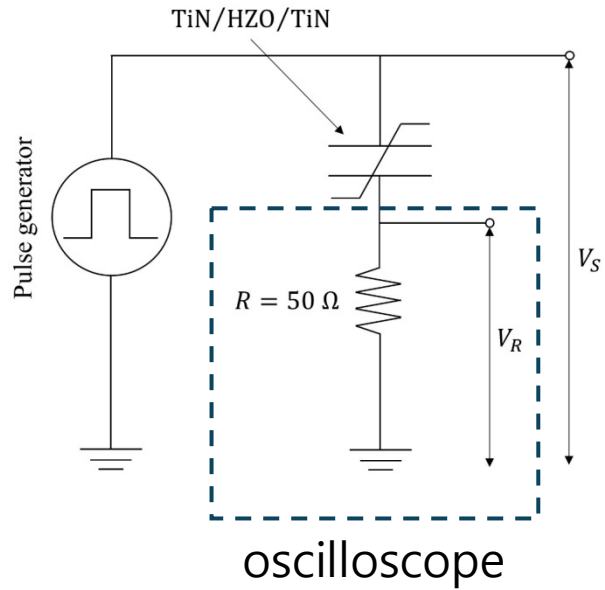


Polarization switching current i_{sw} measured using a reading voltage pulse.

$$\int i_{sw}(t') dt'$$



Polarization obtained by the average of P in the simulated P map.



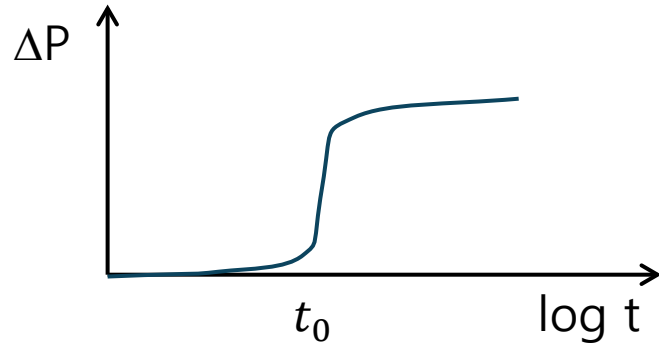
(1) 이전의 분극 상태가 각인되지 않도록 up/down 몇 번 흔들어줌

(2) 한 쪽으로 분극 정렬해서 기준 상태 만듦

(3) 반대 방향으로 펄스 걸어서 스위칭 시킴. 다음번 반복할 때 voltage 또는 펄스폭을 바꾸며 다양하게 측정

(4) 3번 단계에서 얼마만큼의 분극 스위칭이 이루어졌는지 측정

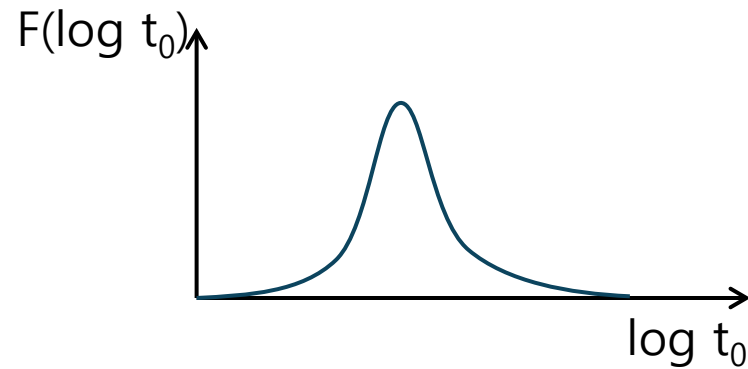
(5) 4번 단계 중 non-ferroelectric한 성분을 빼주기 위한 측정



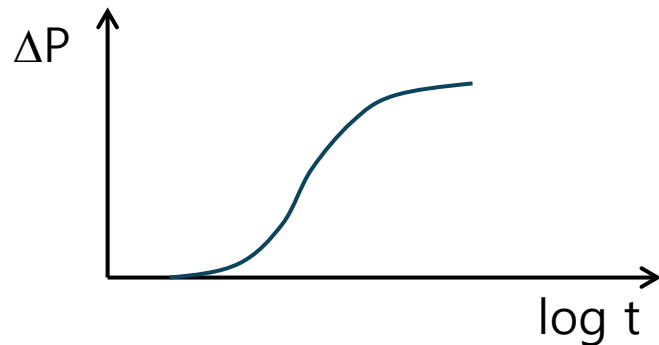
KAI 이론 (Kolmogorov-Avrami-Ishibashi)

: single crystal의 경우, 잘 정의된 characteristic time t_0 를 중심으로, stretched exponential처럼 polarization switching함.

$$\Delta P(t) = 2P_S [1 - \exp\{-(t/t_0)^n\}]$$



그런데, polycrystal이거나 disordered ferroelectric의 경우, t_0 자체가 꽤 분포를 가짐.



Nucleation-limited-switching model

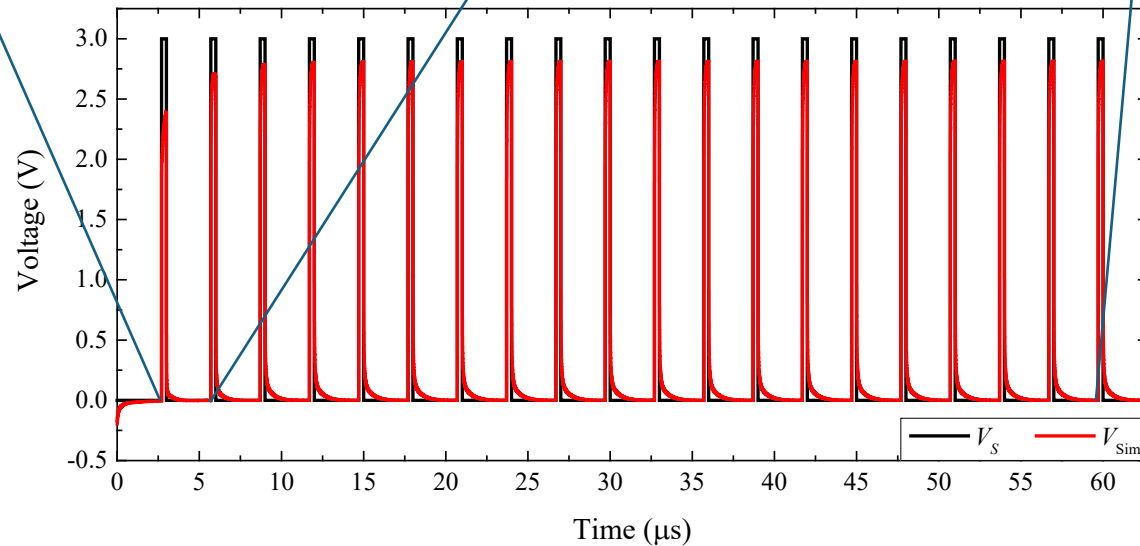
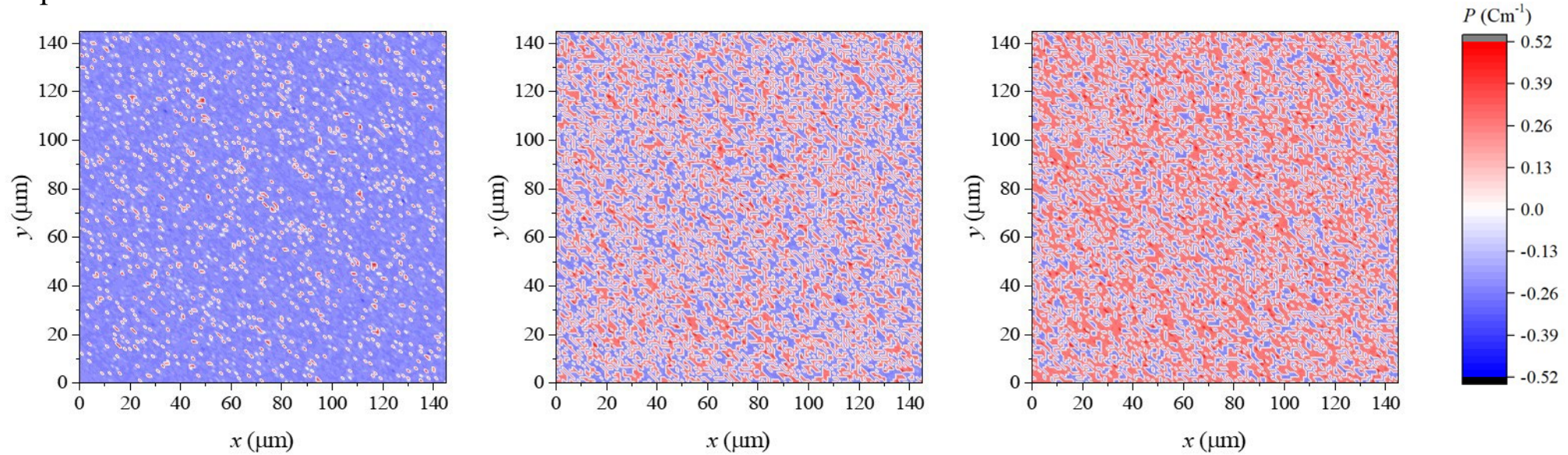
: KAI이론의 ferroelectric domain 성장보다는 nucleation time t_0 의 분포에 의해 polarization switching이 결정됨.

$$\Delta P(t) = 2P_S \int_{-\infty}^{\infty} [1 - \exp\{-(t/t_0)^n\}] F(\log t_0) d(\log t_0)$$

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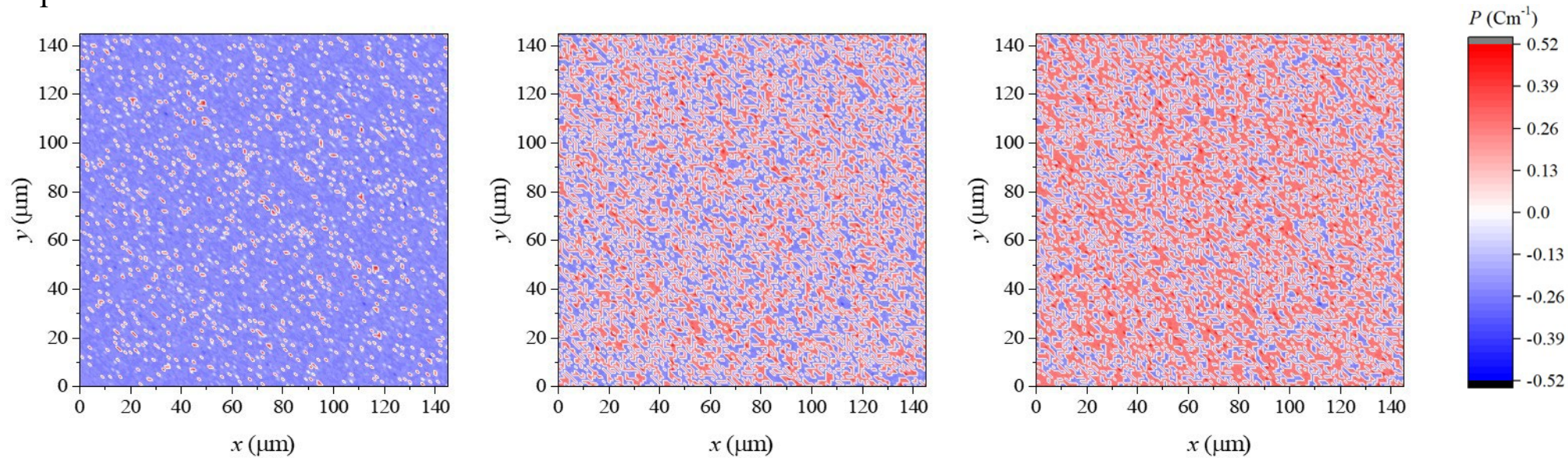
Polarization map of the ferroelectric film



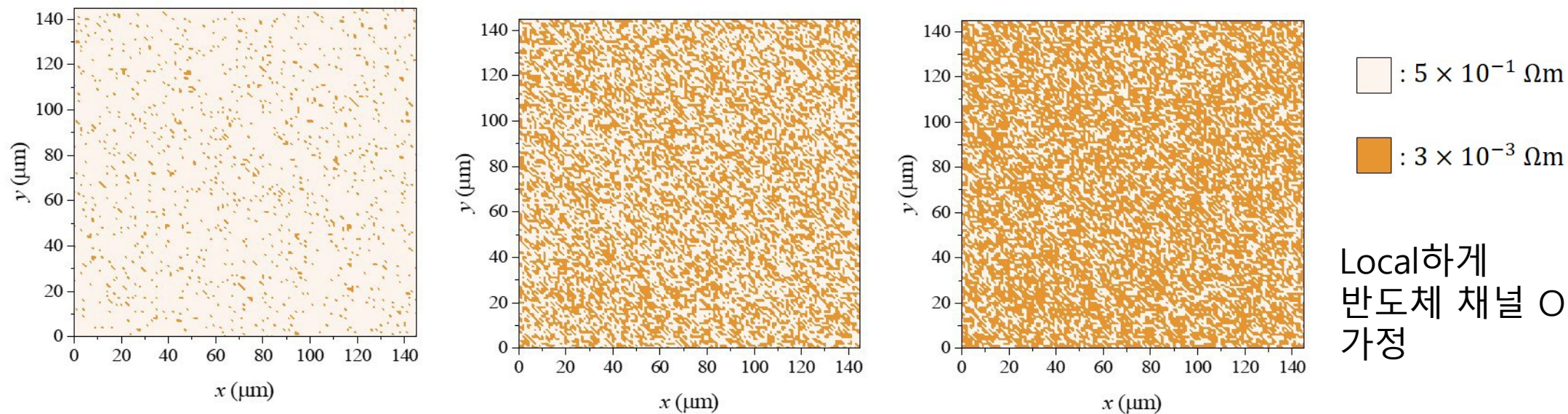
Constant voltage 하에서
시간에 따른 스위칭 말고.

이젠
Pulse 개수에 따른 스위칭.

Polarization map of the ferroelectric film



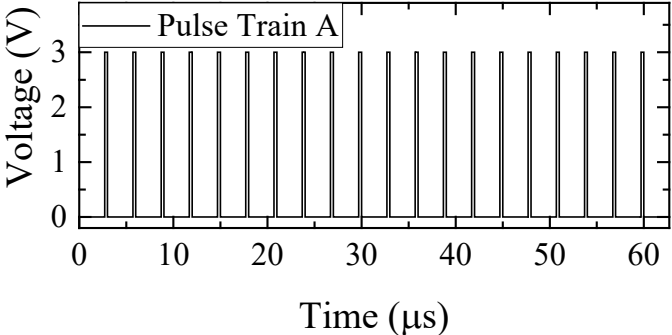
Resistivity map of the channel layer



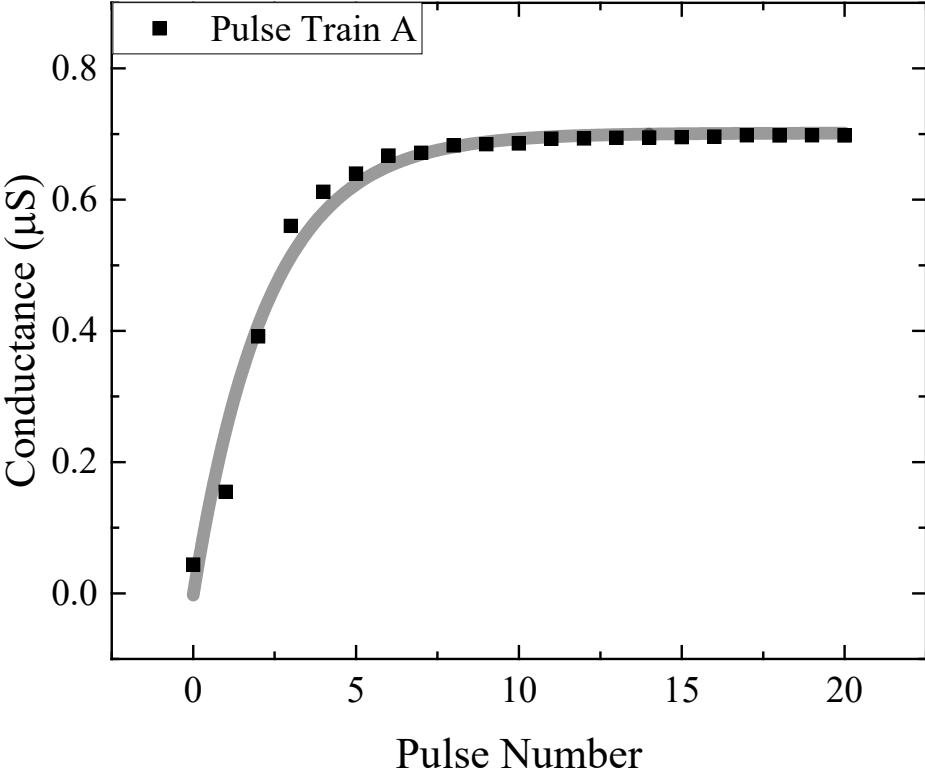
Local하게
반도체 채널 ON!
가정

Conductance Modulation of Neuromorphic Computing

In the potentiation,



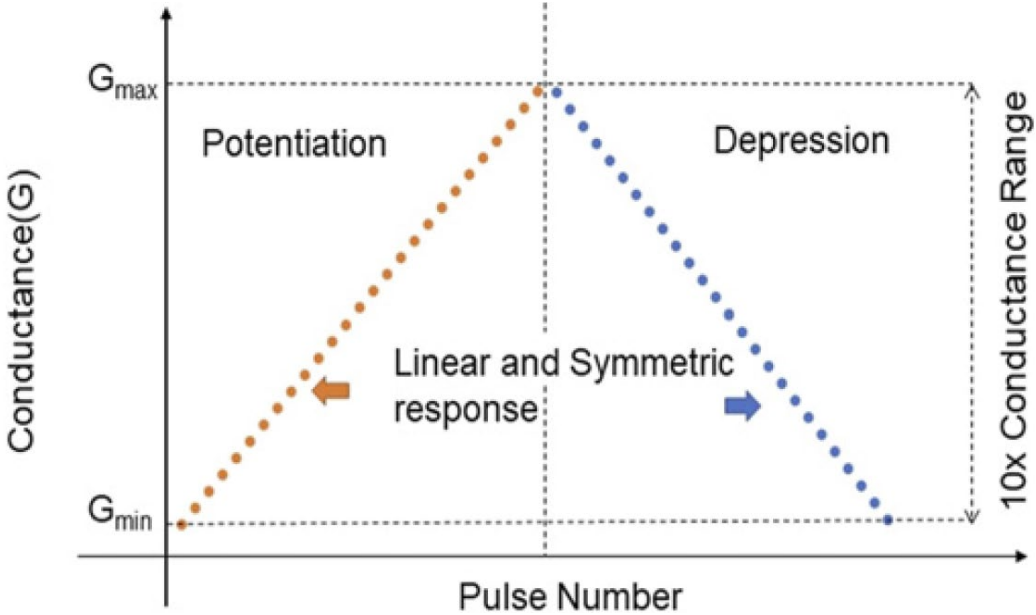
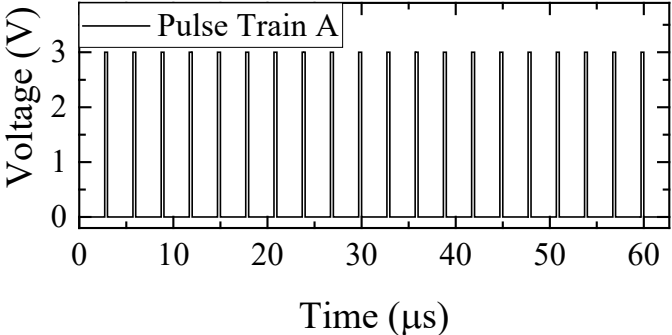
Conductance of the channel layer



Number of Conductance state ↓

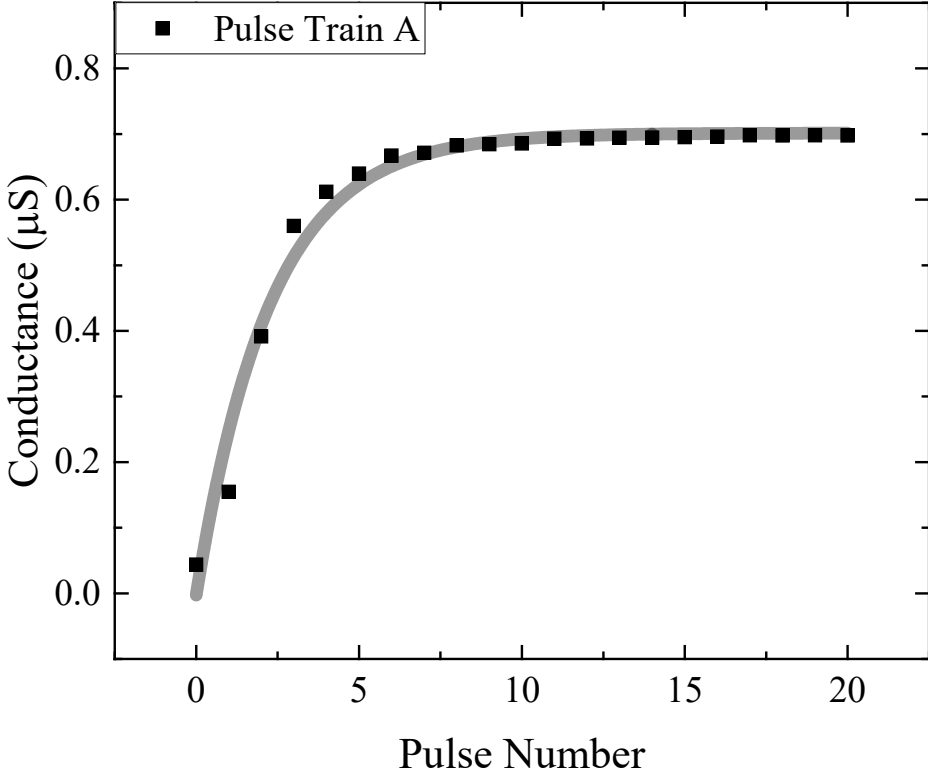
Conductance Modulation of Neuromorphic Computing

In the potentiation,



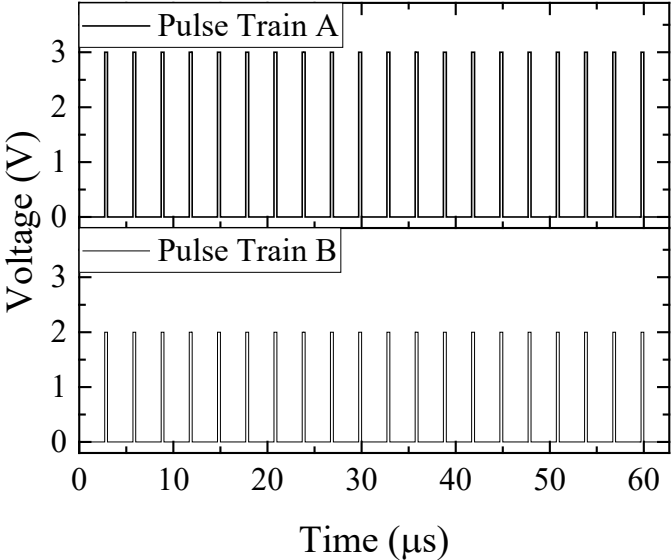
Neuromorph. Comput. Eng. 2, 021002 (2022)

Conductance of the channel layer

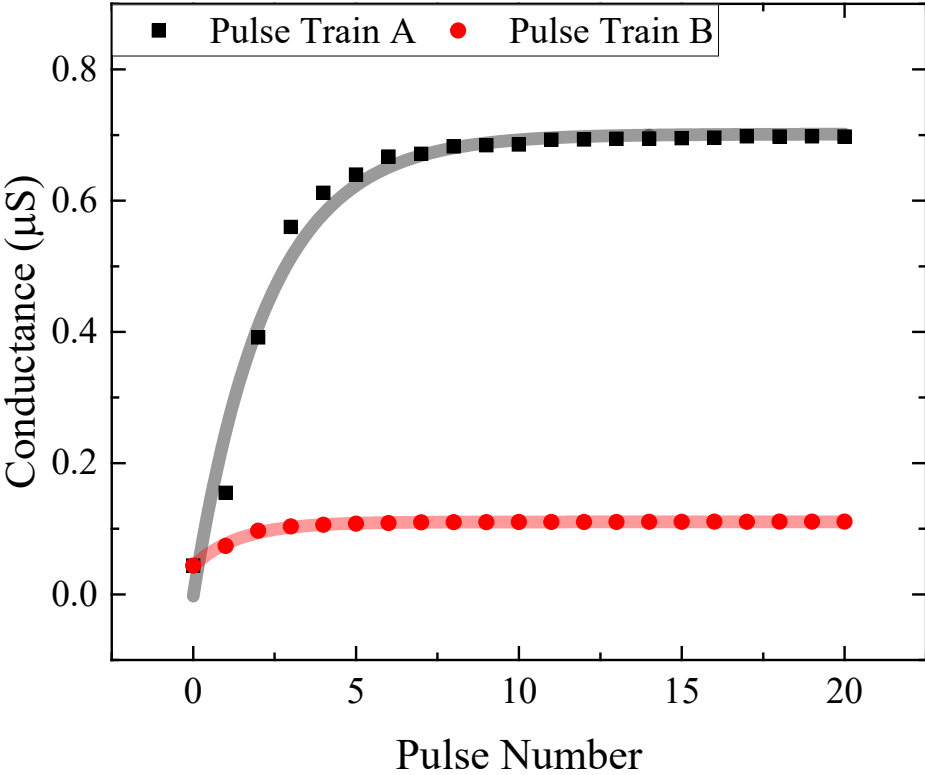


Number of Conductance state ↓

In the potentiation,



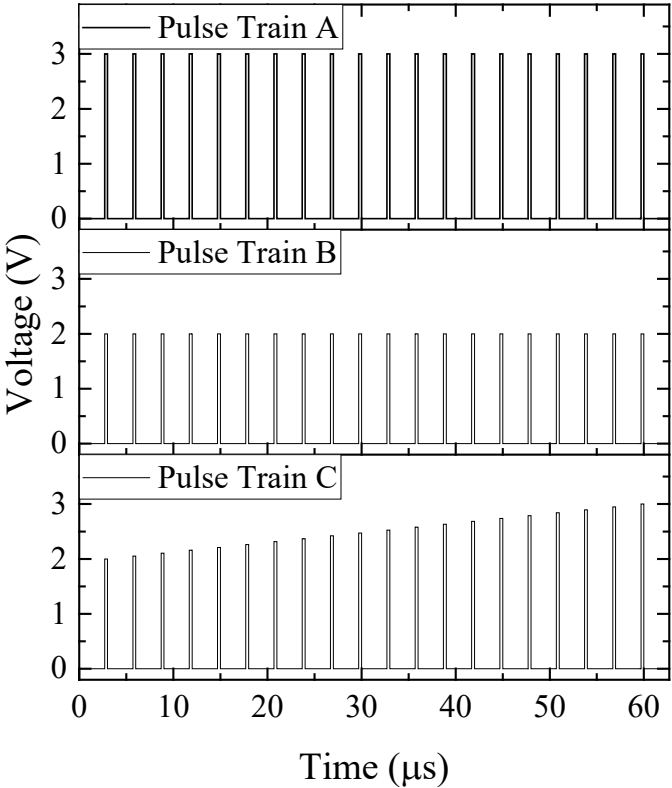
Conductance of the channel layer



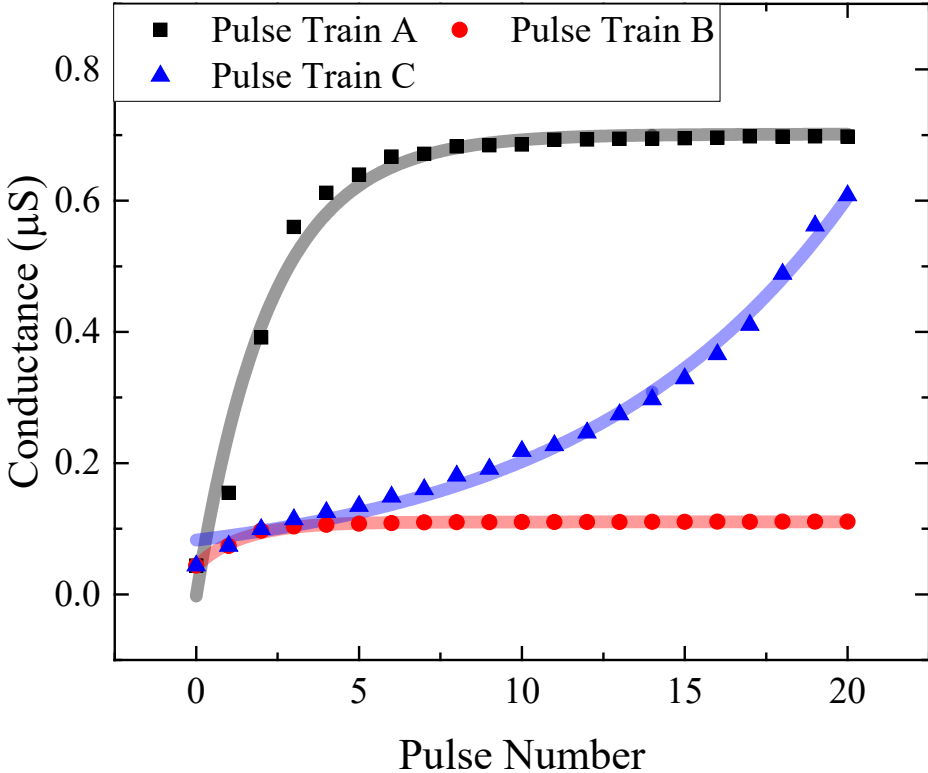
The conductance did not increase significantly.

Conductance Modulation of Neuromorphic Computing

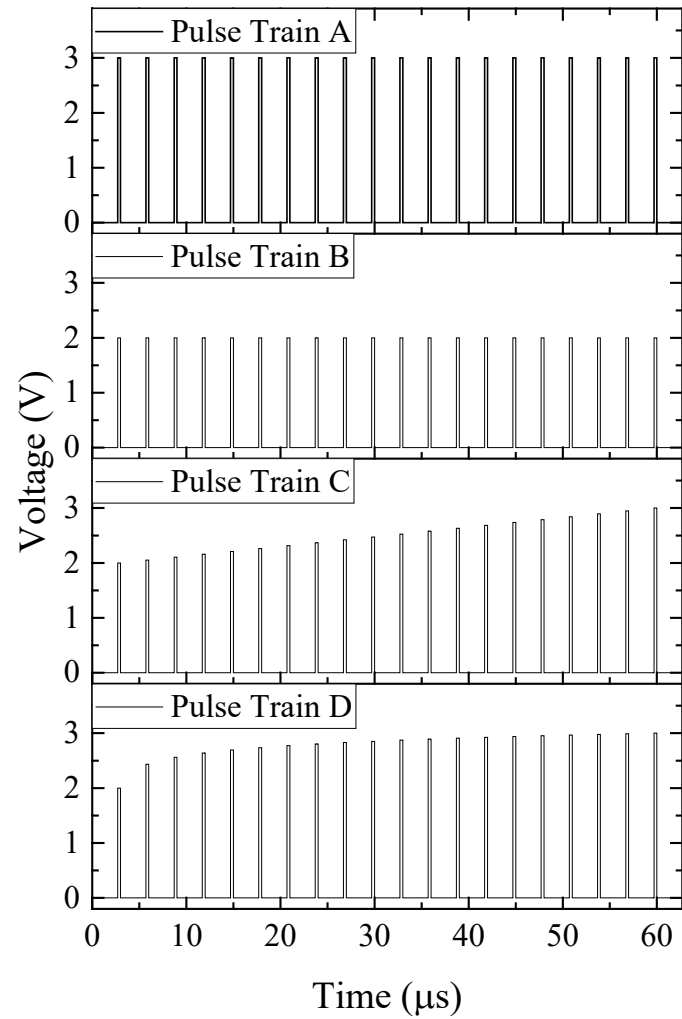
In the potentiation,



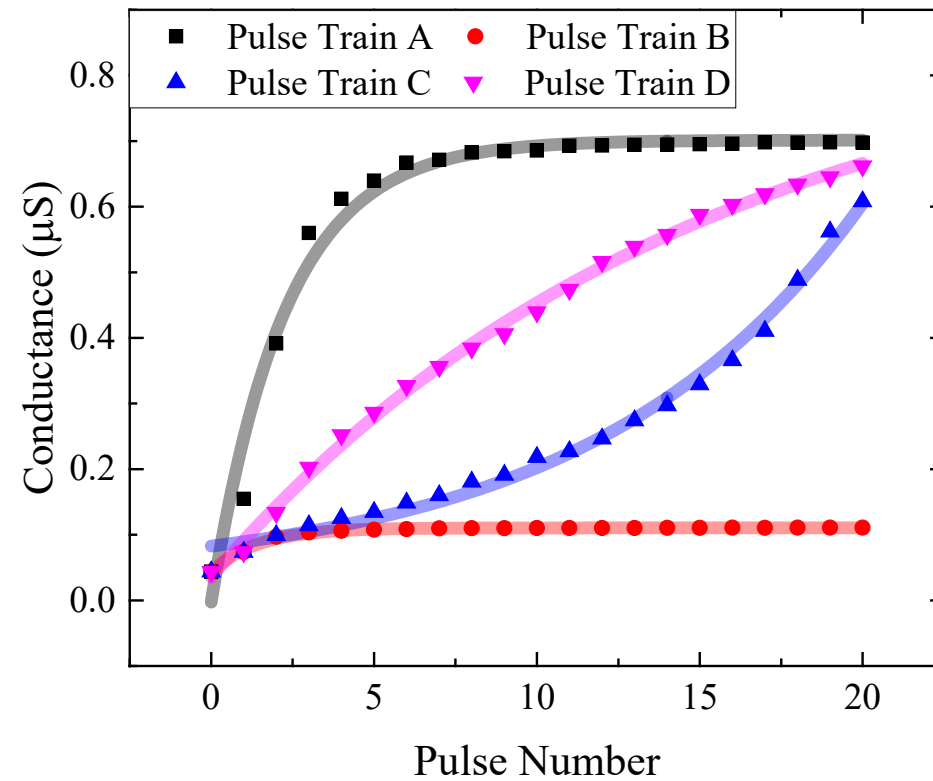
Conductance of the channel layer



In the potentiation,



Conductance of the channel layer



We employed the log function.

$$V(n) = \xi \log((t_0 + t_V)(n - 1) + B) + C$$

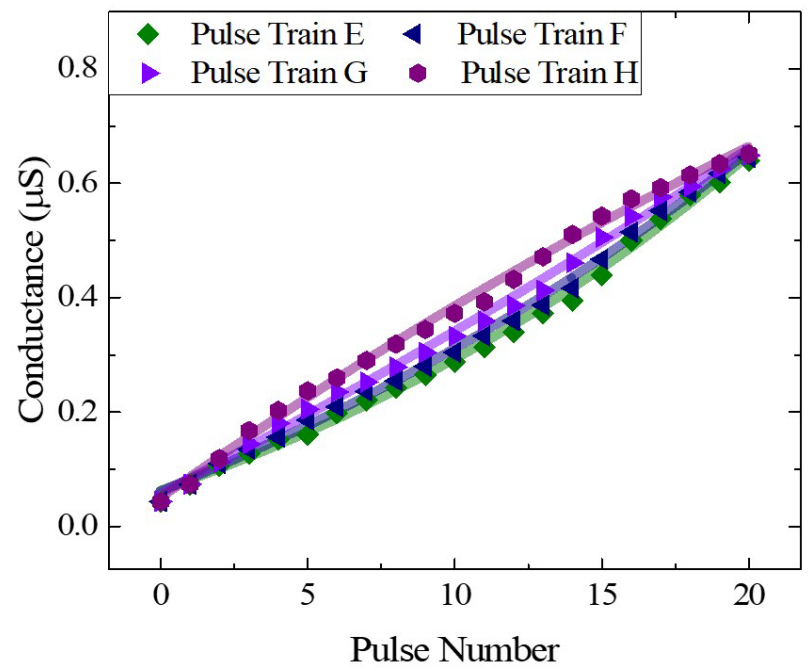
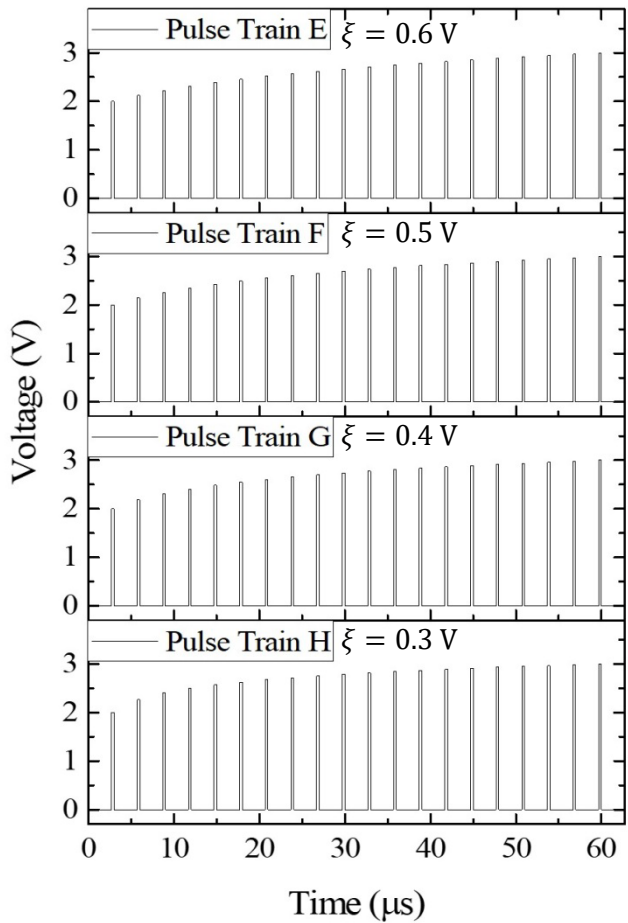
The linearity for pulse train G is better than others.

$$V(n) = \xi \log((t_0 + t_V)(n - 1) + B) + C$$

$$\xi = 0.2 \sim 0.6 \text{ V}$$

$$G(n) = D_0 \left\{ 1 - \exp\left(-\frac{2n}{n_{\max} A_p}\right) \right\} + G_{\min}$$

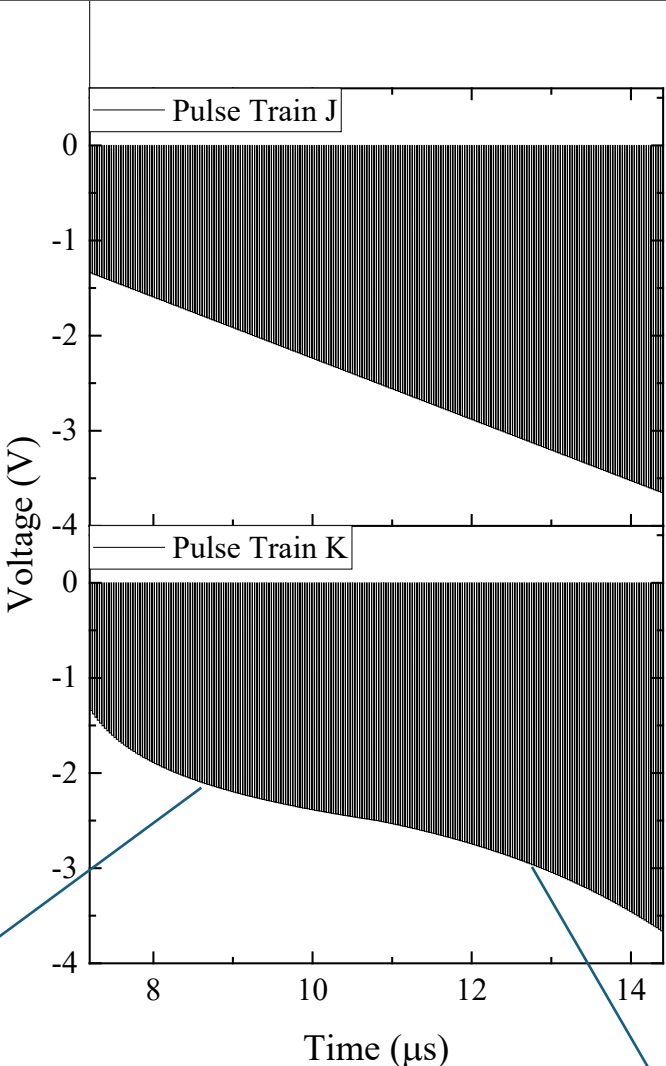
$$D_0 = (G_{\max} - G_{\min}) / \left\{ 1 - \exp\left(-\frac{1}{A_p}\right) \right\}$$



Pulse Train	Linearity $ A_{\text{pot}} $
A	0.11
B	0.07
C	0.41
D	0.74
E	1.14
F	1.54
G	4.25
H	2.71

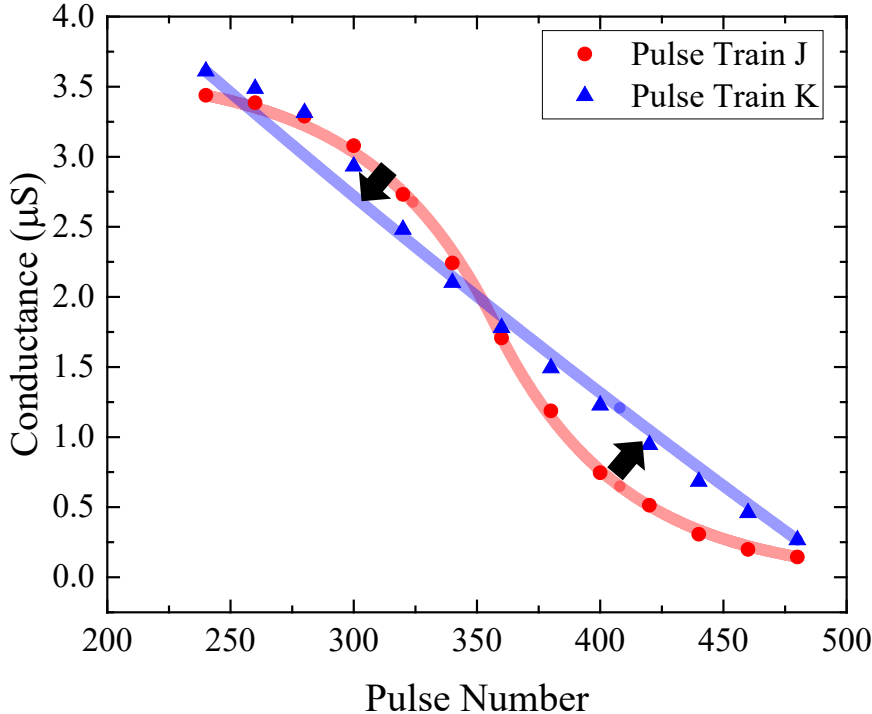
Conductance Modulation of Neuromorphic Computing

In the depression,

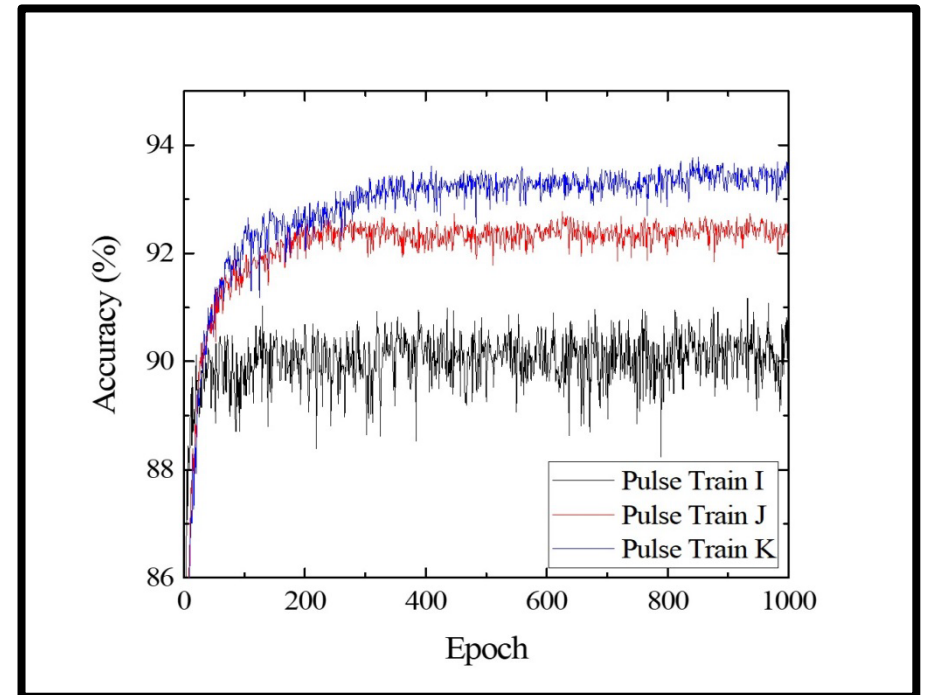
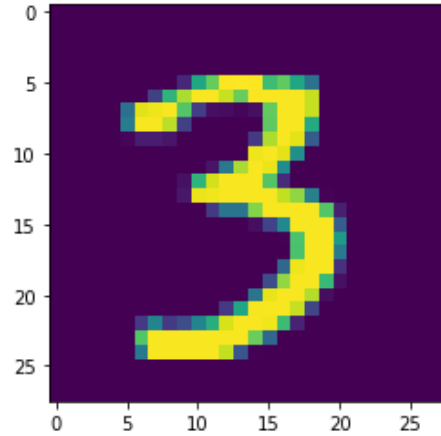
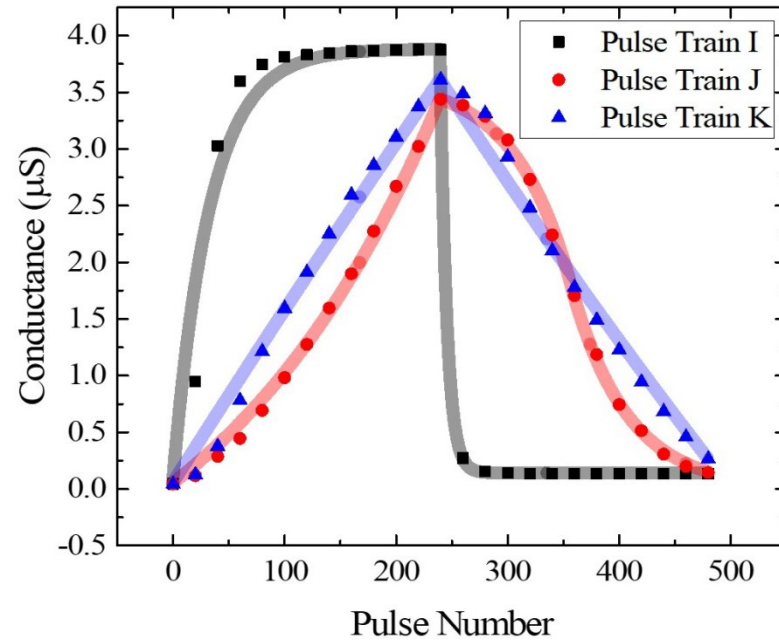
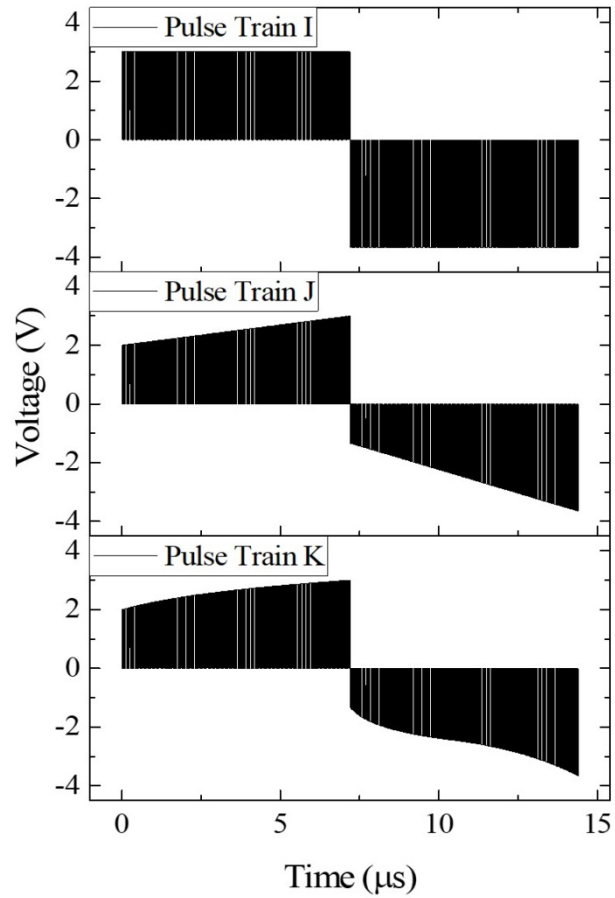


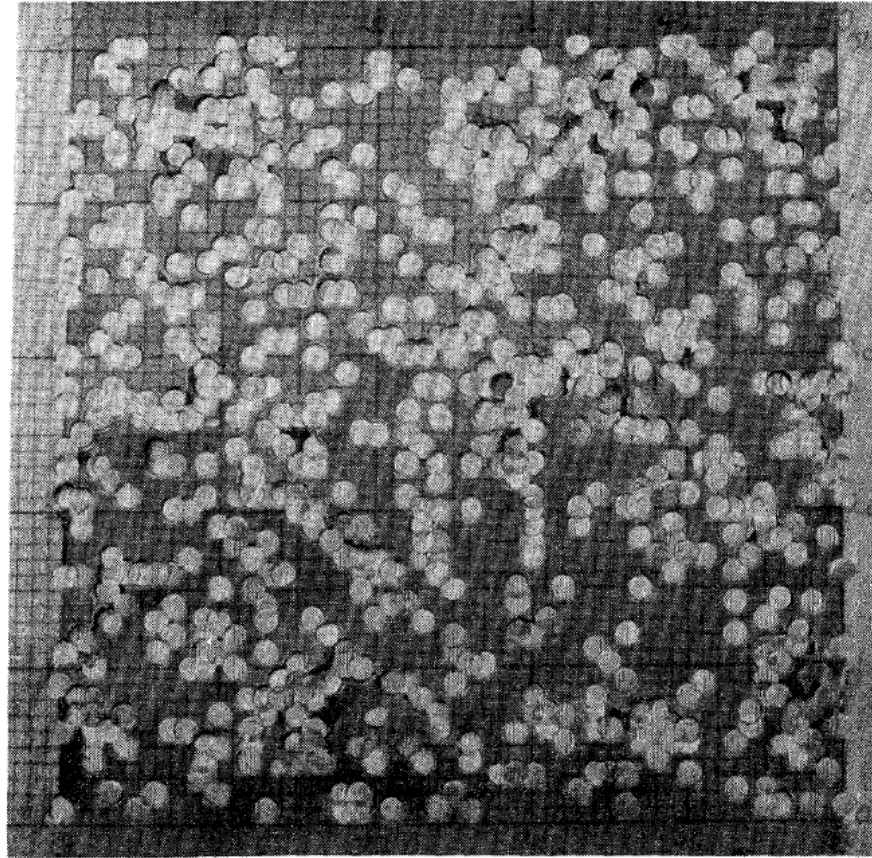
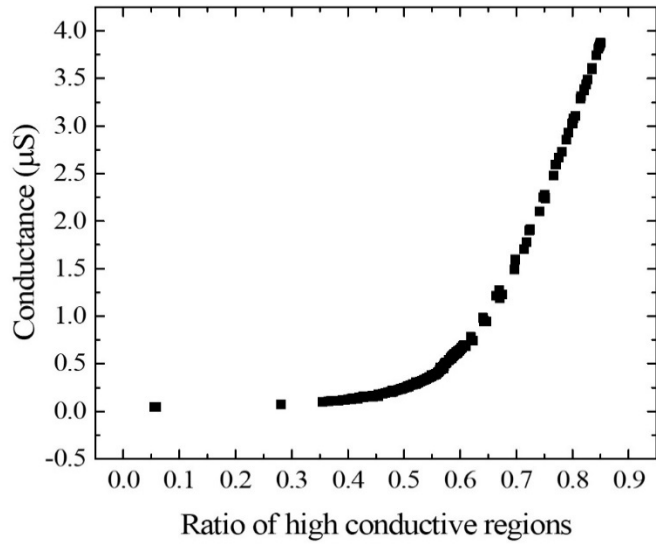
$$V(n) = -\xi_1 \log((t_0 + t_V)(n - 1) + B_1) + C_1$$

$$V(n) = -\exp\left(\frac{(t_0 + t_V)(n - 1) + B_2}{\xi_2}\right) - C_2$$

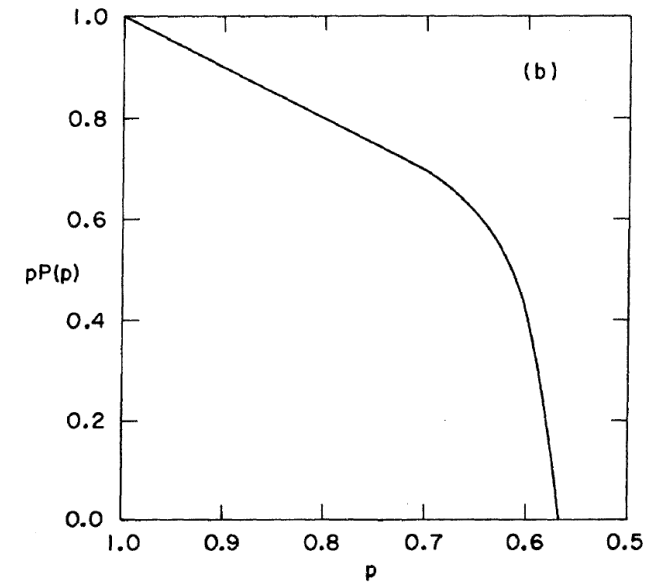
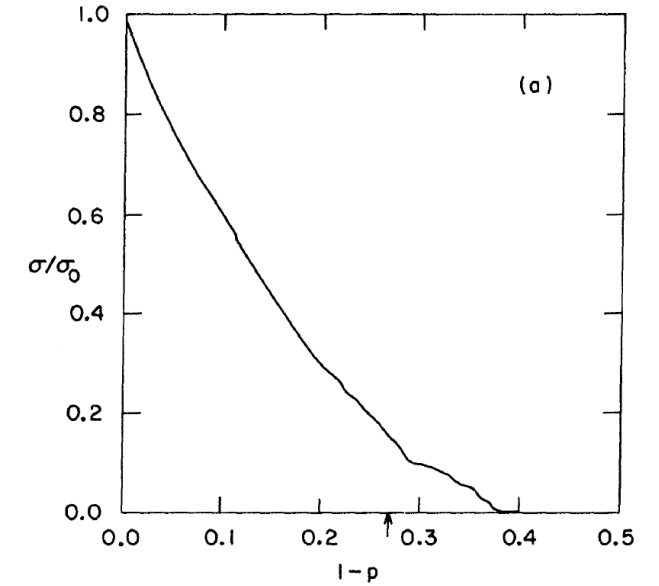


MNIST 손글씨 data 인식의 learning accuracy 계산 by NeuroSim.





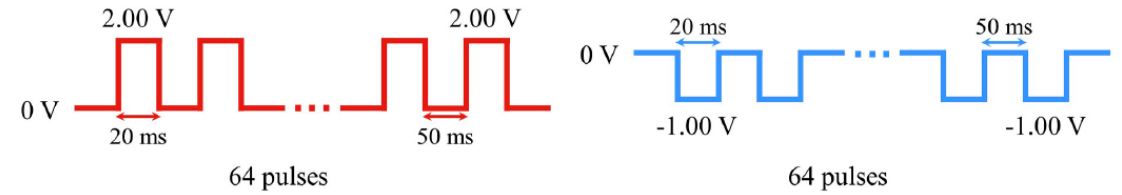
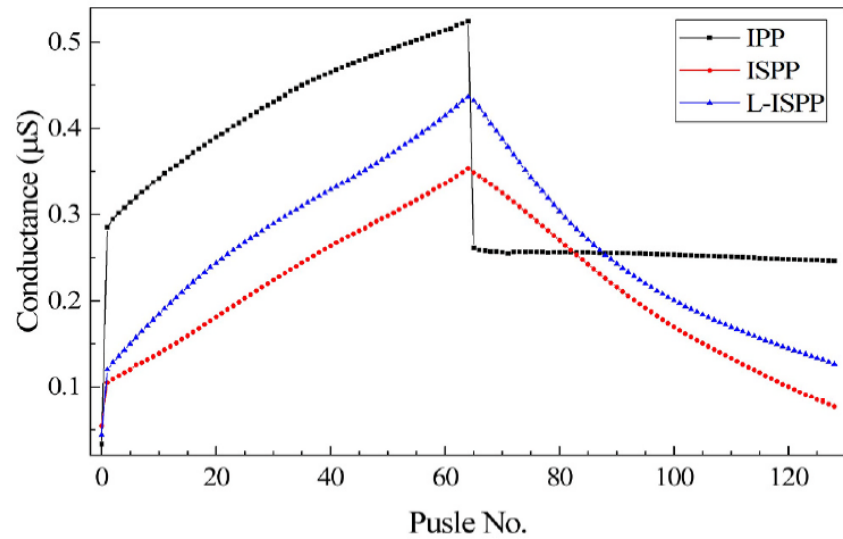
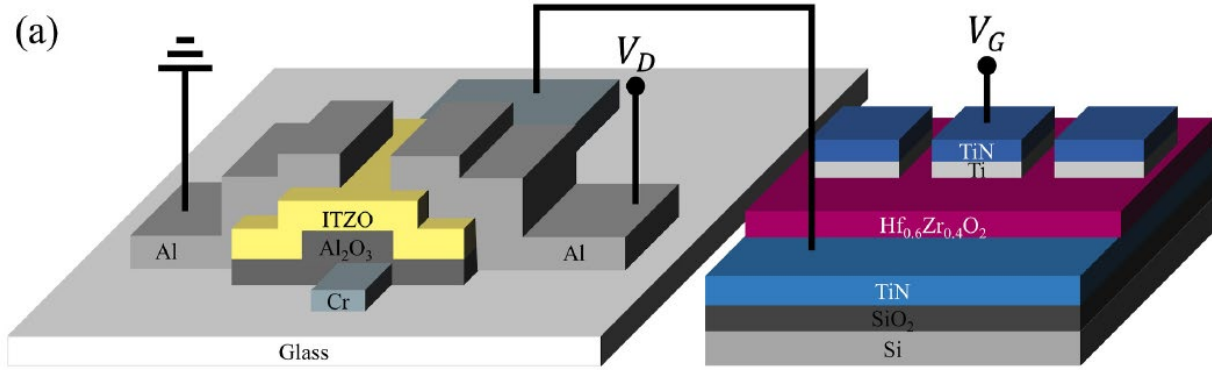
Phys. Rev. Lett. 27, 1719 (1971)



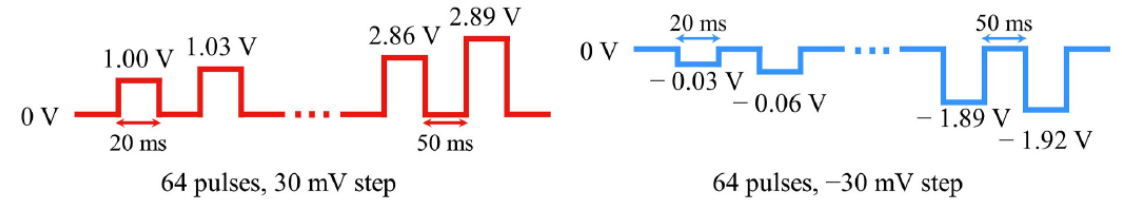
The percolation threshold is known as ≈ 0.593 for 2D square site.

The nucleation is more dominant than the domain growth in the polarization switching.

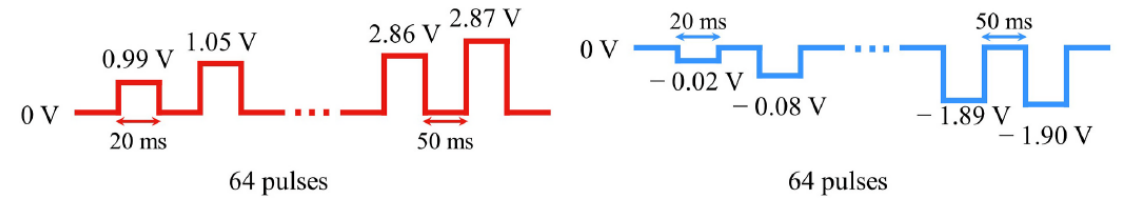




(a) Identical Pulse Program (IPP)



(b) Incremental-Step Pulse Program (ISPP)



(c) Logarithmic-Incremental-Step Pulse Program (L-ISPP)

Pulse program	Dynamic range	Linearity		Programming energy consumption (nJ)	Learning accuracy (%)
		Potentiation	Depression		
IPP	2.1	0.4	≈0	13.9	87
ISPP	3.4	2.9	-7.0	8.22	92.8
L-ISPP	3.6	1.1	-1.6	10.3	93.2

Conclusion

- 강유전체 하프늄 산화물 박막 내 분극 반전을 시뮬레이션하여, 전압 펄스에 따라 분극 도메인이 성장하고 융합되는 과정을 확인했다.
- 적절한 전압 펄스 트레인 설계를 통해 전도 변조의 선형성과 대칭성을 크게 향상시켰으며, 이는 뉴로모픽 소자의 성능 개선에 기여한다.
- 폴리 박막이라 그런지 도메인 성장보다 핵 생성이 분극 반전에 더 우세한 영향을 미친다.