



KoALICE



Sentaurus TCAD Tutorial

Giyeong Kim

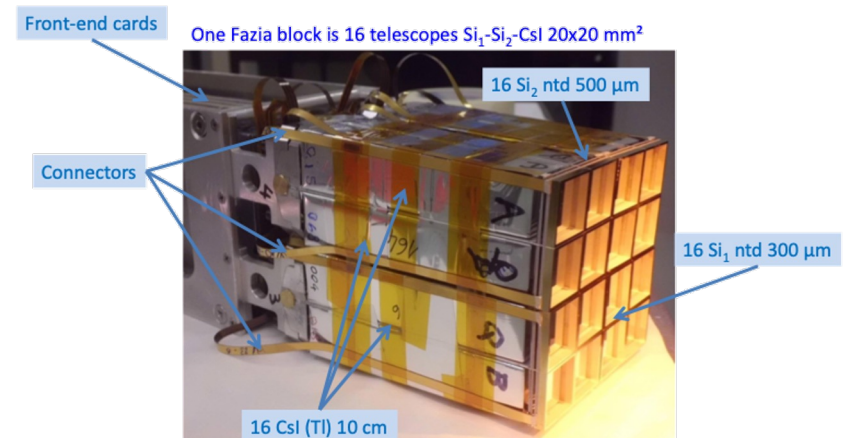
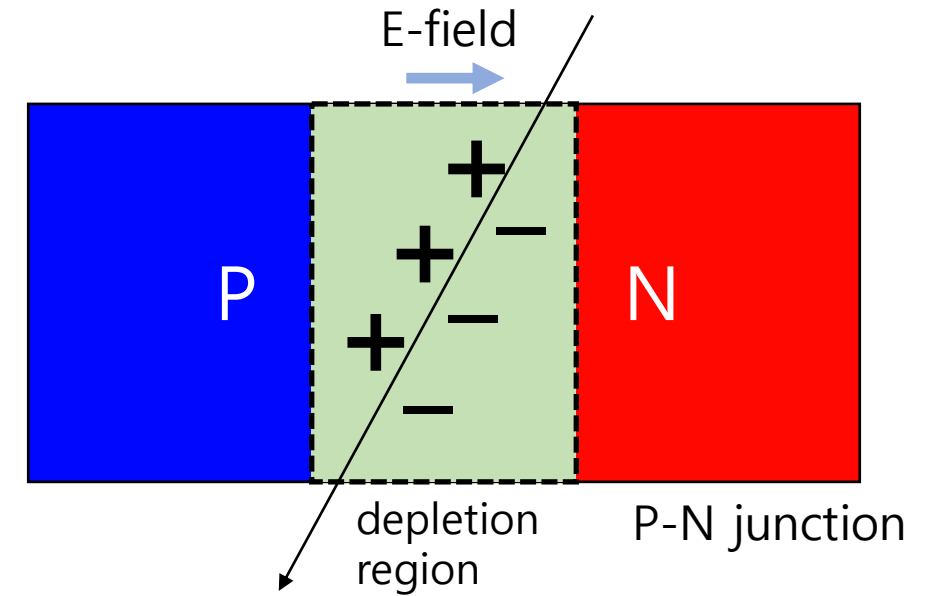
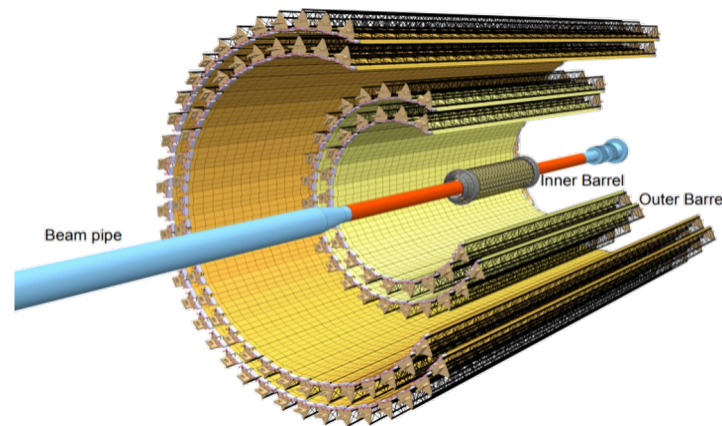
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index

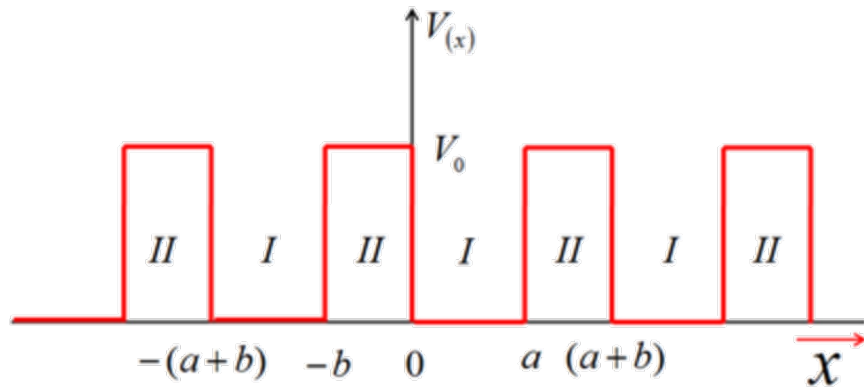
- Introduction to semiconductor detector
- Summary of TCAD tool
- Design of PiN sensor
- Silicon sensor fabrication
- Hands on session

Introduction to semiconductor detectors

- Semiconductor detectors have good energy resolution, so these detectors are widely used in high-energy collision experiments.
- When charged particles pass through the depletion region, they create electron-hole pairs.
- The created electron-hole pairs drifted in the electric field, thereby generating the signal.
- To increase the depletion region, reverse bias voltage is applied to the device.



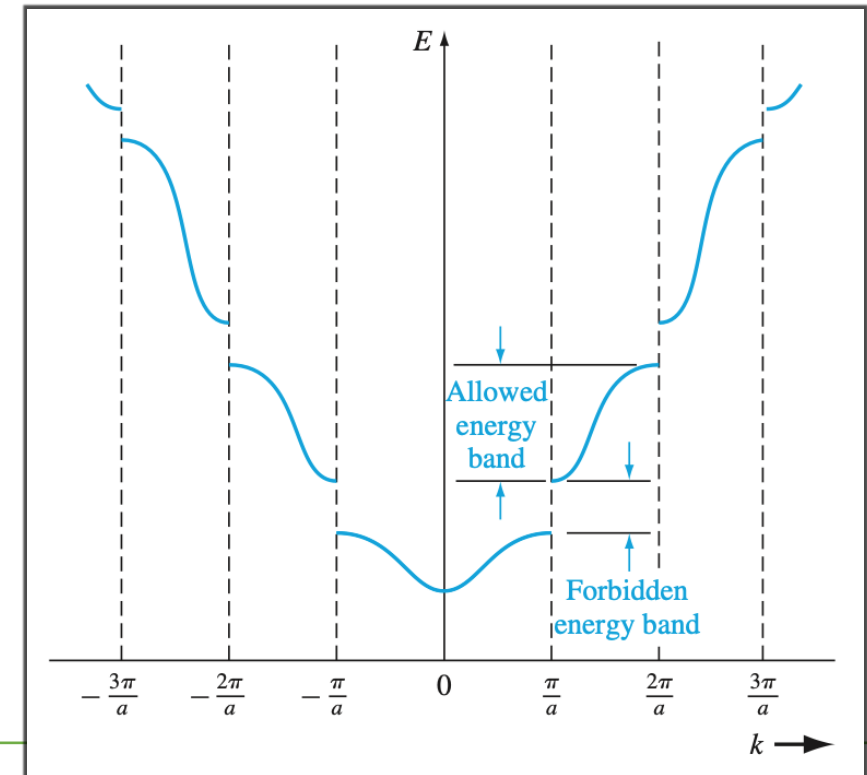
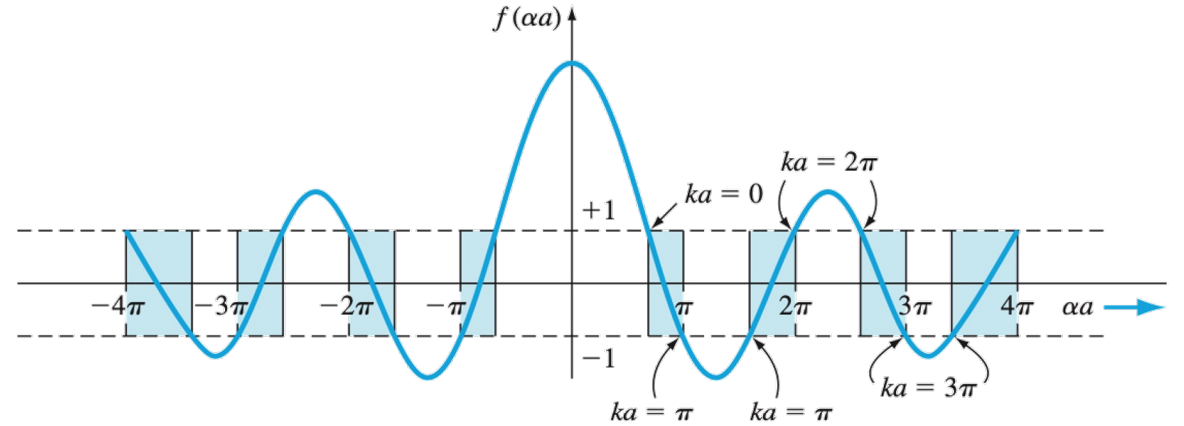
Band gap



$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U\psi = E\psi$$

Using Bloch's function

$$\Psi(x, t) = u(x)e^{i(kx - (E/\hbar)t)}$$



Density of state

$$\frac{2mE}{\hbar^2} = k^2 = k_x^2 + k_y^2 + k_z^2 = (n_x^2 + n_y^2 + n_z^2) \left(\frac{\pi^2}{a^2} \right)$$

$$V_k = \left(\frac{\pi}{a} \right)^3$$

~ free electron

$$V(x, y, z) = 0 \quad \text{for } 0 < x < a \\ 0 < y < a \\ 0 < z < a$$

$$V(x, y, z) = \infty \quad \text{elsewhere}$$

$$g_T(k) dk = 2 \left(\frac{1}{8} \right) \frac{4\pi k^2 dk}{\left(\frac{\pi}{a} \right)^3}$$

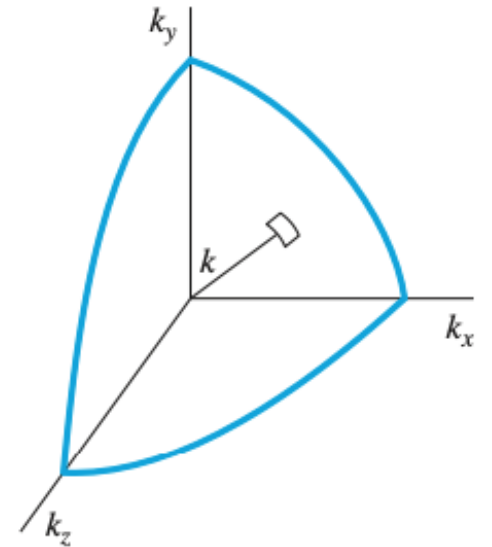
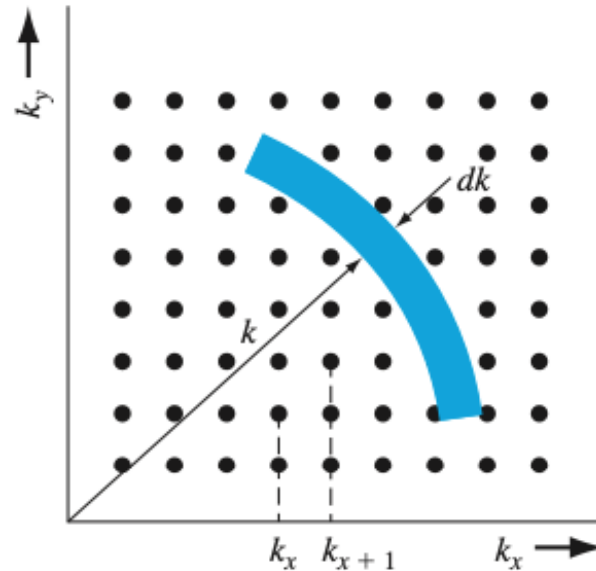
one octant
Spin

Total state in k-space

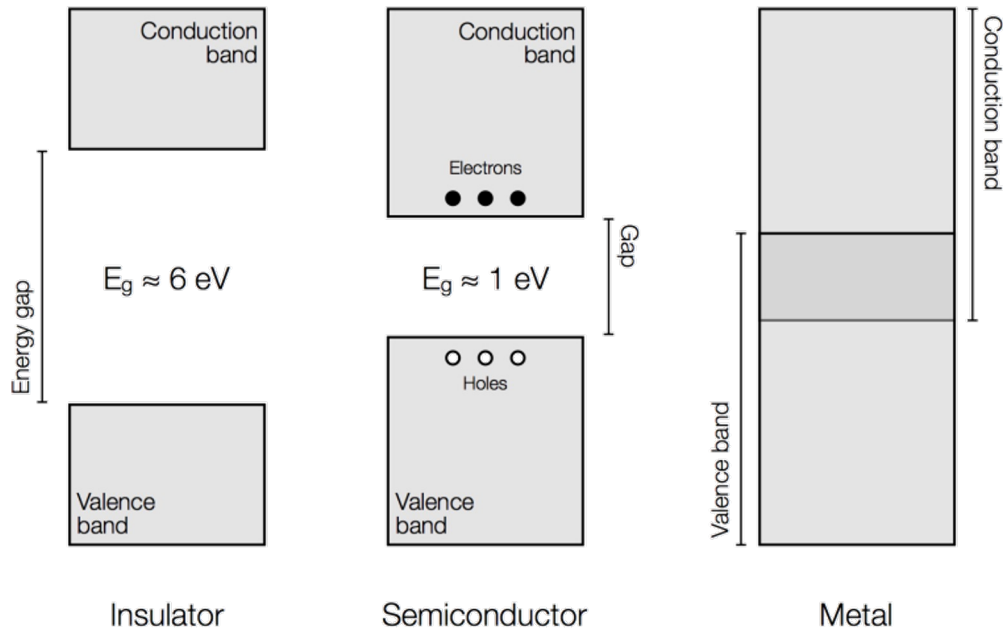
$$g_T(E) dE = \frac{4\pi a^3}{h^3} \cdot (2m)^{3/2} \cdot \sqrt{E} dE$$

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3} \sqrt{E}$$

Energy density of state



Intrinsic semiconductor



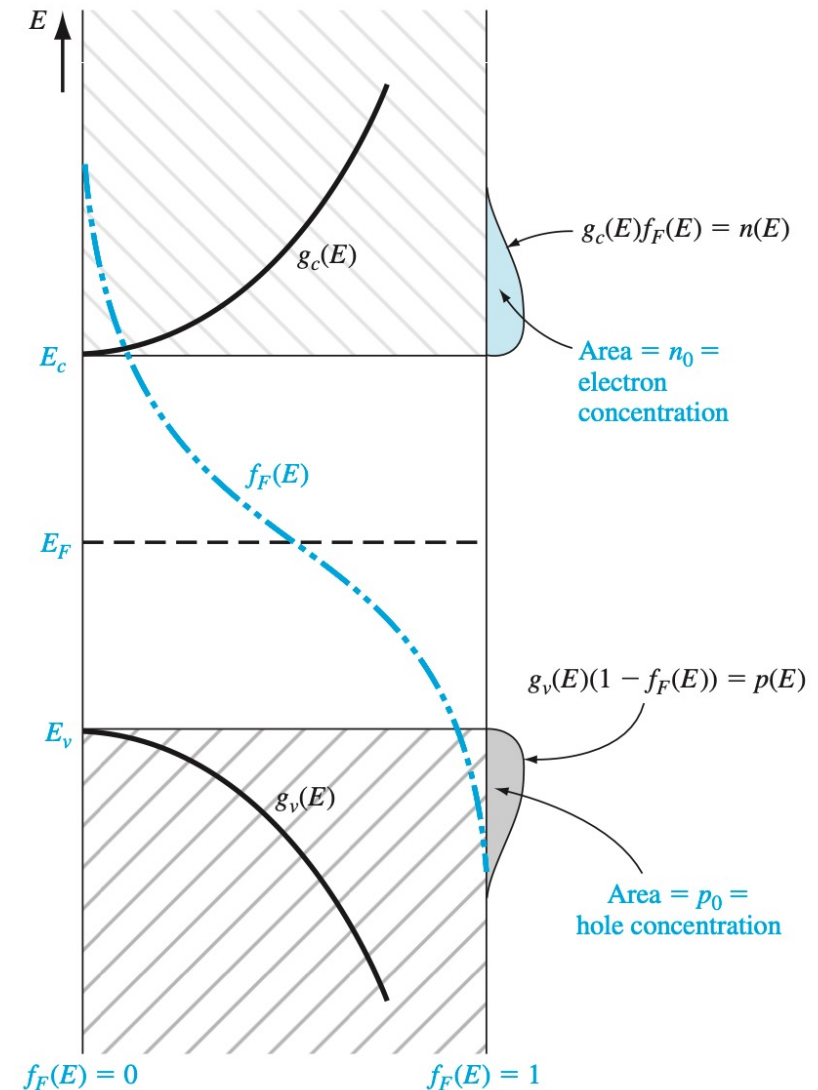
$$n(E)dE = g(E)f(E)dE \quad , g(E) : \text{density of state}$$

$$p(E)dE = g(E)[1 - f(E)]dE \quad f(E) : \text{Fermi-Dirac function}$$

$$n(E) = N_c \exp\left(\frac{E_F - E_c}{kT}\right) \quad , E_F : \text{fermi energy}$$

$$p(E) = N_v \exp\left(\frac{E_v - E_F}{kT}\right) \quad N_c, N_v : \text{effective density of state}$$

$$n=p \Rightarrow np = n_i^2 \text{ .from intrinsic semiconductor}$$



Intrinsic semiconductor

Intrinsic silicon detector에서의 S/N

실리콘에 입자가 지나갔을 때 생기는 *signal*과 *background*를 계산해보자.

Mean ionization energy $I_0 = 3.62$ eV,

$dE/dx = 3.87$ MeV/cm,

$n_i \sim 1.45 \cdot 10^{10} \text{cm}^{-3}$ at $T = 300$ K (Ge는 대략 $1.5 \cdot 10^{13} \text{cm}^{-3}$)

⊙ 두께 $d = 300\mu\text{m}$, 면적 $A = 1\text{cm}^2$ 의 검출기에 MIP 입자가 지나간다면,

$$\frac{dE/dx \cdot d}{I_0} = \frac{3.87 \cdot 10^6 \text{eV/cm} \cdot 0.03\text{cm}}{3.62\text{eV}} \approx 3.2 \cdot 10^4 e^-h^+ \text{ pairs}$$

⊙ 같은 검출기 부피 내의 intrinsic charge carrier ($T=300$ K),

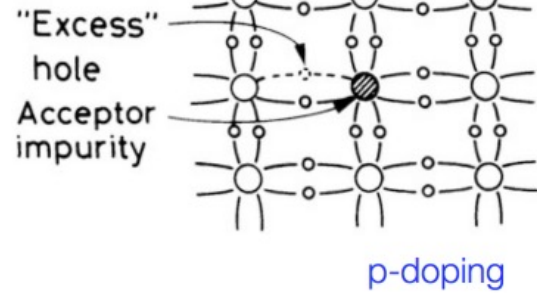
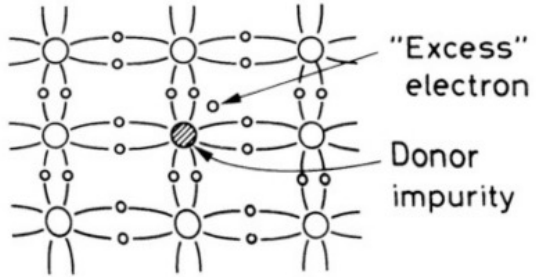
$$n_i dA = 1.45 \cdot 10^{10} \text{cm}^{-3} \cdot 0.03\text{cm} \cdot 1\text{cm}^2 \approx 4.35 \cdot 10^8 e^-h^+ \text{ pairs}$$

Thermal e^-h^+ 쌍의 수가 MIP 입자 *signal* 보다 만배정도나 더 많다!

⇒ 실리콘을 이용해 검출기를 만들려면 "depletion zone in reverse biased pn junctions"이 필요하다. Doping이 필요하다.

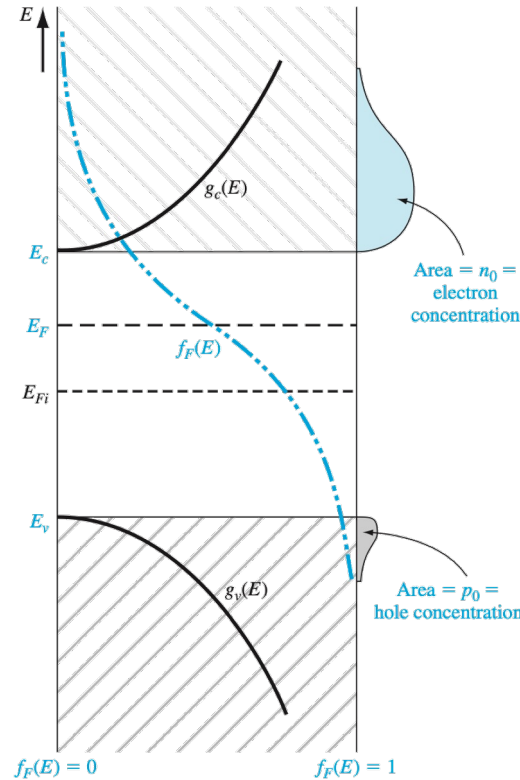
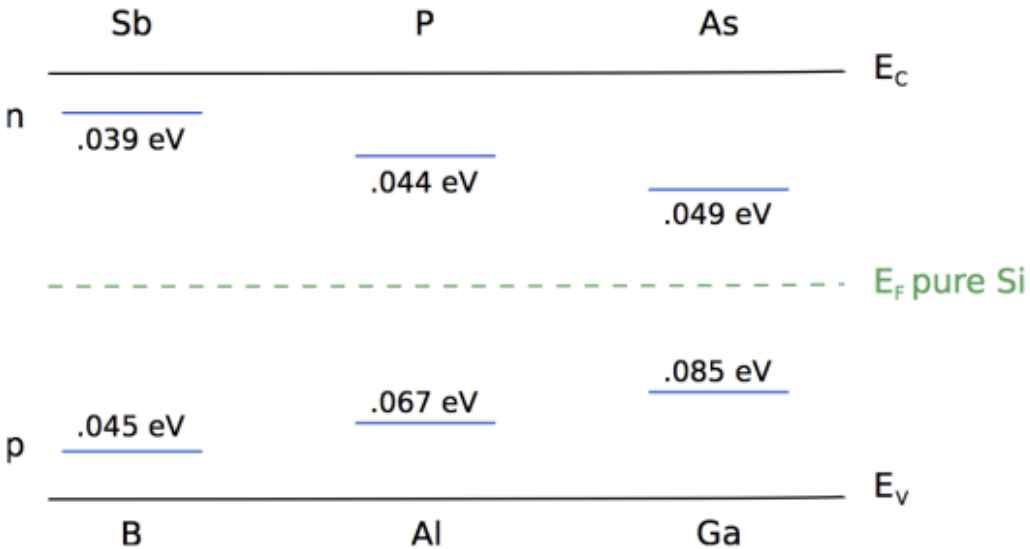
Extrinsic semiconductor

n-doping

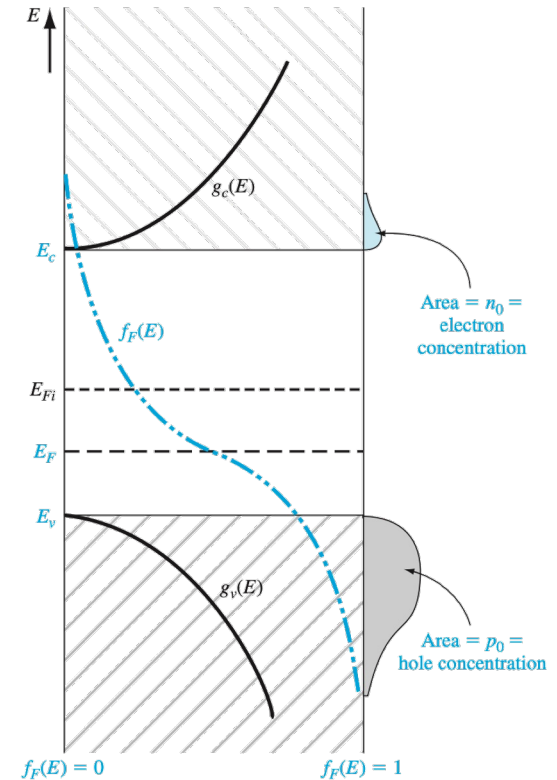


Doping group 5 atoms
: P, Ar, Sb

Doping group 3 atoms
: B, Al, Ga, In

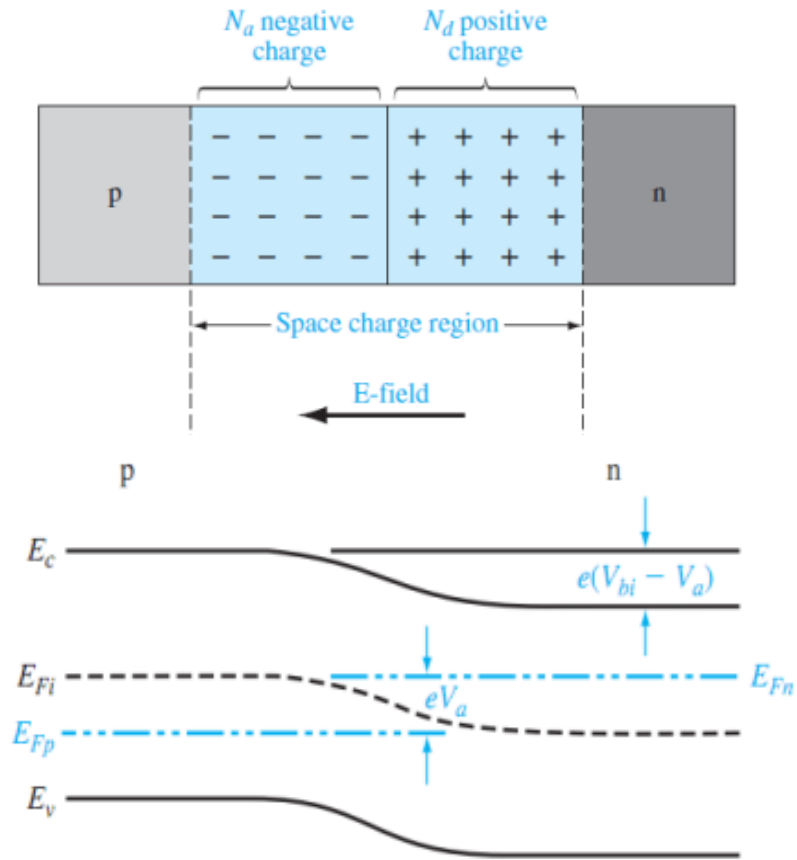


n-doping

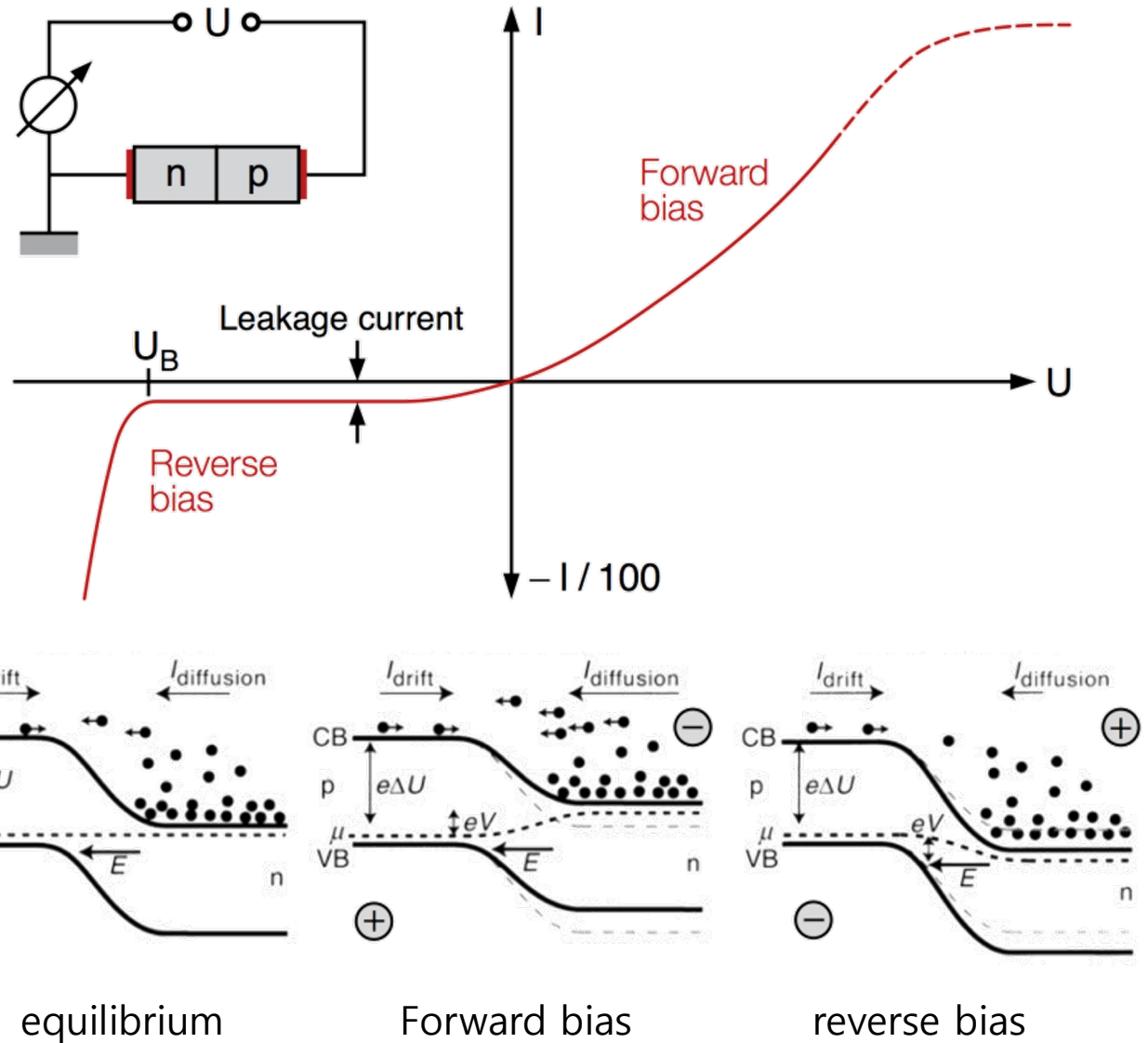


p-doping

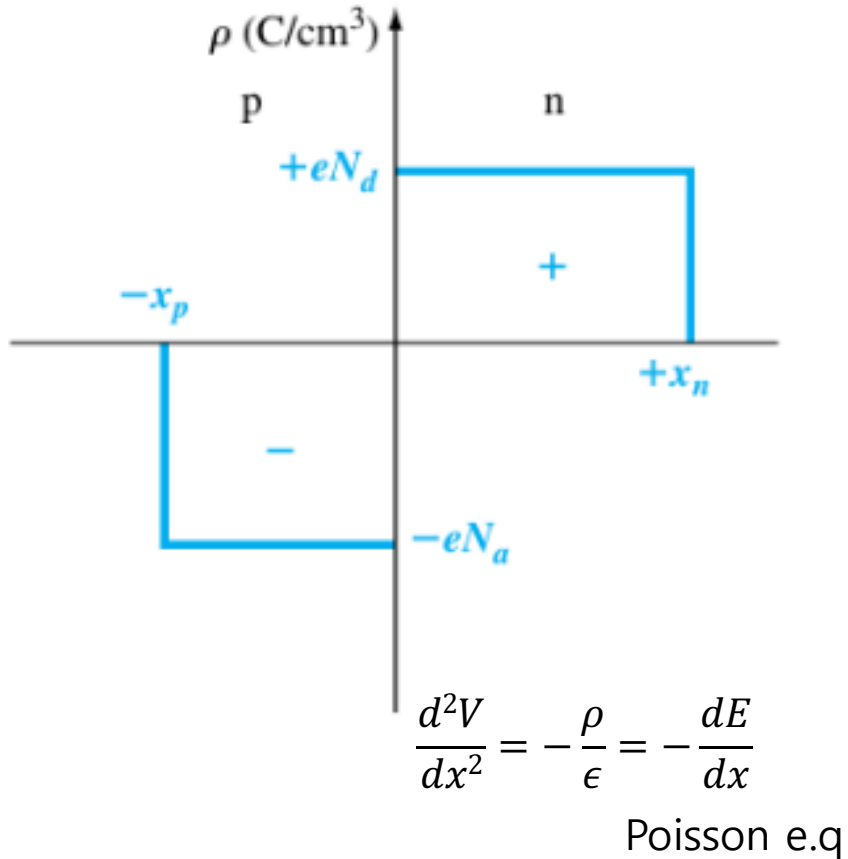
The p-n junction



Intrinsic electric field structure of semiconductor due to the diffusion of majority carrier at the junction



The p-n junction



overall region, space-charge neutral

$$\rho(x) = \begin{cases} 0 & x > x_n \\ eN_D & 0 < x < x_n \\ -eN_A & -x_p < x < 0 \\ 0 & x < -x_p \end{cases}$$

$$\frac{dV}{dx} = \begin{cases} -eN_D/\epsilon \cdot x + C_n & 0 < x < x_n \\ eN_A/\epsilon \cdot x + C_p & -x_p < x < 0 \end{cases}$$

$$= \begin{cases} -eN_D/\epsilon \cdot (x - x_n) & 0 < x < x_n \\ eN_A/\epsilon \cdot (x + x_p) & -x_p < x < 0 \end{cases}$$

as electric field $E = -dV/dx$ must vanish for $x = x_n$ and $x = -x_p$

$$W_{scr} = \left[\frac{2\epsilon(V_{bi} + V_0)}{e} \left(\frac{N_a + N_d}{N_a N_d} \right) \right]^{1/2} \quad \begin{matrix} N_d \ll N_a \\ W_{scr} \approx 0.53\sqrt{\rho V_0}, (\mu m) \end{matrix}$$

$$\begin{matrix} N_a < N_d \\ W_{scr} \approx 0.32\sqrt{\rho V_0}, (\mu m) \end{matrix}$$

The p-n junction

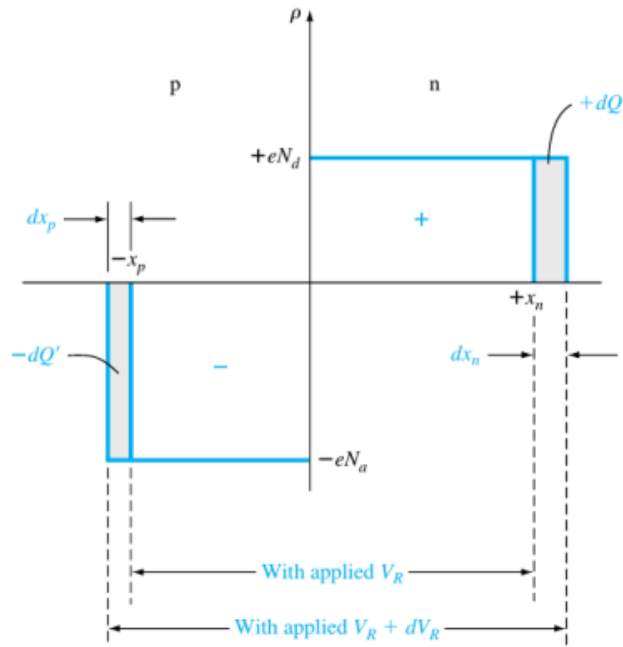


Figure 7.9 | Differential change in the space charge width with a differential change in reverse-biased voltage for a uniformly doped pn junction.

junction capacitance

$$C = \frac{\epsilon A}{W_{scr}}$$

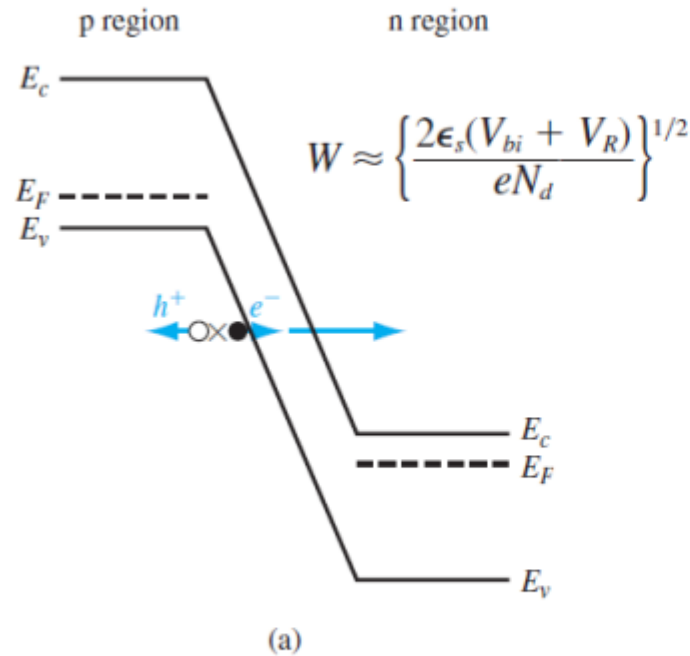
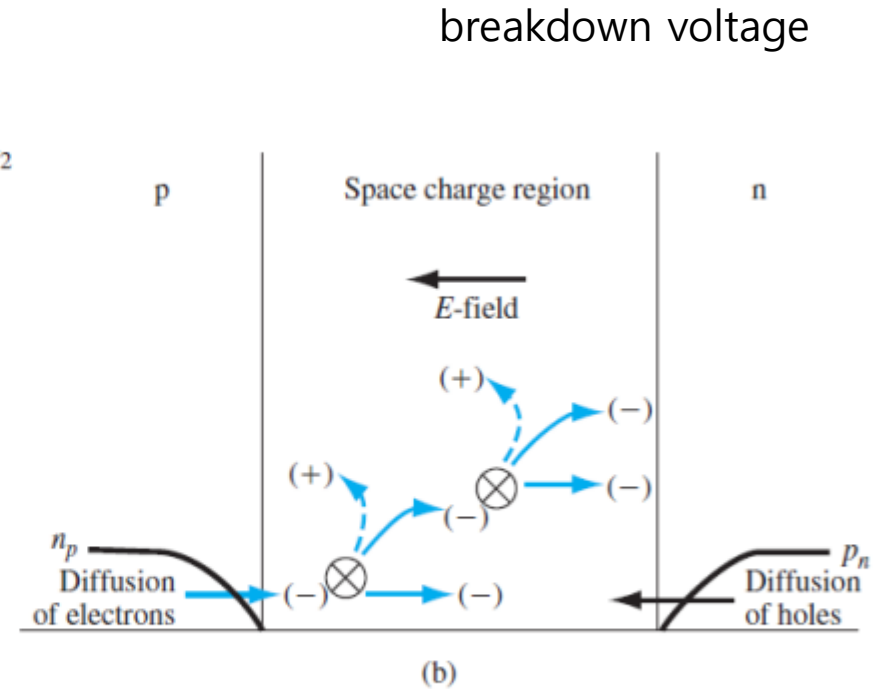
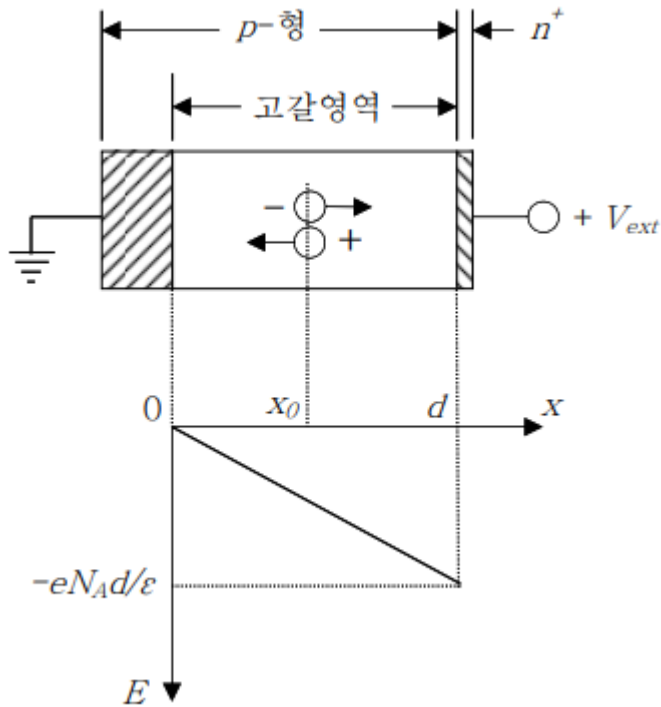


Figure 7.12 | (a) Zener breakdown mechanism in a reverse-biased pn junction; (b) avalanche breakdown process in a reverse-biased pn junction.

Zener breakdown : high doped
Avalanche breakdown : high electric field



Signal



n+p 다이오드 내부 전기장 :
 $E = -\frac{eN_A d}{\epsilon} x = -\frac{x}{\mu_p \tau}, \tau = \frac{\epsilon}{\sigma}$

전자의 속도
 $v = \frac{dx}{dt} = -\mu_n E$

전극에 유도되는 전하
 $dQ = \frac{q}{d} dx$

$$Q_n = \frac{e}{d} x_0 (1 - \exp \frac{\mu_n t}{\mu_p \tau})$$

$$\rightarrow Q_p = -\frac{e}{d} x_0 (1 - \exp \frac{-t}{\tau})$$

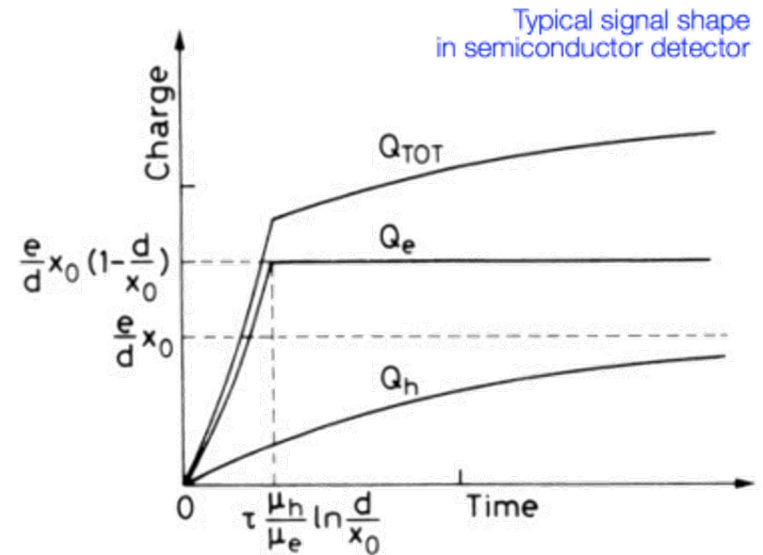
$$Q_{tot} = Q_n + Q_p = -e$$

ehp 한 쌍이 생겨났을 경우의 시그널

$$J_{drift} \approx e\mu_p N_A E = \sigma E = \frac{1}{\rho} E$$

$$\frac{d^2 V}{dx^2} = -\frac{\rho}{\epsilon} = -\frac{dE}{dx}$$

Poisson e.q



[Using:
 $t = \tau \frac{\mu_h}{\mu_e} \cdot \ln \frac{x}{x_0}$ and $d = x$]

Signal

	ϵ_0 [@ 300 K]	ϵ_0 [@ 77 K]	E_{gap}
Si	3.6 eV	2.8 eV	1.1 eV
Ge	-	2.9 eV	0.7 eV

ϵ_0 : mean energy per electron-hole pair

energy conservation

$$E_0 = E_i \cdot N_i + E_x \cdot N_x$$

$$E_i \cdot \Delta N_i + E_x \cdot \Delta N_x = 0$$

$E_0 = \text{const}$

E_i : ionization energy

E_x : phonon excitation

on average

$$E_x \sigma_x = E_i \sigma_i$$

$$\sigma_i = \sqrt{N_i}, \sigma_x = \sqrt{N_x}$$

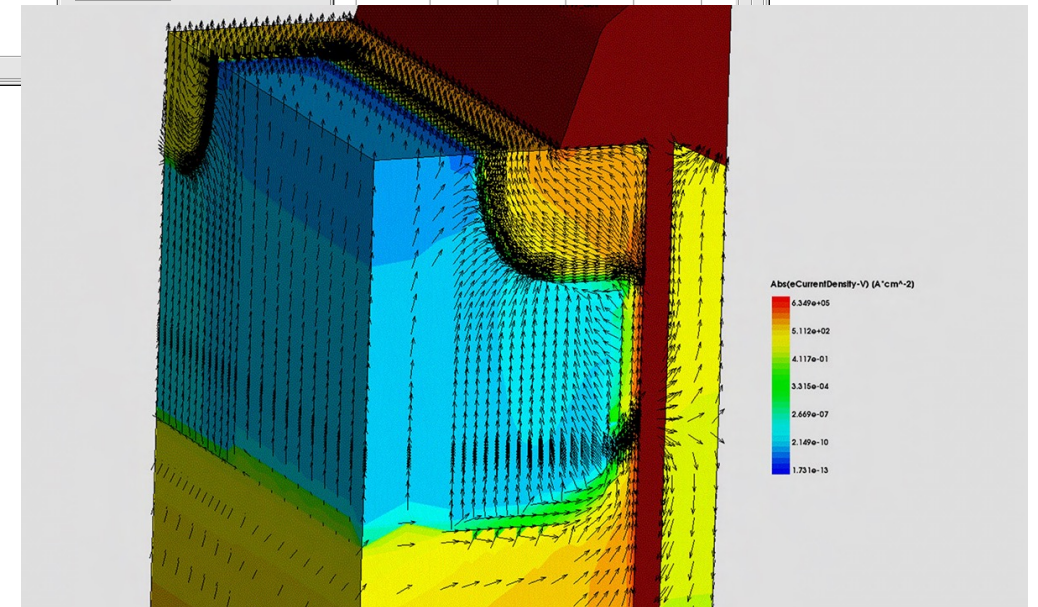
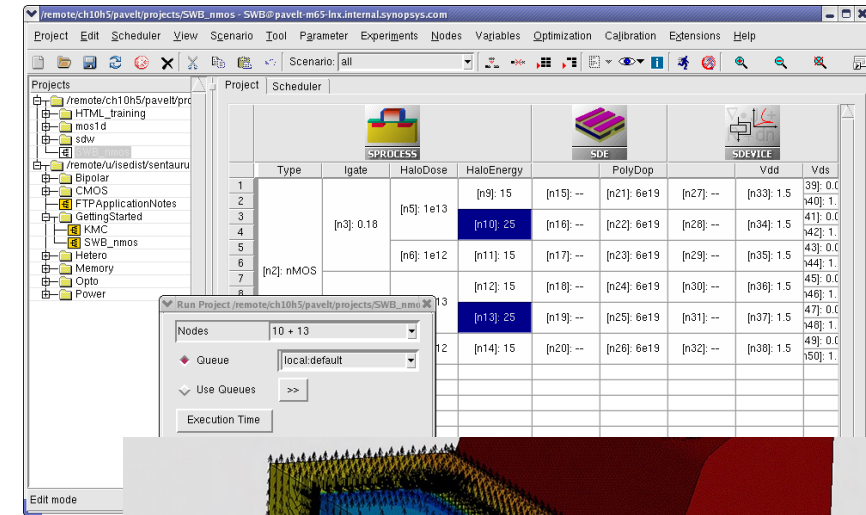
$$\sigma_i = \frac{E_x}{E_i} \sqrt{\frac{E_0}{E_x} - \frac{E_i}{E_x} N_i}, \quad N_i = \frac{E_0}{\epsilon_0}$$

$$\sigma_i = \sqrt{N_i F}, \quad F = \sqrt{\frac{E_x}{E_i} \left(\frac{\epsilon_0}{E_i} - 1 \right)}$$

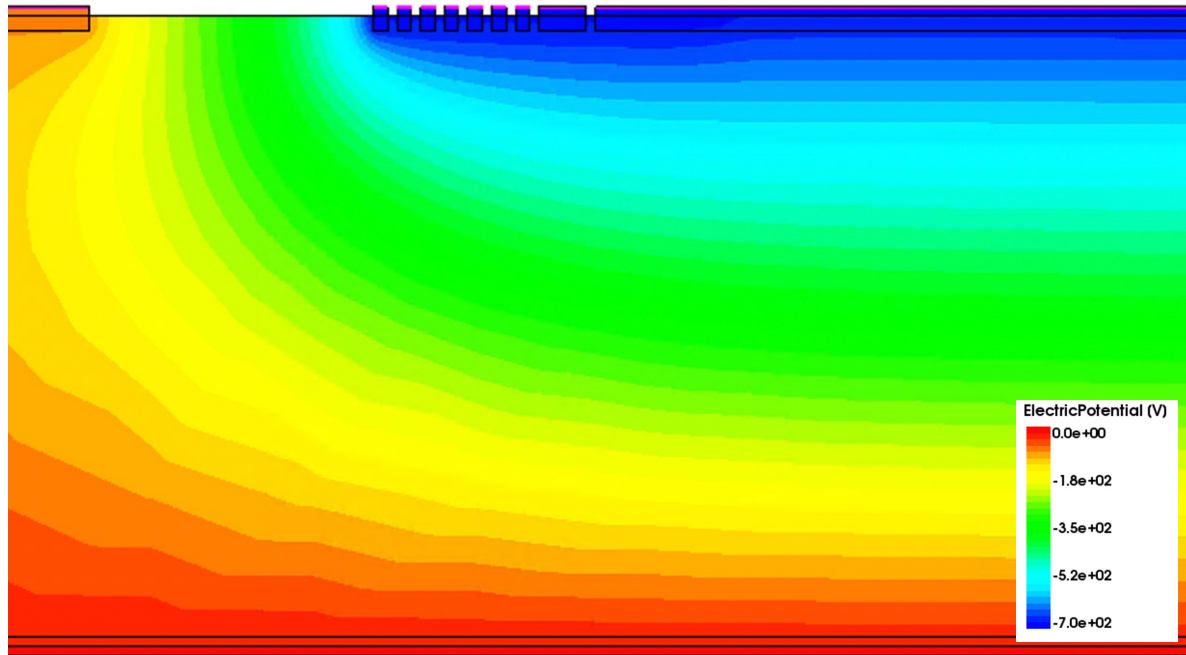
: fano factor, 실리콘의 경우(300K) ~0.1

TCAD(Technology Computer Aided Design) simulation

- ▶ TCAD simulators calculate the Poisson equation of the semiconductor properties in the numerical analysis method.
- ▶ TCAD simulators can visualize physical characteristics of semiconductors, such as electric field, potential, and current density.



Synopsys TCAD tool



ϵ : electrical permittivity

\vec{P} : ferroelectric polarization

$n(p)$: electron(hole) density

q : elementary charge

$\mu_{n(p)}$: electron(hole) carrier mobility

▶ Electrostatic Potential

$$\nabla \cdot (\epsilon \nabla \phi + \vec{P}) = -q(p - n + N_D - N_A) - \rho_{\text{trap}}$$

▶ Carrier transport model

$$\nabla \cdot \vec{J}_{n(p)} = q(R_{\text{net},n(p)} - G_{\text{net},n(p)}) + q \frac{\partial n(p)}{\partial t}$$

▶ Drift-diffusion model

$$\vec{J}_{n(p)} = -n(p)\mu_{n(p)}\nabla\Phi_{n(p)} \quad \text{by Einstein relation}$$

$R_{\text{net},n(p)}$: electron(hole) net recombination rate

$G_{\text{net},n(p)}$: electron(hole) net generation rate

$\vec{J}_{n(p)}$: electron(hole) current density

$\Phi_{n(p)}$: electron(hole) quasi_Fermi potential

$N_D (N_A)$: concentration of ionized donors(acceptors)

Synopsys TCAD tool



Senstaurus tools



Sentaurus process

- An advanced 1D, 2D, and 3D process simulator
- Equipped with a set of advanced process models, which include default parameters calibrated with data from equipment vendors



Sentaurus structure editor

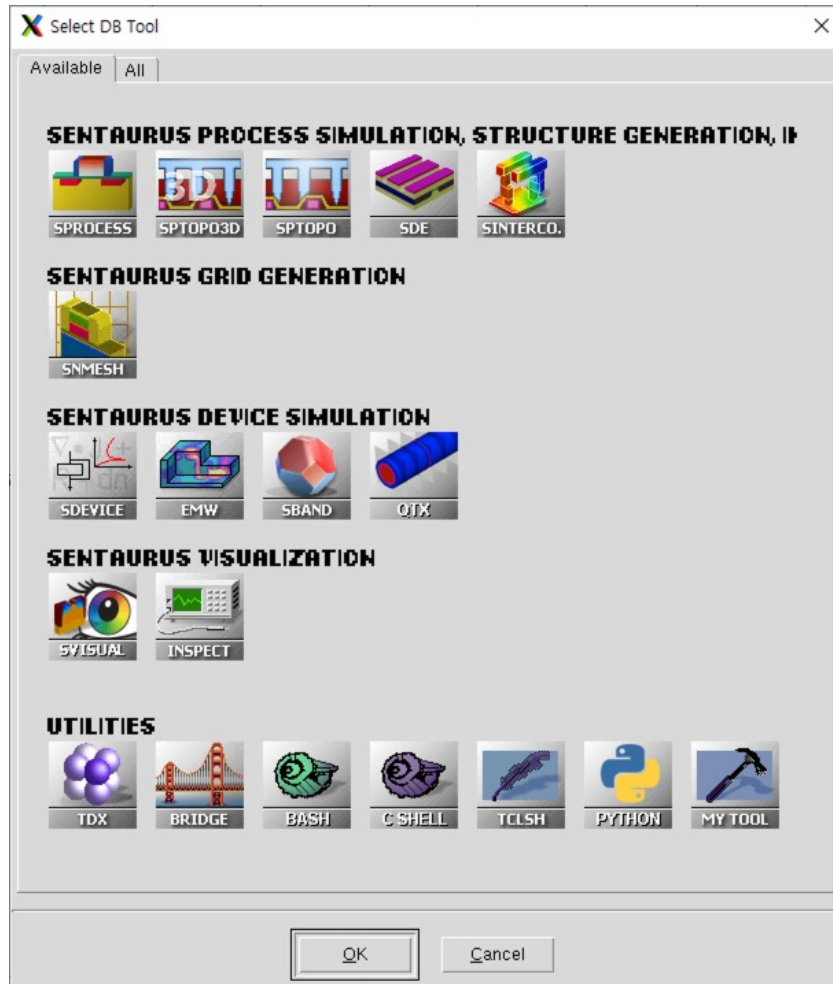
- Tools for creating geometric structures for TCAD simulation
- Direct CAD operations can be used to create 2D and 3D structures



Sentaurus device

- An advanced multidimensional (1D/2D/3D) device simulator
- Characterize electrical, thermal and optical behavior of semiconductor devices

Synopsys TCAD tool



Senstaurus tools



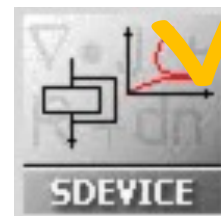
Sentaurus process

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Sentaurus structure editor

- Tools for creating geometric structures for TCAD simulation
- Direct CAD operations can be used to create 2D and 3D structures

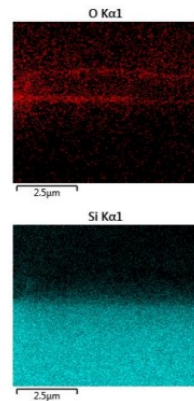
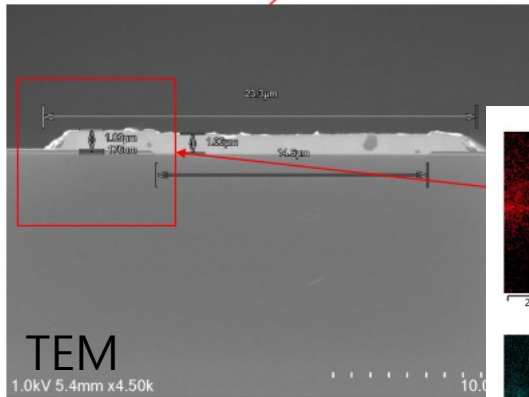
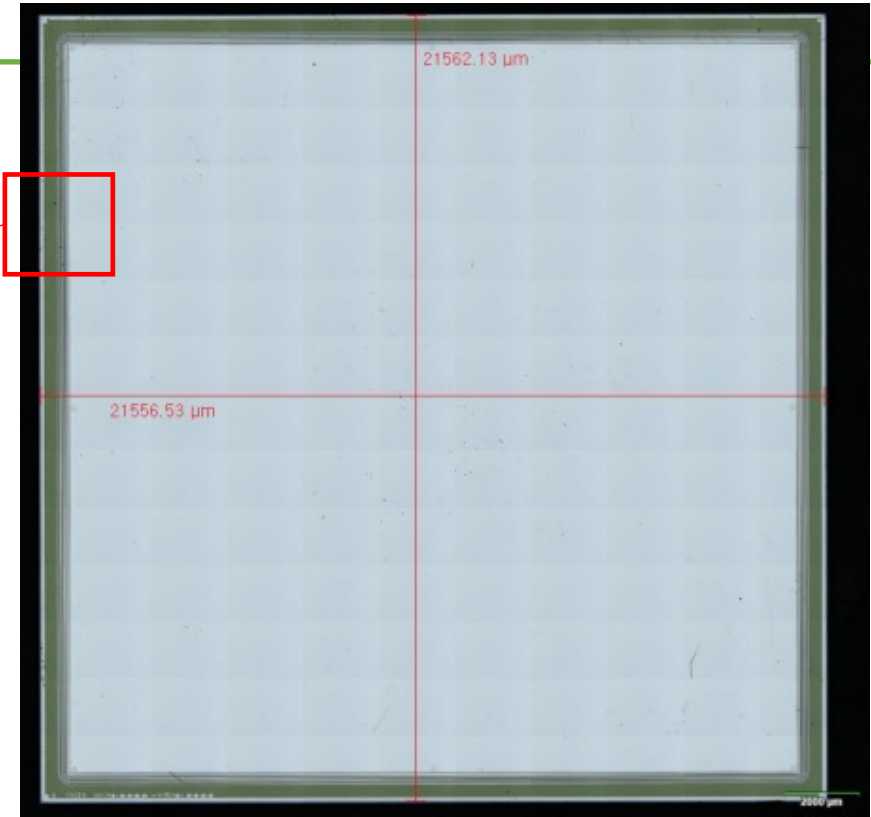
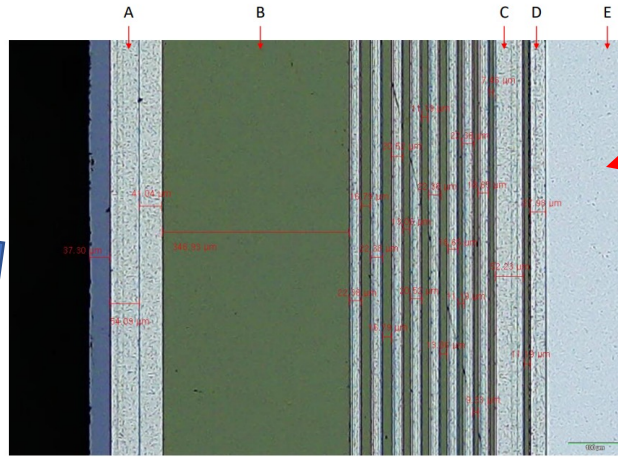
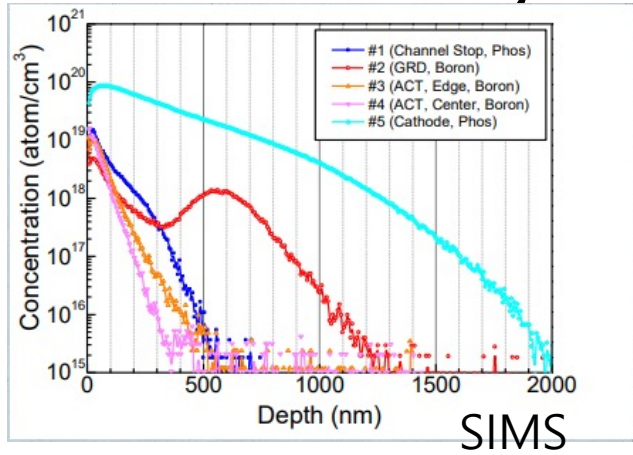


Sentaurus device

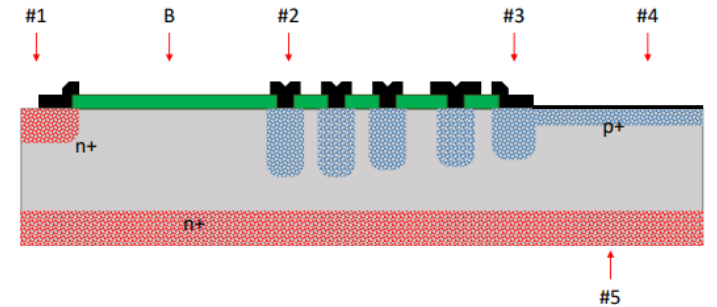
- An advanced multidimensional (1D/2D/3D) device simulator
- Characterize electrical, thermal and optical behavior of semiconductor devices

SDE & SDEVICE

Reverse engineering target chip

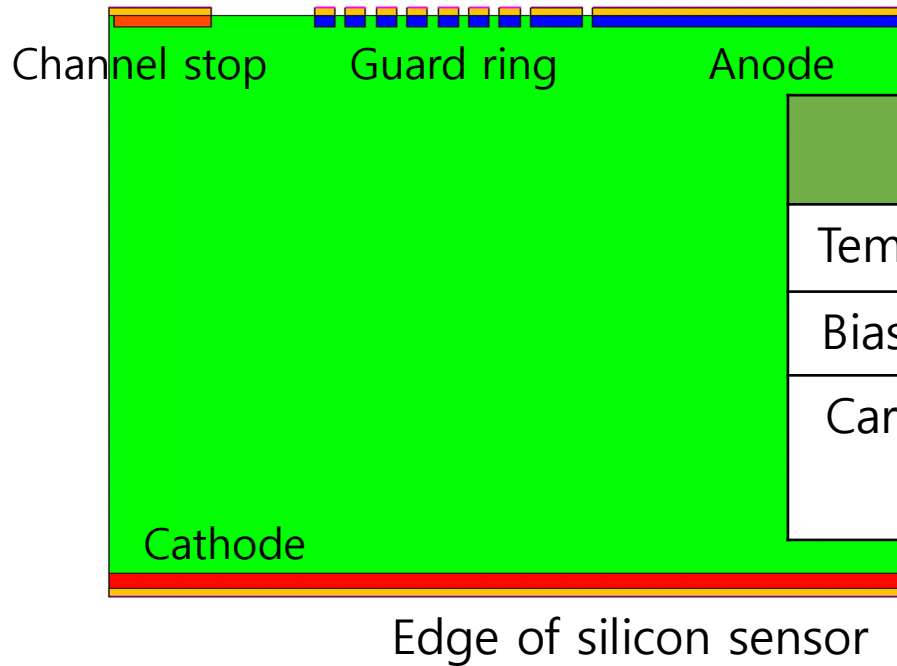
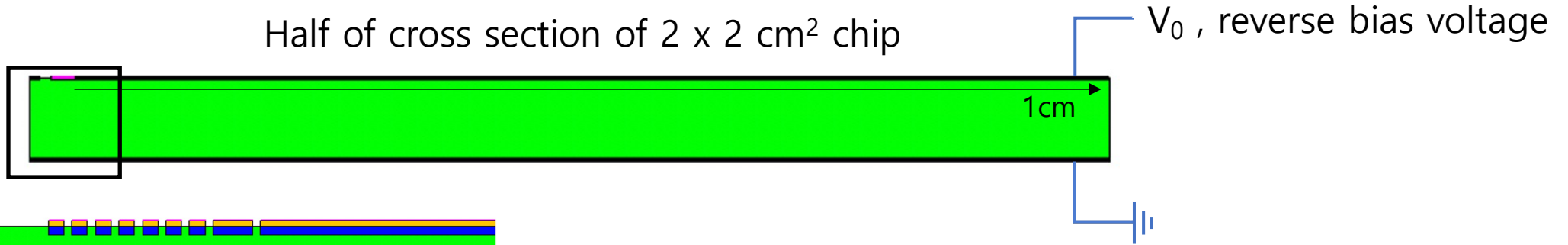


Element	Line Type	Apparent Concentration	k Ratio	Wt%	Wt% Sigma	Standard Label	Factory Standard	Standard Calibration Date
C	K series	0.09	0.00091	13.19	0.50	C Vit	Yes	
O	K series	0.40	0.00135	7.01	0.18	SiO ₂	Yes	
Al	K series	2.07	0.01485	18.70	0.15	Al ₂ O ₃	Yes	
Si	K series	5.33	0.04221	60.34	0.38	SiO ₂	Yes	
Ti	K series	0.03	0.00031	0.44	0.06	Ti	Yes	
Ag	L series	0.02	0.00020	0.33	0.10	Ag	Yes	
Total:				100.00				



Simulation setup

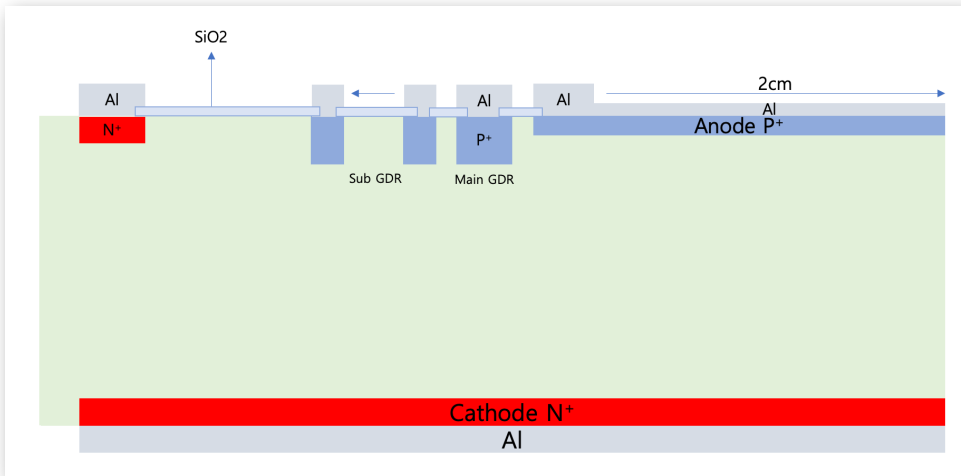
Half of cross section of 2 x 2 cm² chip



Input parameter				
Temperature	300K		Doping density	
Bias voltage	0 ~ -700V		P-type	1x10 ¹⁹ cm ⁻³
Carrier lifetime	electron	1x10 ⁻⁴ s ⁻¹	N-type	5x10 ¹¹ cm ⁻³
	hole	3x10 ⁻⁴ s ⁻¹	N-type	1x10 ²⁰ cm ⁻³

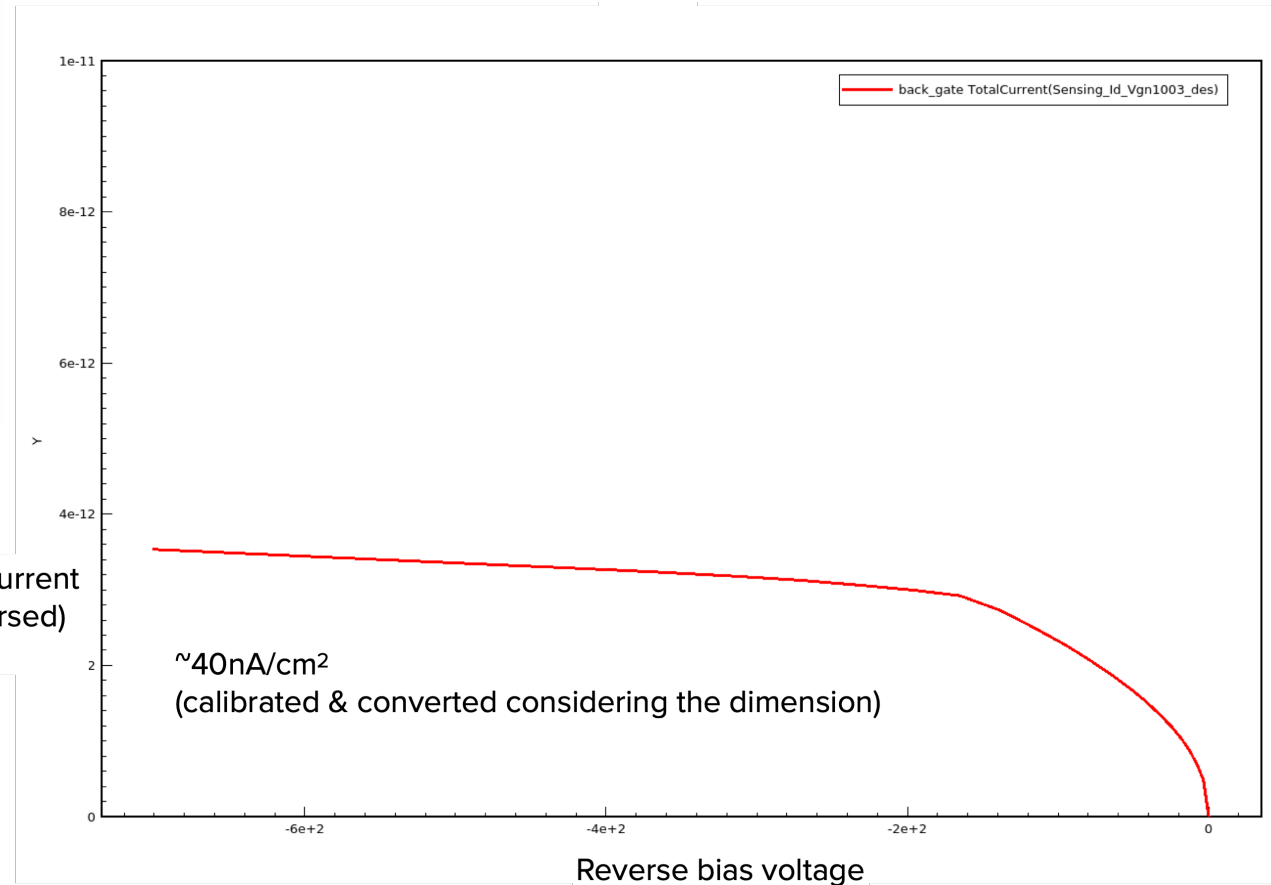
Design of PiN sensor using TCAD simulation

Leakage current result with the final design

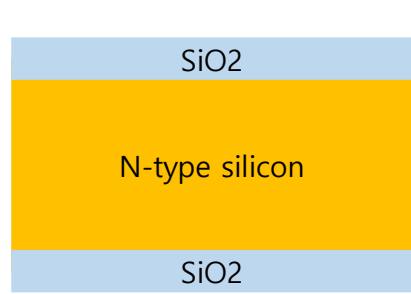


► We calculated the leakage current of the final design based on the calibrated parameters.

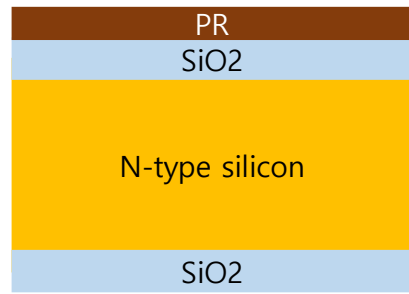
Leakage current
(sign reversed)



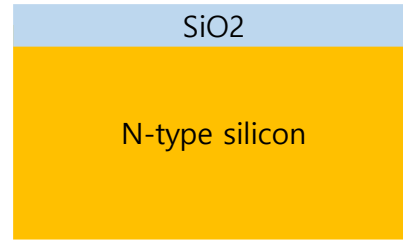
Process flow co- ETRI



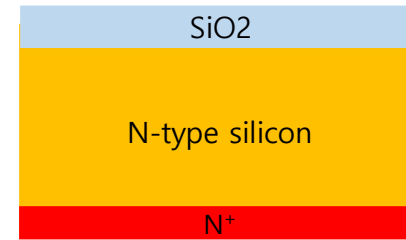
1. Oxidation [900°C, 6000Å]



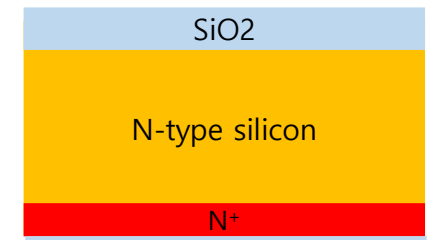
2. PR coating



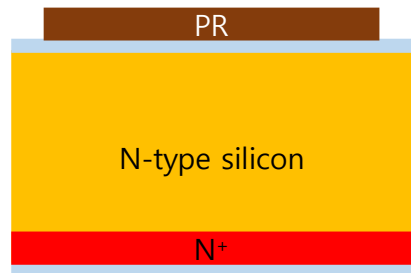
3. Backside Oxide strip
PR strip



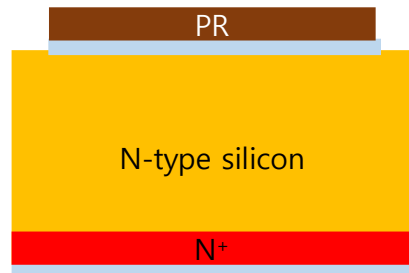
4. POCl3 Doping
Deglase PSG



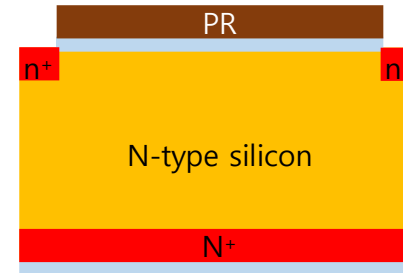
5. Oxidation [900°C, 1000Å]



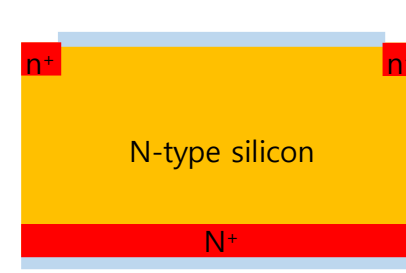
6. #Channel Stop Patterning



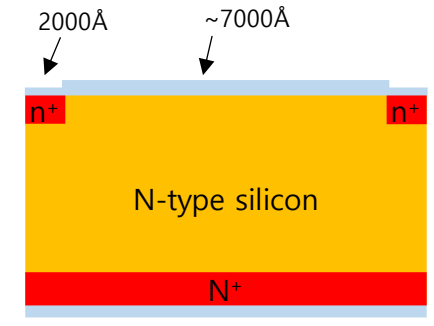
7. Oxide etch ~6000Å



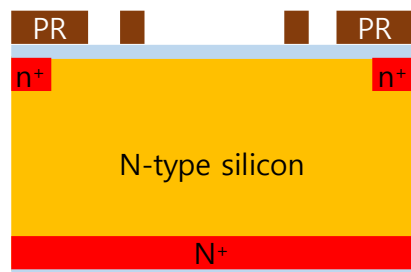
8. N+ implant [channel stop]
P31, 50KeV, 4.0E14/cm2



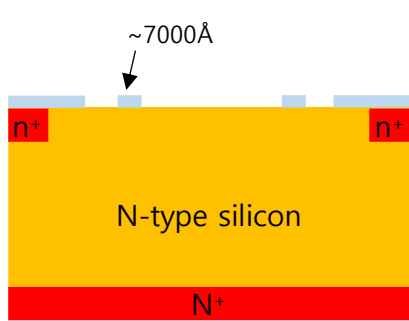
9. PR strip



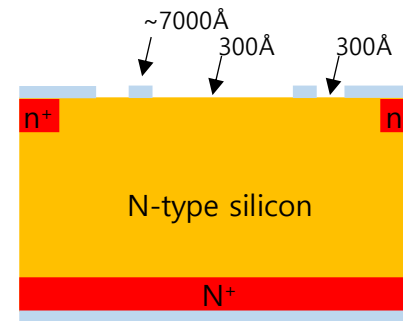
10. Oxidation [900°C, 2000Å]



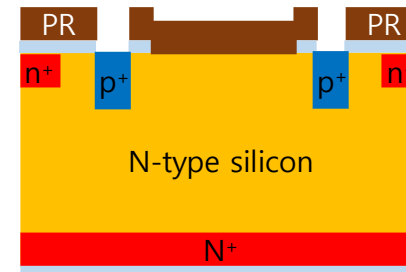
11. #Active Patterning



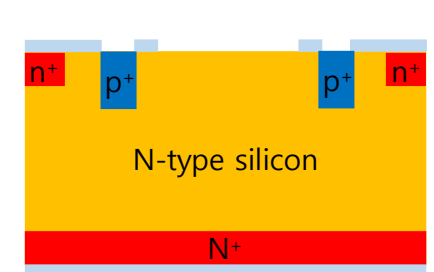
12-1. Oxide etch (Dry + Wet)
12-2. PR strip



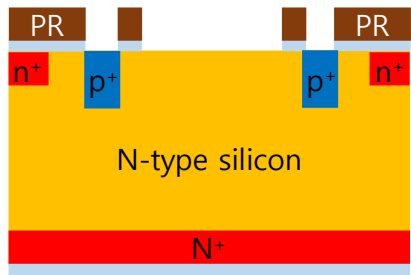
13. Oxidation [850°C, 300Å]



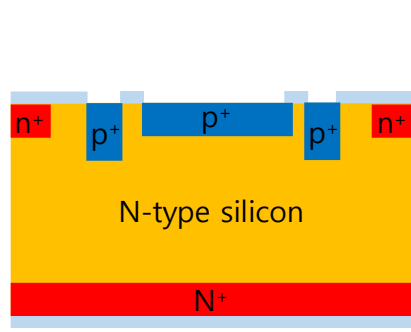
14-1. #GRD Patterning
14-2. P+ implant [GRD]
B11, 180KeV, 1.0E14/cm2



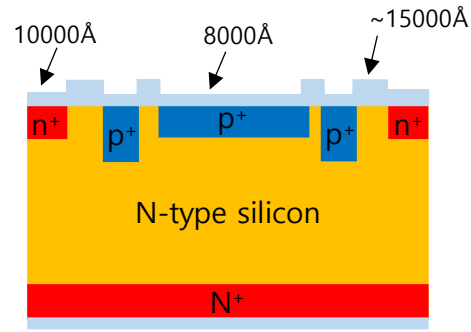
15-1. PR strip
15-2. Anneal (950°C, 60min)



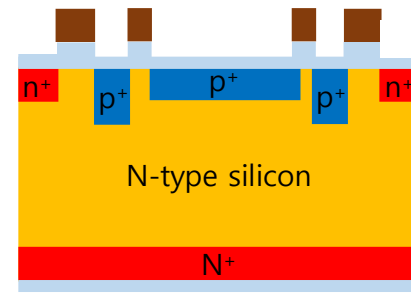
16-1. Active Patterning
 16-2. P⁺ implant [Active]
 B11, 50KeV, 1.0E15/cm²



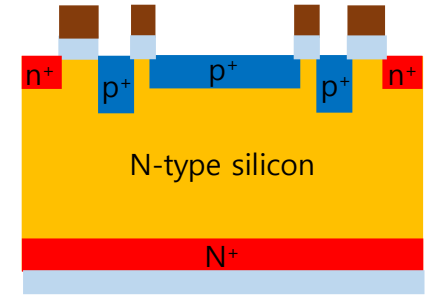
17. PR strip



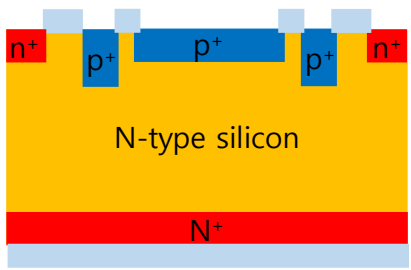
18-1. TEOS 8,000Å
 18-2. Anneal (950°C, 30min)



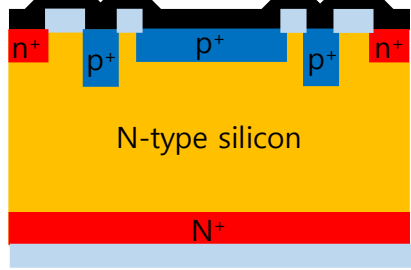
19. #CONT Patterning



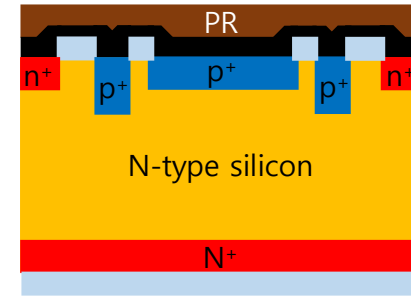
20. Oxide etch (Dry+Wet)
 Target: ~10000Å (oxide on n+)



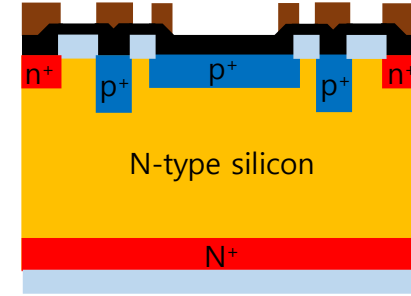
21. PR strip



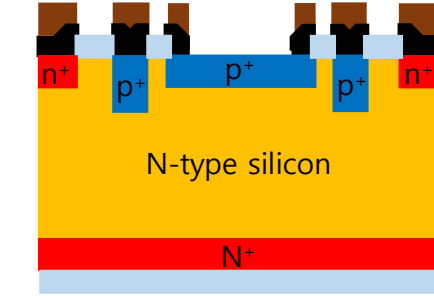
22. metal deposit
 [10000Å]



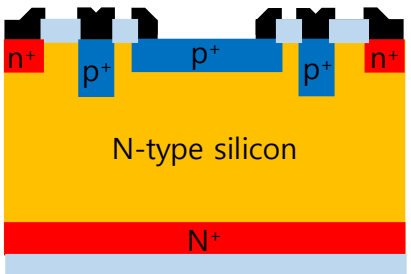
23. PR coating



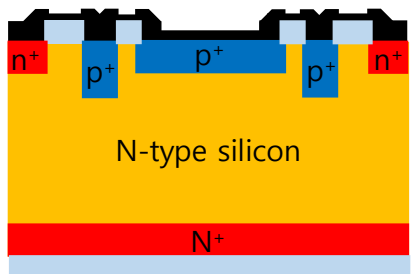
24. #GRD metal Patterning



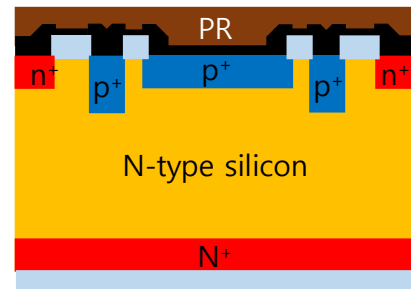
25. metal etching



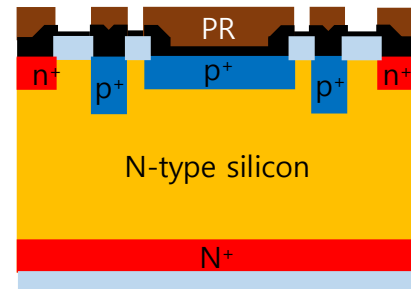
26. PR strip



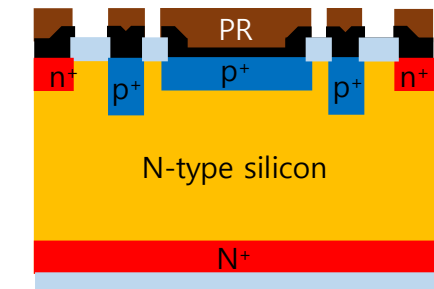
27. metal deposit[400Å]
 barrier metal split



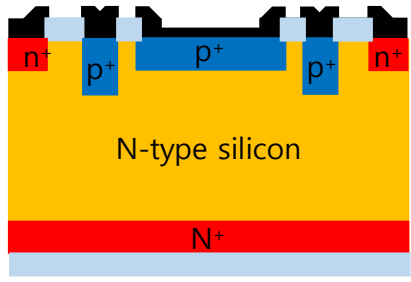
28. PR coating



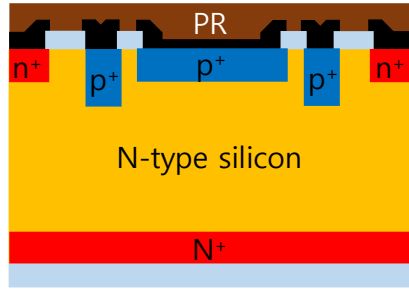
29. #ACT metal Patterning



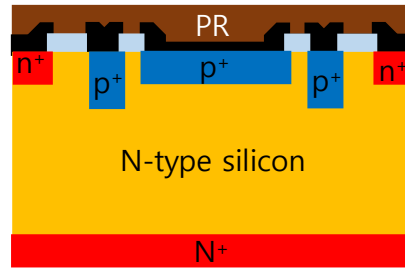
30. metal etching



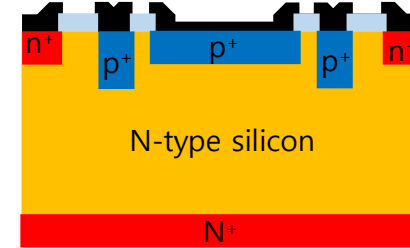
31. PR strip



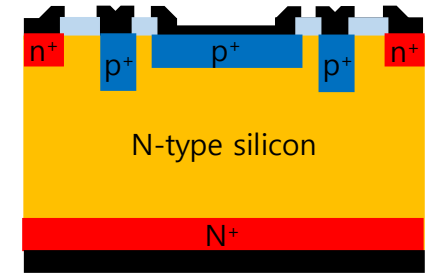
32. PR coating



33. oxide etching

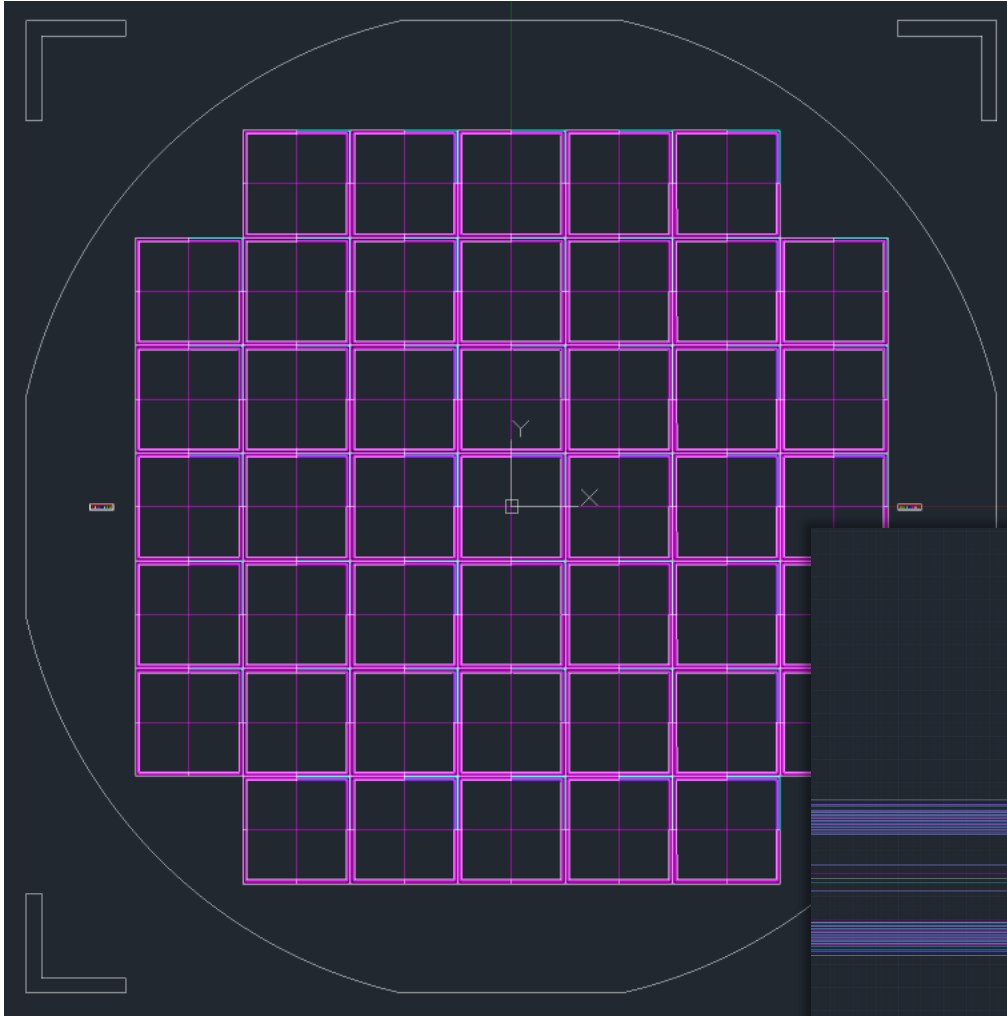


34. PR strip

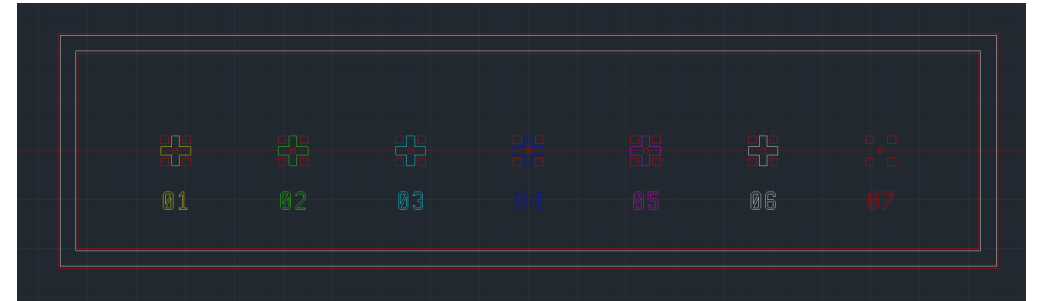


35-1. metal deposit [10000Å]
35-2. Alloy (420°C, 30min)

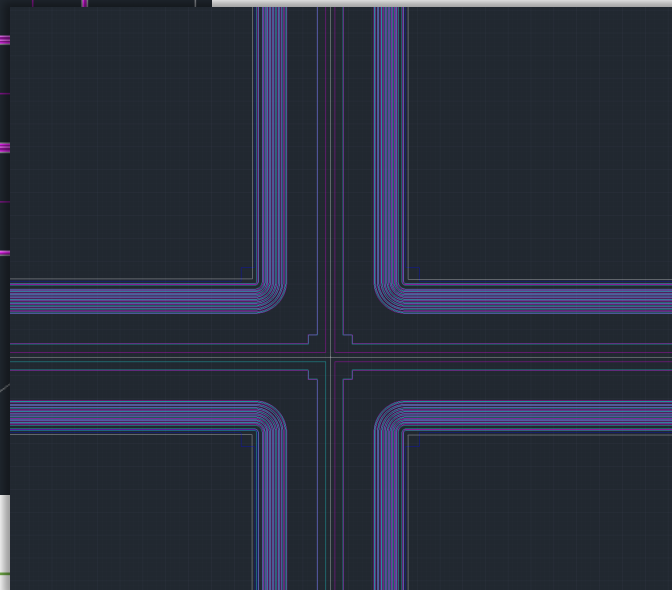
Photomask designed



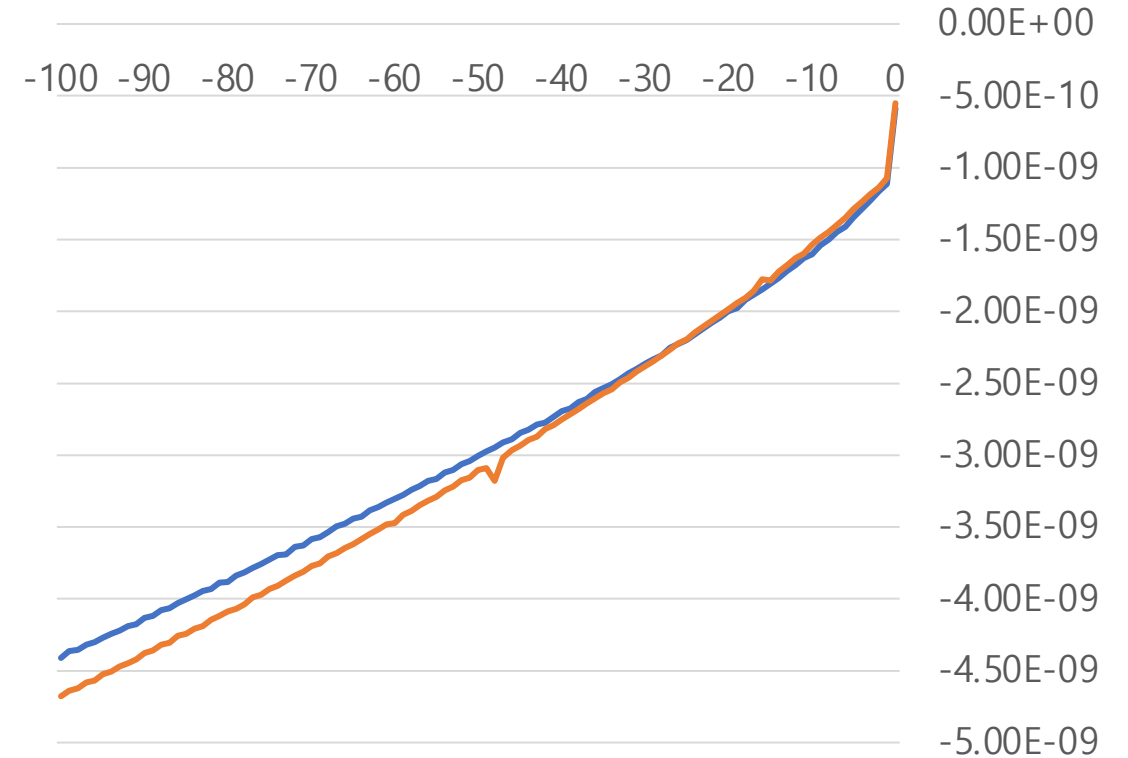
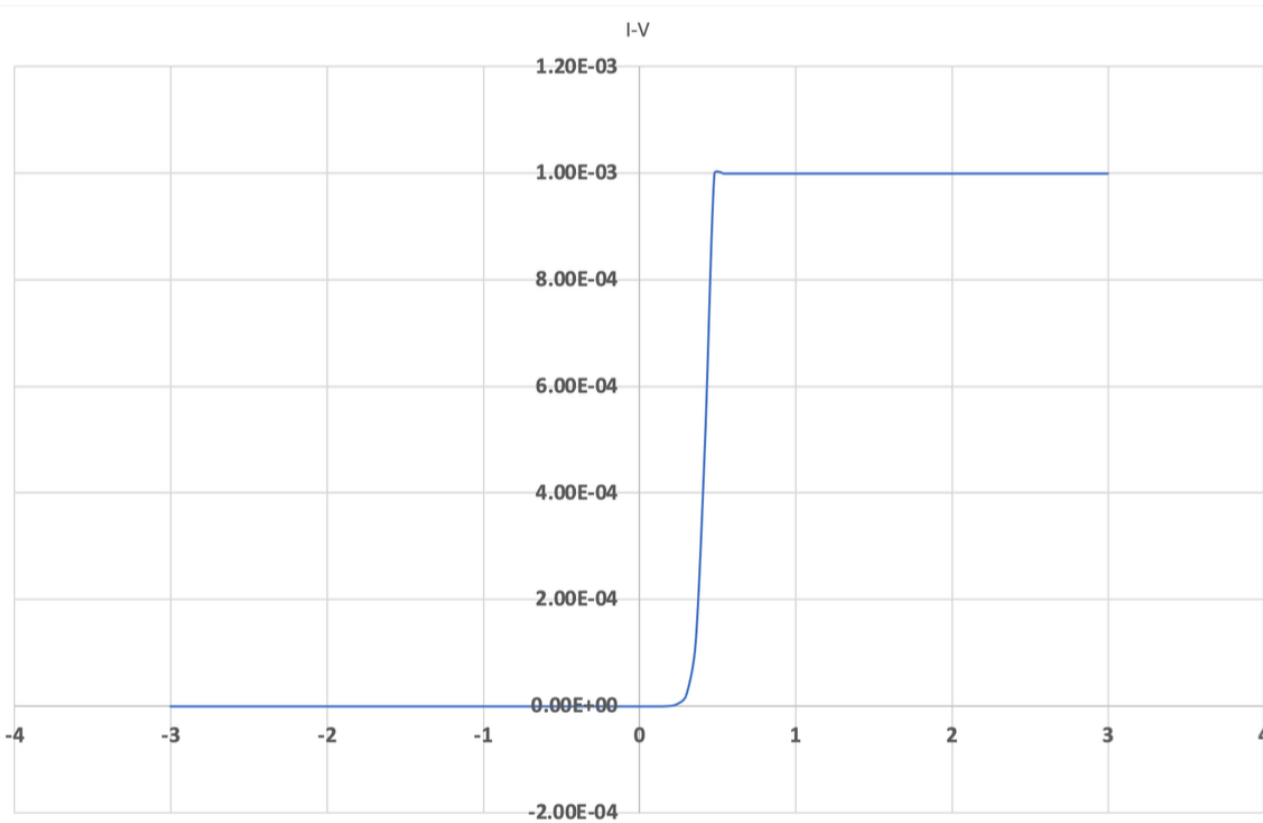
Photomask layout of 8" wafer using AutoCAD tool



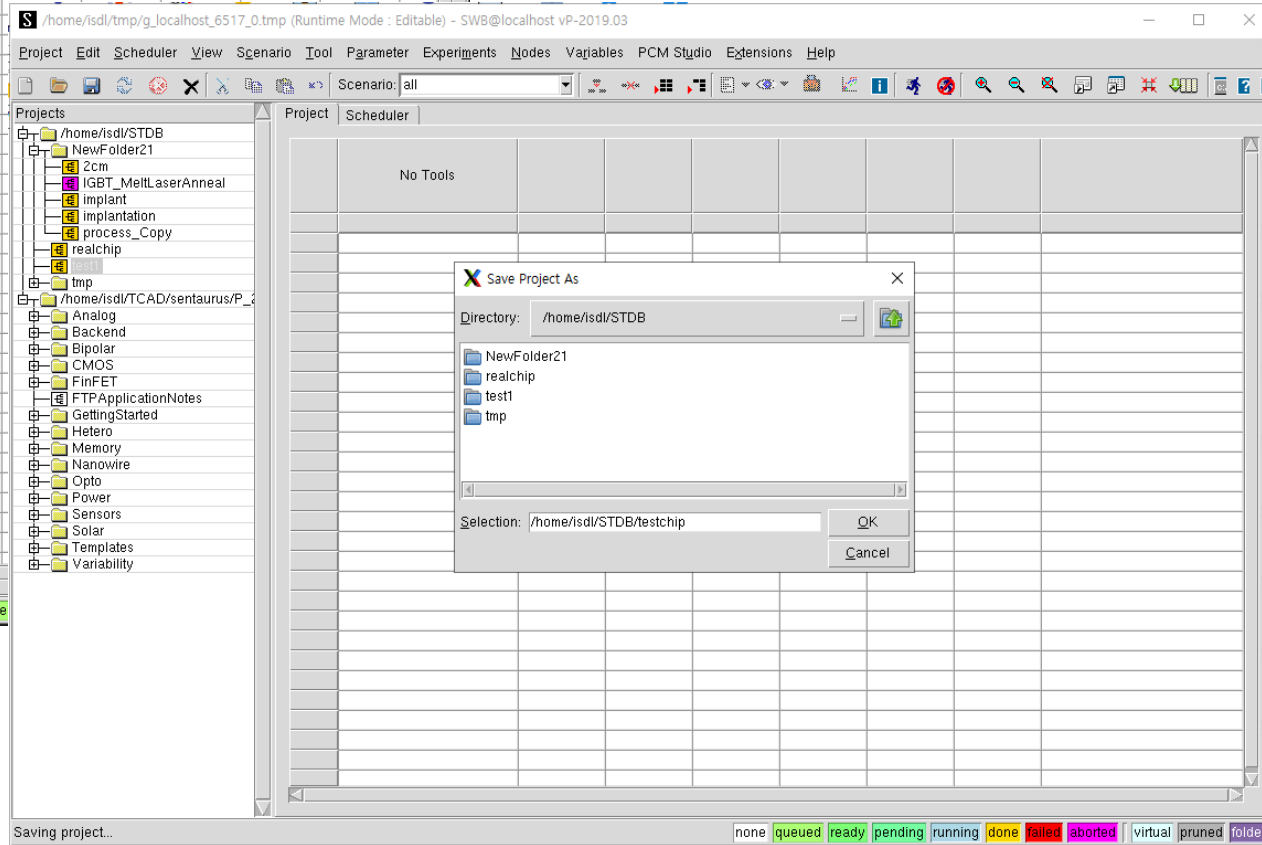
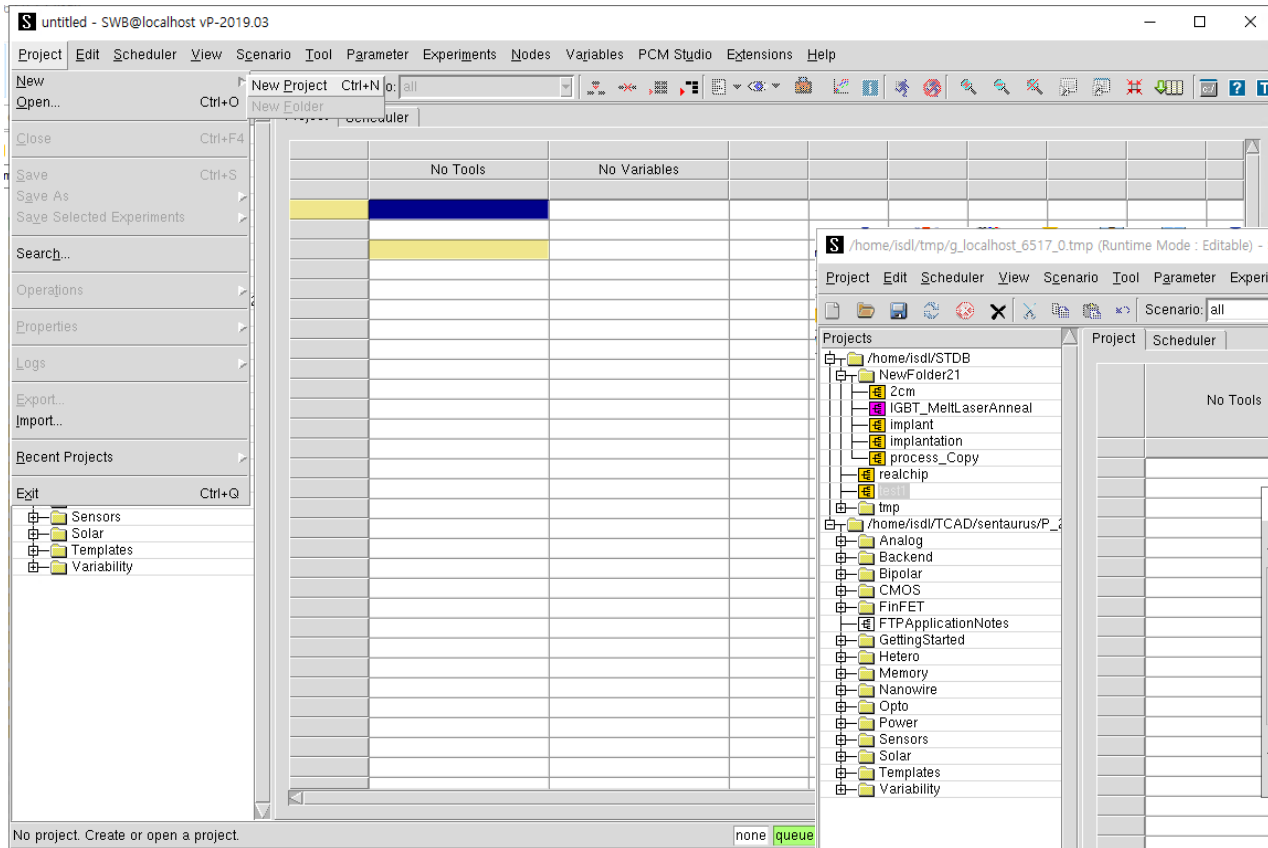
Align key for NNFC



Performance of fabricated chip

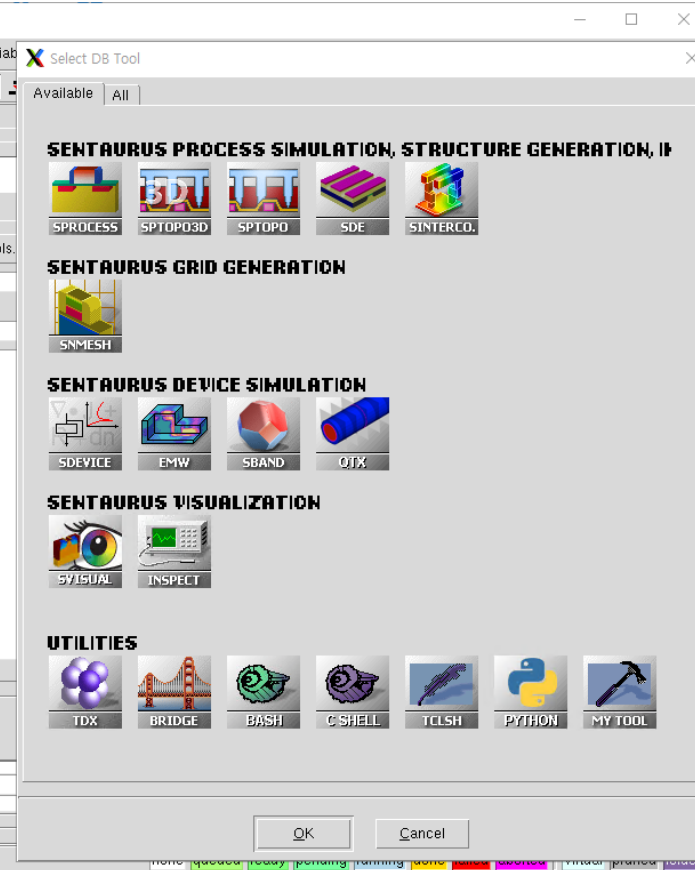
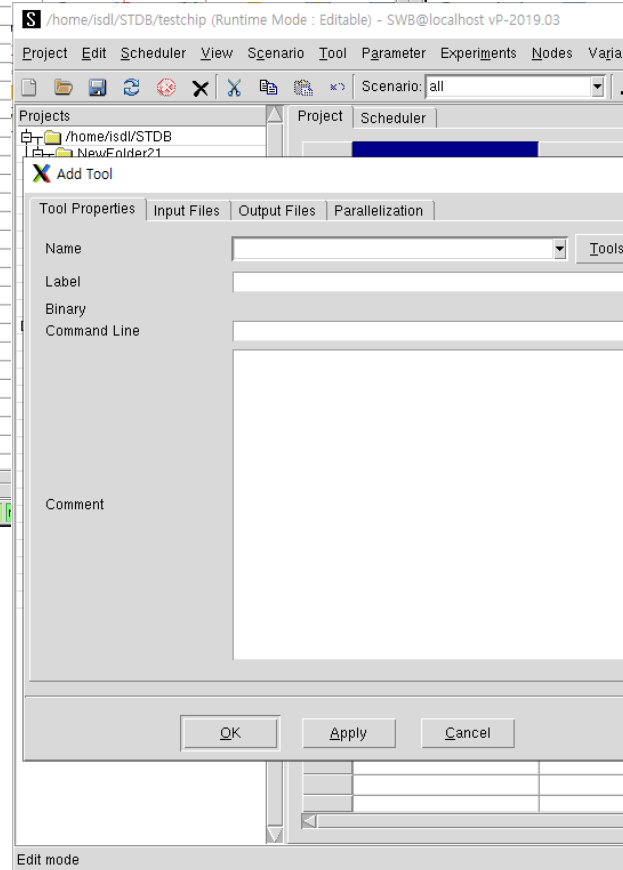
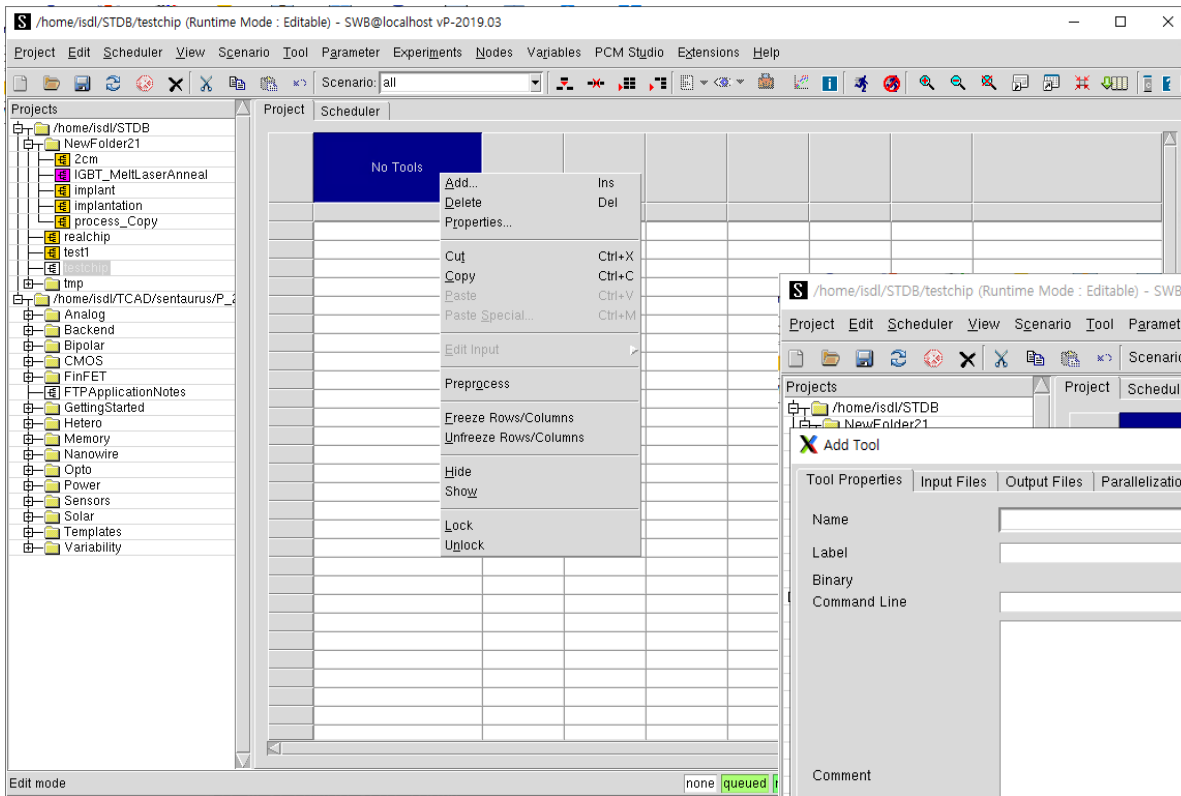


Hands on session

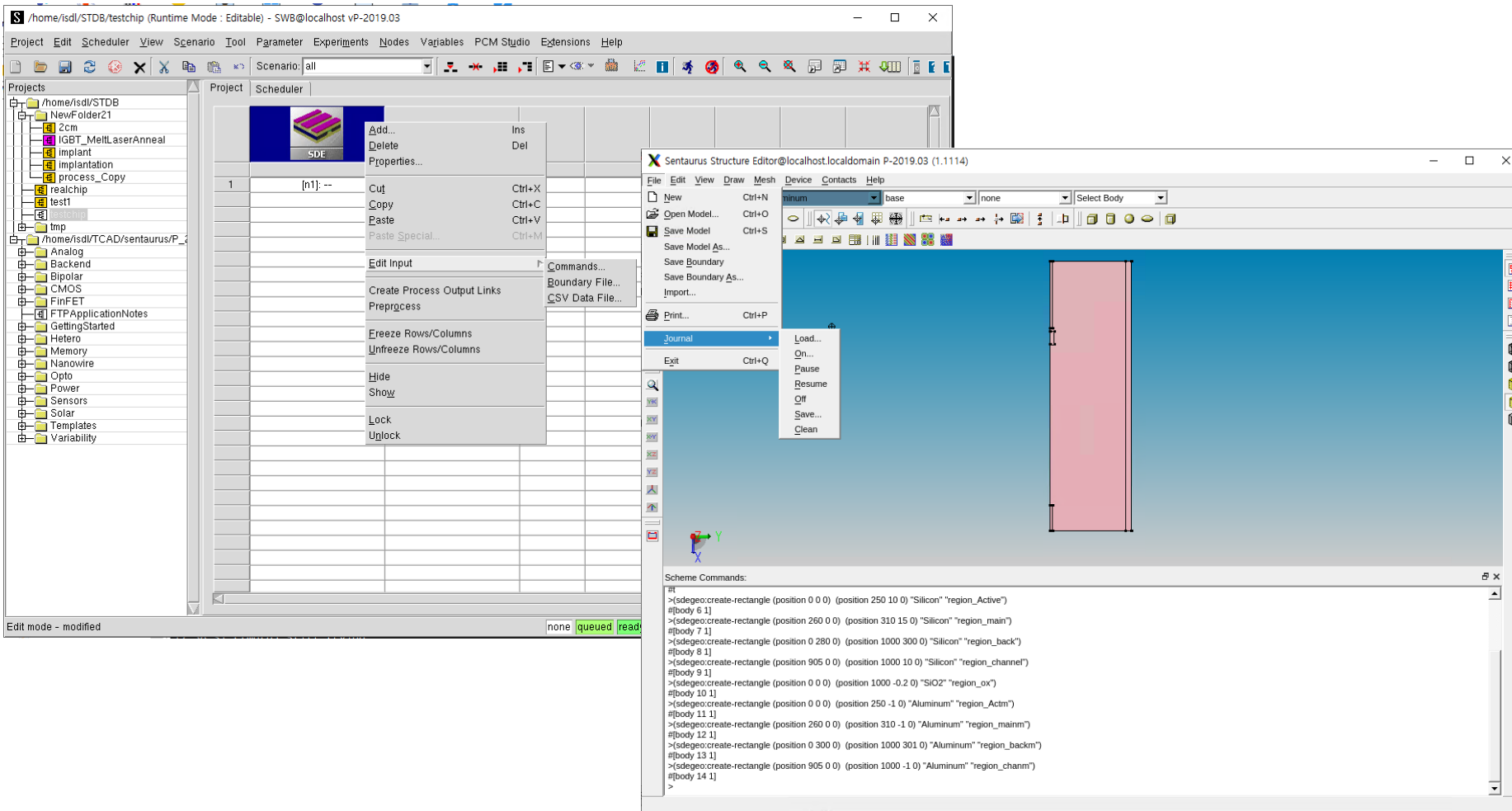


swb -> new project

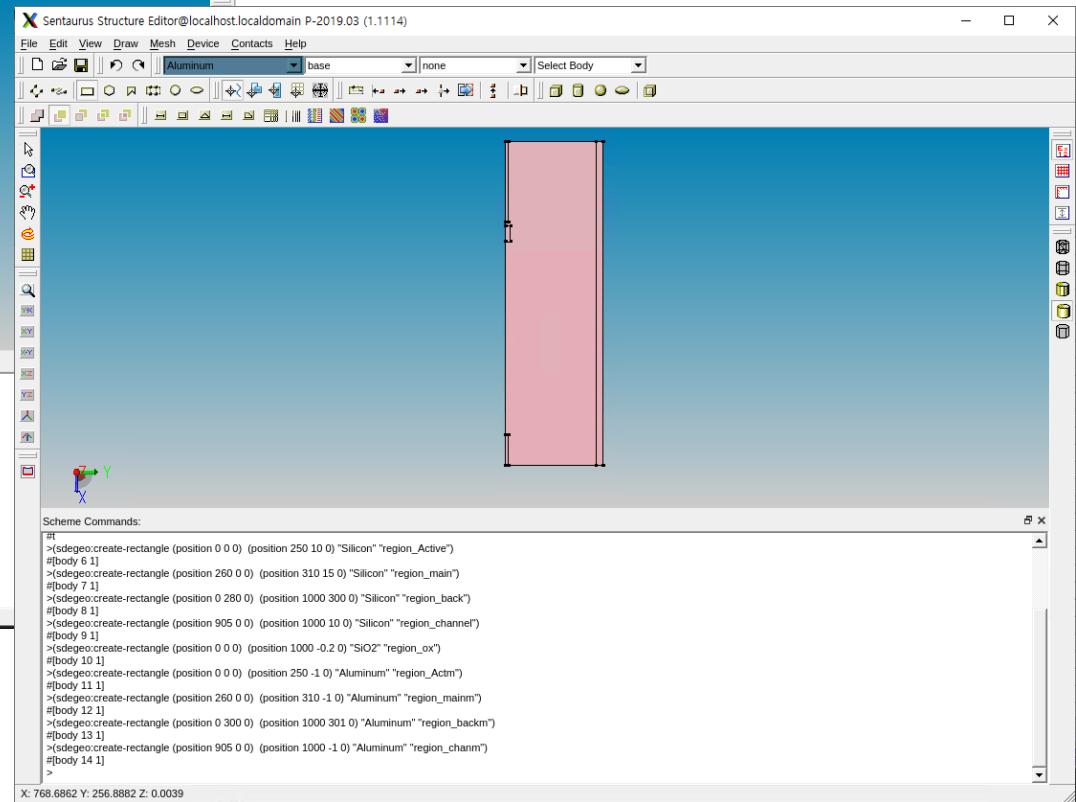
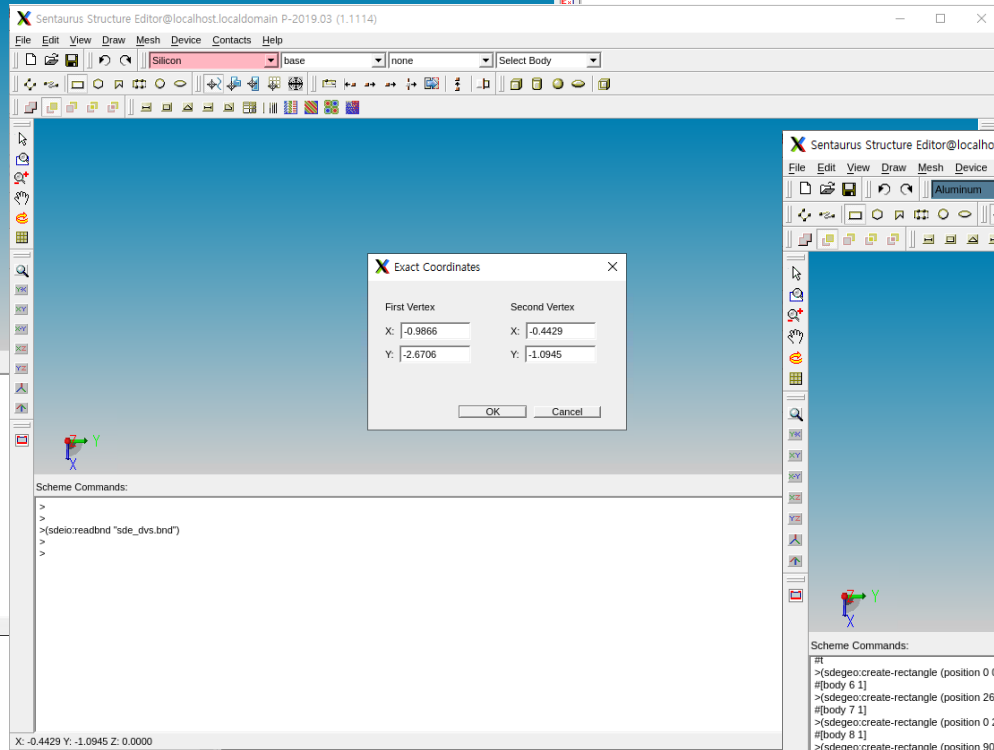
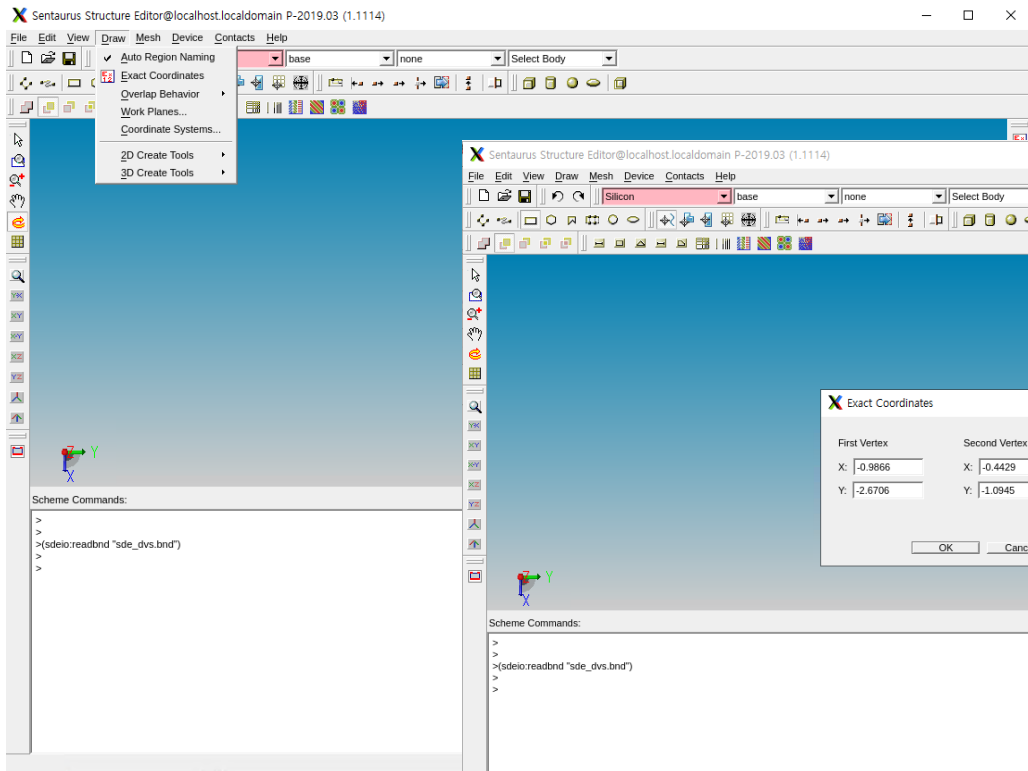
-> Save (경로 STDB)



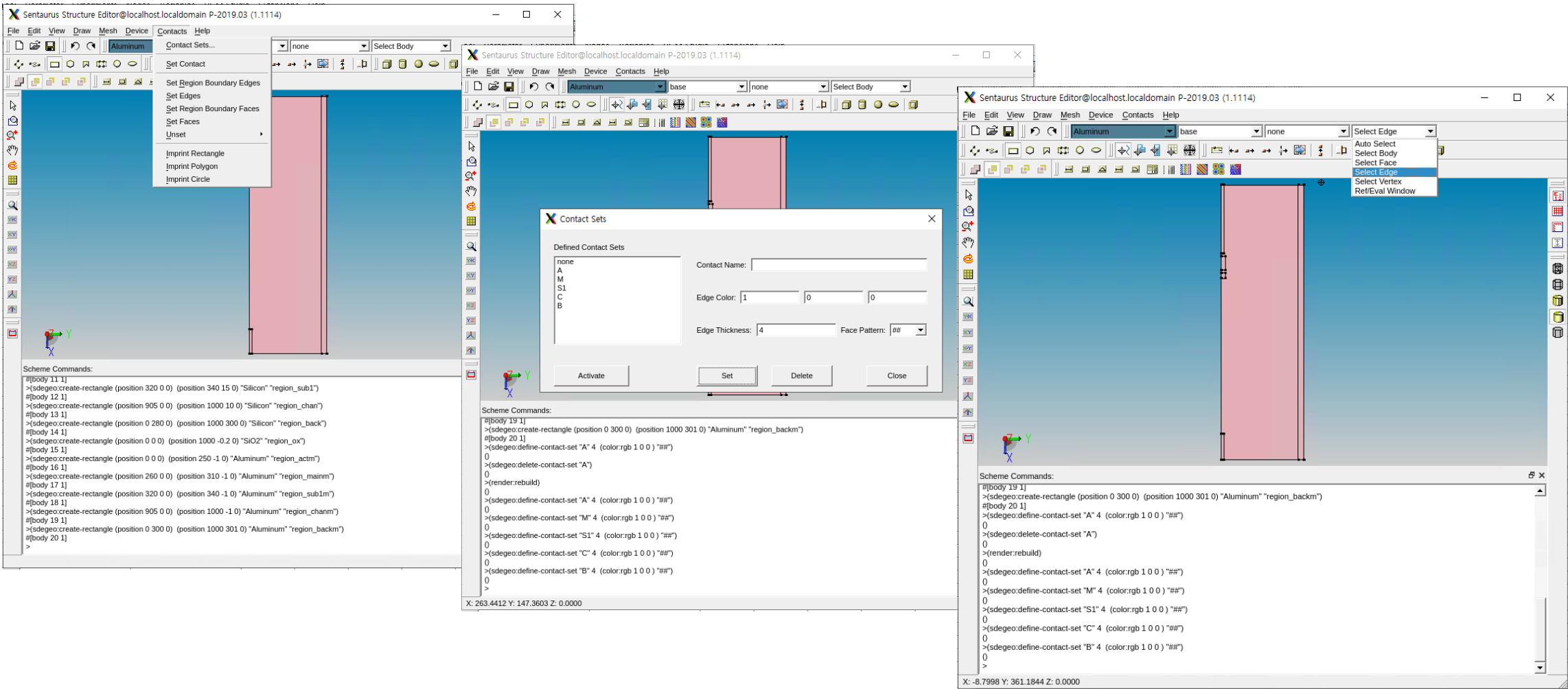
Tools -> Add -> SDE



Boundary File 클릭 -> SDE 창이 뜨면 file -> Journal -> on 클릭(기록용)

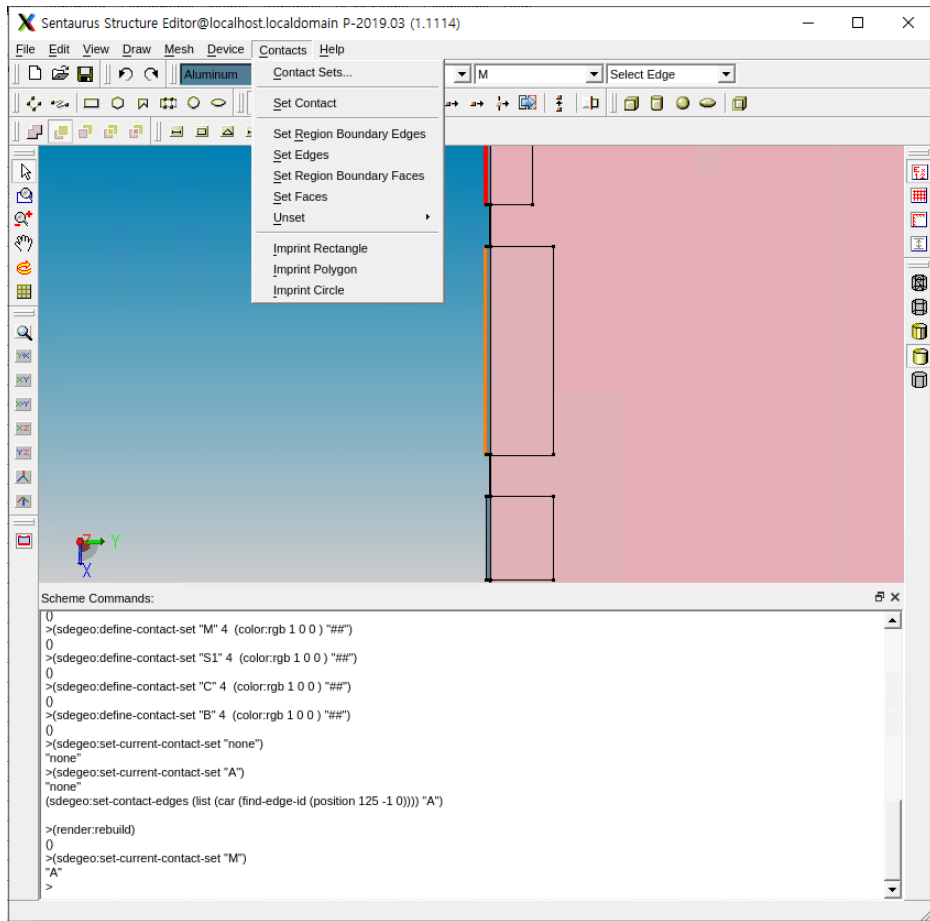


Draw -> exact coordinate -> 사각형 클릭, 단위는 um,
silicon, aluminum 등 선택

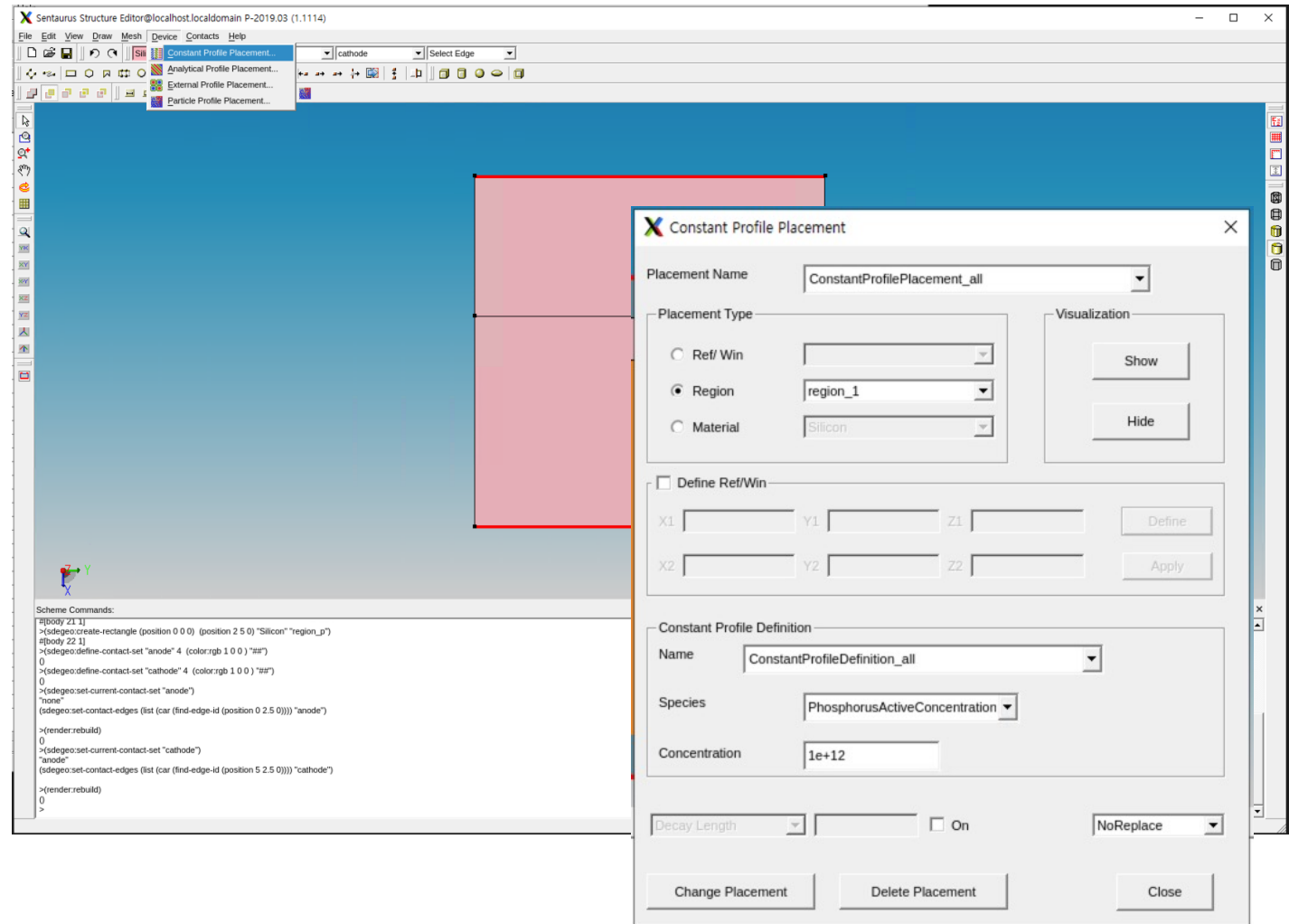


Contacts -> contact Sets -> electrode 만들기

-> select body에서 select edge로 바꾸고 none부분을 지정하고자 하는 이름으로 변경



Electrode 라인 클릭 후 Set contact 클릭



Doping concentration 정하기

Sentaurus Structure Editor@localhost.localdomain P-2019.03 (1.1114)

File Edit View Draw Mesh Device Contacts Help

Define Ref/Eval Window
Delete Ref/Eval Window

Refinement Placement...
Multibox Placement...
Offsetting Parameters...
Clear All

Tools Parameters...
Tensor Parameters...
Delaunizer Parameters...
Axis-Aligned Parameters...
IOControls and Interpolate Parameters...
Quality Report...

Global Refinement...
Facewise Refinement...
Build Mesh

cathode Select Edge

Refinement Specification

Placement Name: RefinementPlacement_all

Placement Type

Ref/Eval Window	Materials	Regions
RefEvaWin_all	Silicon Aluminum	region_1 p_region anode cathode

Define Ref/Eval Window

X1: 0.000000 Y1: 0.000000 Z1: Create

X2: 10.000000 Y2: 10.000000 Z2: Modify

Refinement Definition

Name: RefinementDefinition_all

	X Direction	Y Direction	Z Direction
Max Element Size	0.5	0.5	<input type="text"/>
Min Element Size	0.5	0.5	<input type="text"/>

More >>

Create Refinement Delete Refinement Close

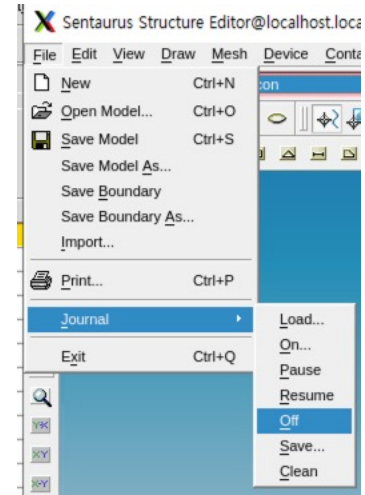
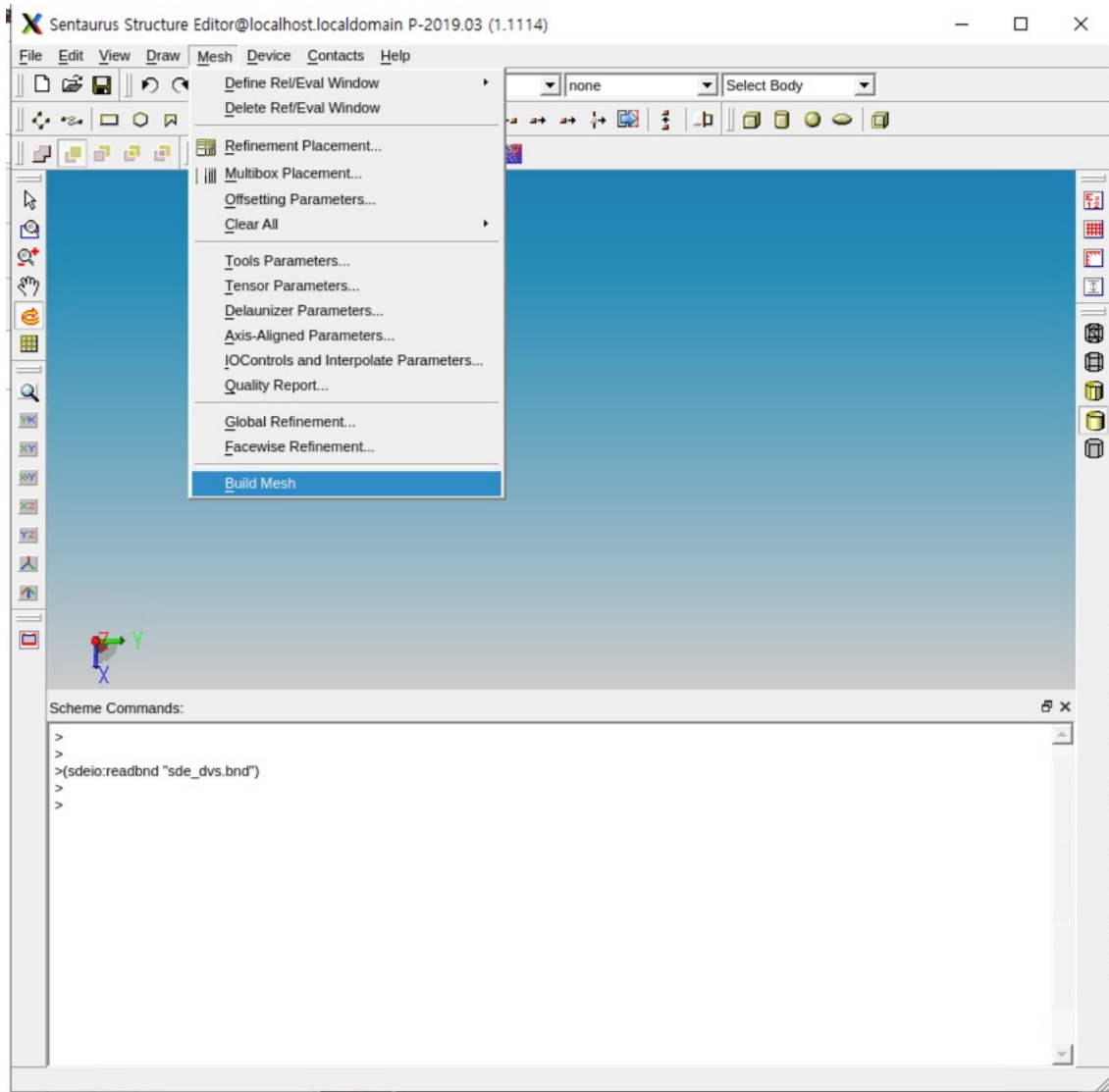
Scheme Commands:

```

0
(sdegeo:set-contact-edges (list (car (find-edge-id (position -1 5 0)))) "anode")
>(render:rebuild)
0
>(sdegeo:set-current-contact-set "cathode")
"anode"
(sdegeo:set-contact-edges (list (car (find-edge-id (position 11 5 0)))) "cathode")
>(render:rebuild)
0
>(sdedr:define-constant-profile "ConstantProfileDefinition_all" "PhosphorusActiveConcentration" 1E+12)
#t
>(sdedr:define-constant-profile-region "ConstantProfilePlacement_all" "ConstantProfileDefinition_all" "region_1")
#t
>(sdedr:define-constant-profile "ConstantProfileDefinition_pdop" "BoronActiveConcentration" 1e+20)
#t
>(sdedr:define-constant-profile-region "ConstantProfilePlacement_pdop" "ConstantProfileDefinition_pdop" "p_region")
#t
>

```

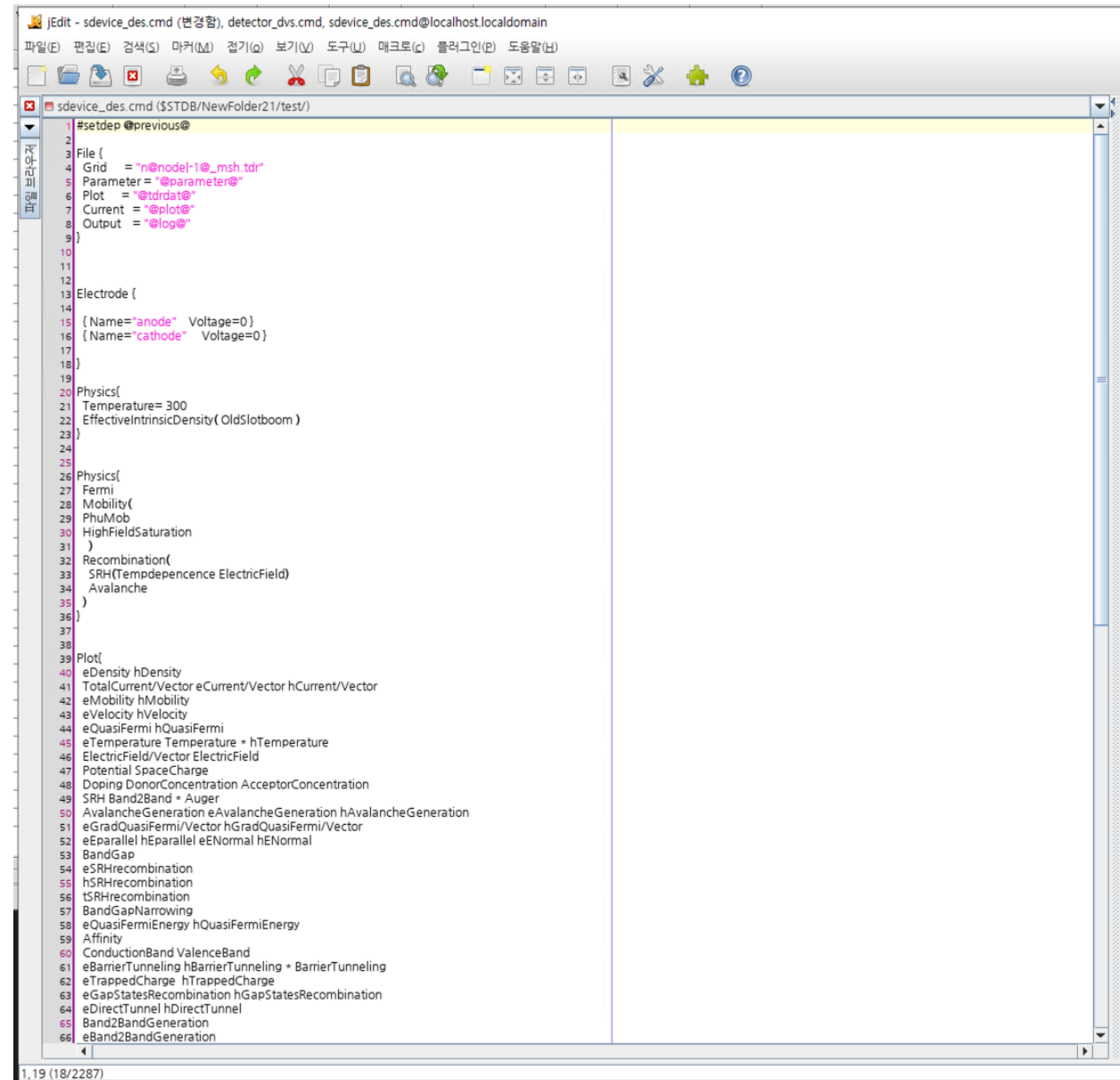
Mesh 설정



완성된 구조 저장하기
Mesh -> Build Mesh

File -> Journal -> off

sdevice



```
JEdit - sdevice_des.cmd (변경됨), detector_dvs.cmd, sdevice_des.cmd@localhost.localdomain
파일(F) 편집(E) 검색(S) 마커(M) 찾기(O) 보기(V) 도구(U) 매크로(C) 플러그인(I) 도움말(H)
sdevice_des.cmd ($STDB/NewFolder21/test/)
1 #setdep @previous@
2
3 File {
4   Grid = "n@node1-1@_msh.tdr"
5   Parameter = "@parameter@"
6   Plot = "@tdrdat@"
7   Current = "@plot@"
8   Output = "@log@"
9 }
10
11
12 Electrode {
13
14
15   {Name="anode" Voltage=0}
16   {Name="cathode" Voltage=0}
17
18 }
19
20 Physics{
21   Temperature= 300
22   EffectiveIntrinsicDensity( OldSlotboom )
23 }
24
25
26 Physics{
27   Fermi
28   Mobility(
29     PhuMob
30     HighFieldSaturation
31   )
32   Recombination(
33     SRH(Tempdependence ElectricField)
34     Avalanche
35   )
36 }
37
38
39 Plot{
40   eDensity hDensity
41   TotalCurrent/Vector eCurrent/Vector hCurrent/Vector
42   eMobility hMobility
43   eVelocity hVelocity
44   eQuasiFermi hQuasiFermi
45   eTemperature Temperature * hTemperature
46   ElectricField/Vector ElectricField
47   Potential SspaceCharge
48   Doping DonorConcentration AcceptorConcentration
49   SRH Band2Band * Auger
50   AvalancheGeneration eAvalancheGeneration hAvalancheGeneration
51   eGradQuasiFermi/Vector hGradQuasiFermi/Vector
52   eEparallel hEparallel eENormal hENormal
53   BandGap
54   eSRHrecombination
55   hSRHrecombination
56   tSRHrecombination
57   BandGapNarrowing
58   eQuasiFermiEnergy hQuasiFermiEnergy
59   Affinity
60   ConductionBand ValenceBand
61   eBarrierTunneling hBarrierTunneling * BarrierTunneling
62   eTrappedCharge hTrappedCharge
63   eGapStatesRecombination hGapStatesRecombination
64   eDirectTunnel hDirectTunnel
65   Band2BandGeneration
66   eBand2BandGeneration
```

1,19 (18/2287)