Advanced TCAD Simulation Techniques

For Wide Bandgap Power Devices

With a Focus on GaN HEMTs

NovaTCAD 20 years ANNIVERSARY

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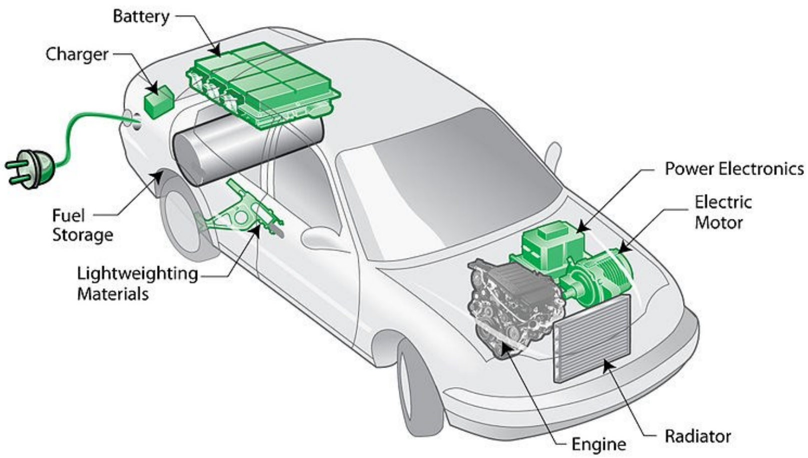
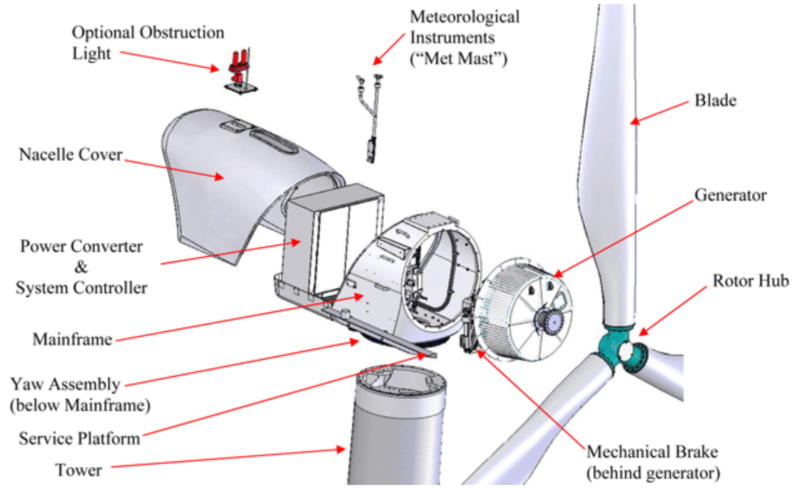
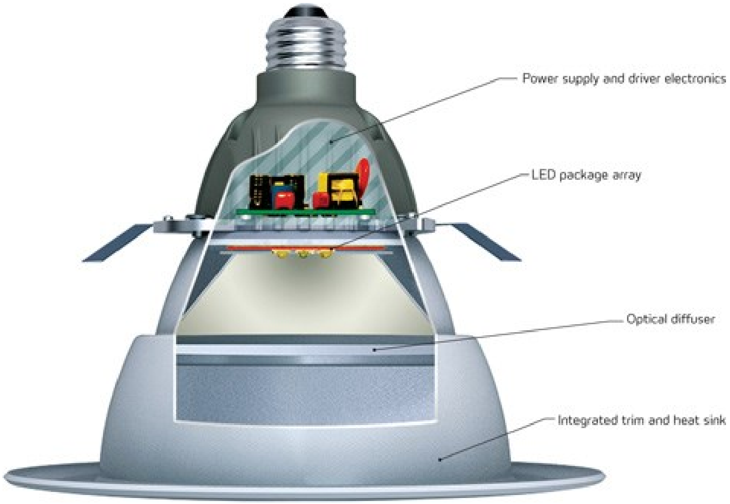
Contents

Power Electronics: *An Enabling Green Technology*







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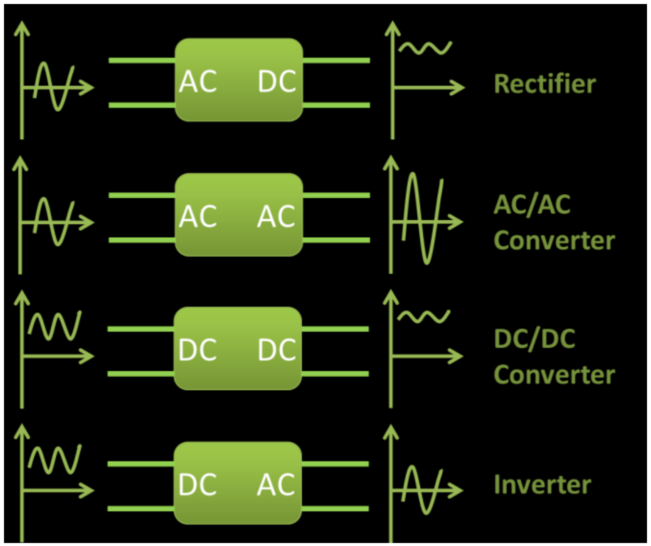
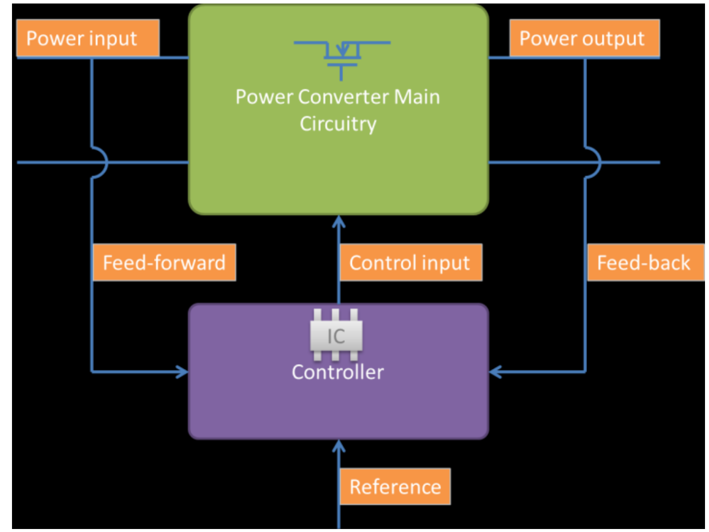
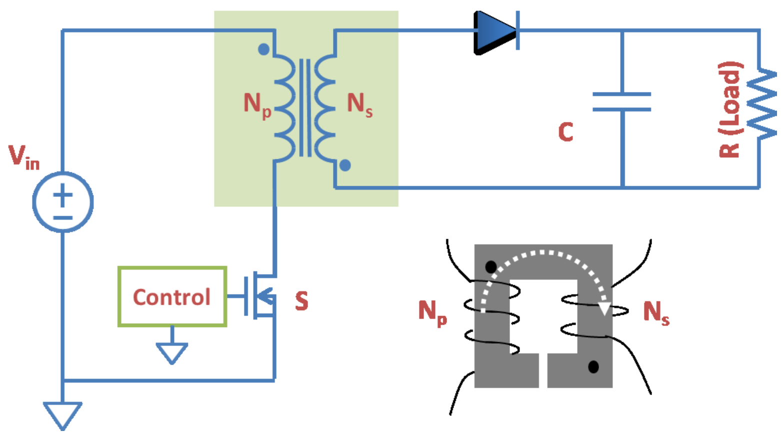
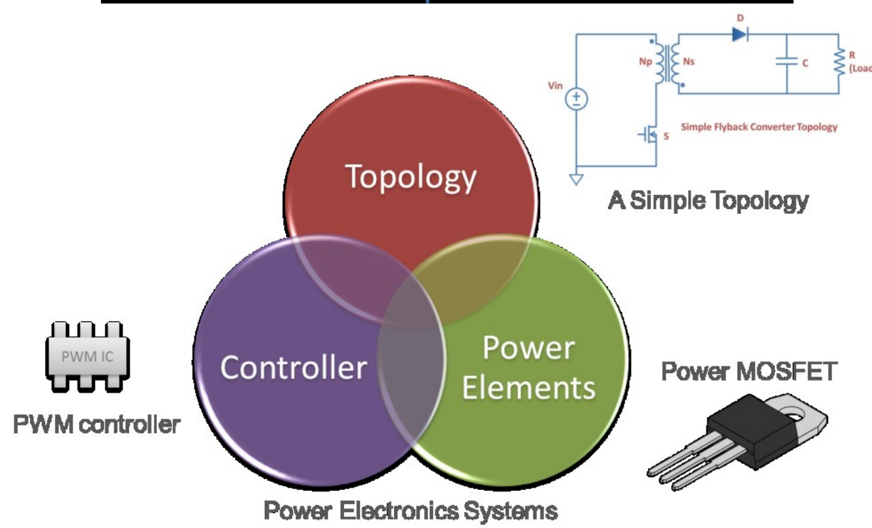
Power Electronics: *The Basics*

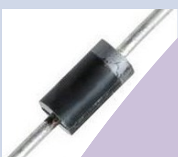
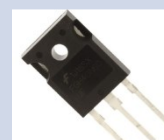
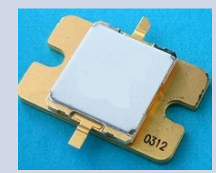








Power Devices: *History of Evolvements*

1952	1957			1980s	1990s~2000s	Now
						
Power Diode Germanium	Thyristor Silicon	Power Bipolar Silicon	Power MOSFET Silicon	IGBT Silicon	Schottky diode Silicon Carbide	Power HEMT GaN

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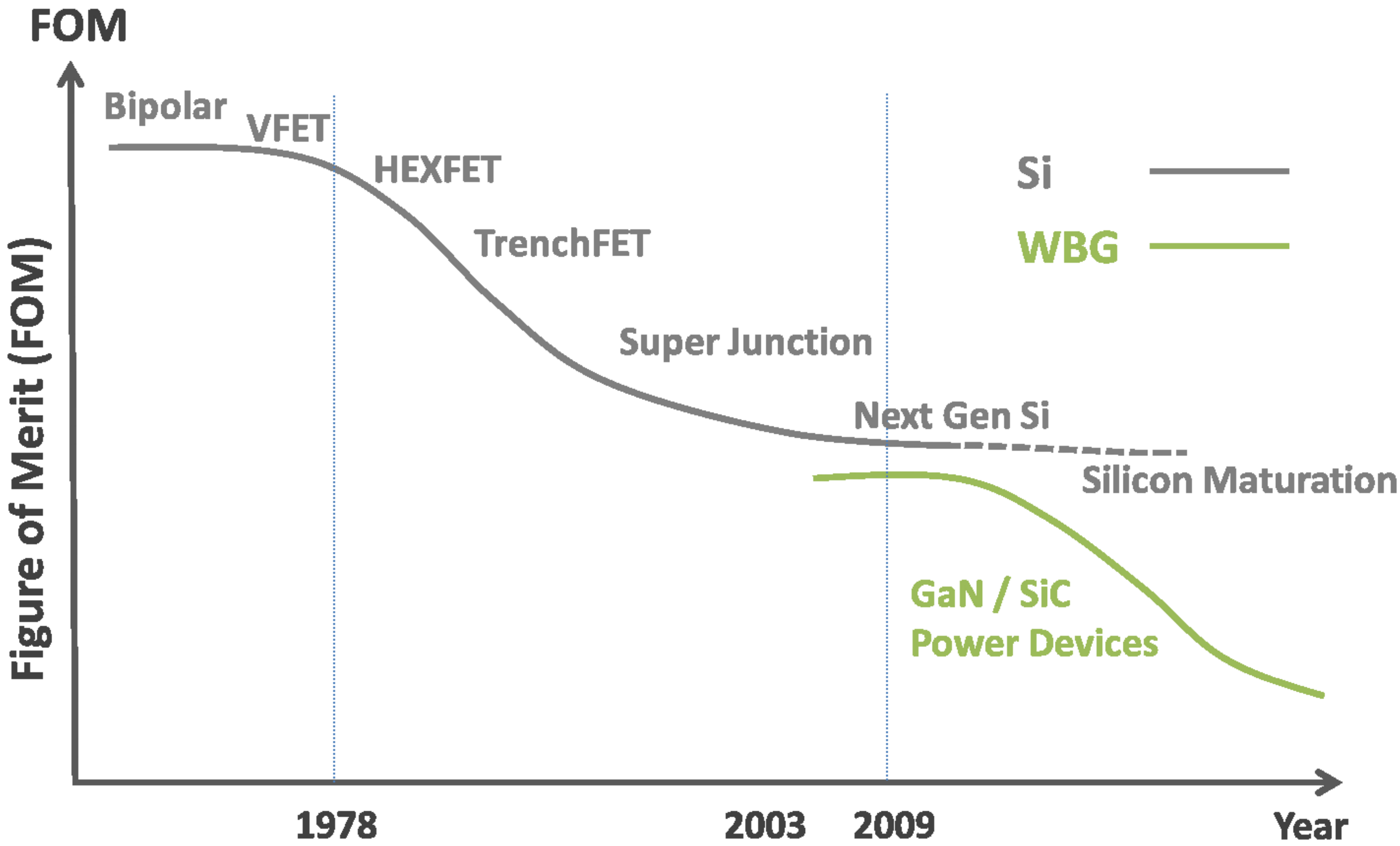
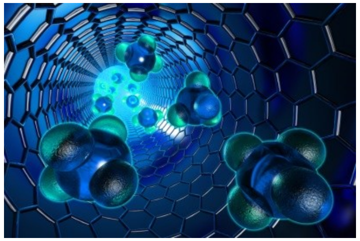
It's time to move on…



Material Properties Comparison



Material Property	Silicon	SiC-4H	GaN
Band-gap (eV)	1.1	3.2	3.4
Critical Field (1E+6V/cm)	0.3	3	3.5
Electron Mobility (cm^2/V-Sec.)	1450	900	2000
Electron Saturation Velocity (1E+6 cm/Sec.)	10	22	25
Thermal Conductivity (W/cm^{2}K)	1.5	3.8	1.3
Baliga Figure of Merit (FOM)=$\varepsilon_s \mu E_c^3$	1	675	3000

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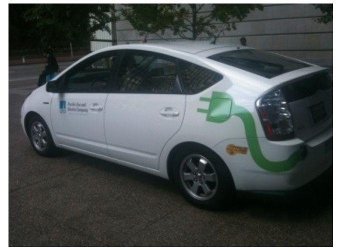
WBG Power Devices: Applications



Consumer Electronics		Automotive		Industrial	
Power Supplies	UPS	DC/AC Inverter	DC/DC Converter	Motor Control	Wind Turbine
< 5KW		30 – 350 KW		100 KW – 1 MW	
GaN and SiC in Competition				SiC Only	

Reference: Jian-Jang Huang, NTU, “GaN/Si HEMT power devices” III-V Nitride Material and Device Modeling workshop, Taiwan, 2014

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Substrate Materials for GaN HEMT

Attributes	Si substrate	SiC substrate	GaN substrate
Defect density (cm^{-2})	1E+9	5E+8	1E+3 to 1E+5
Lattice mismatch (%)	17	3.5	0
Thermal conductivity (W/cm-k at 25 ^{o}C)	1.5	3.0~3.8	1.3
Coefficients of thermal expansions (%)	54	25	0
Off-state leakage	high	high	low
Reliability and yield	low	low	high
Lateral or Vertical device	lateral	lateral	lateral or vertical
Integration possibility	Very high	Moderate	-
Substrate size (mm) (as of 2012)	300	150	50
Substrate cost (relative)	Low	high	Very high

Power RF

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Global Research Activities for GaN HEMTs

** Due to limited space, this diagram is by far not showing the complete companies and institutions that are active in GaN HEMT research*

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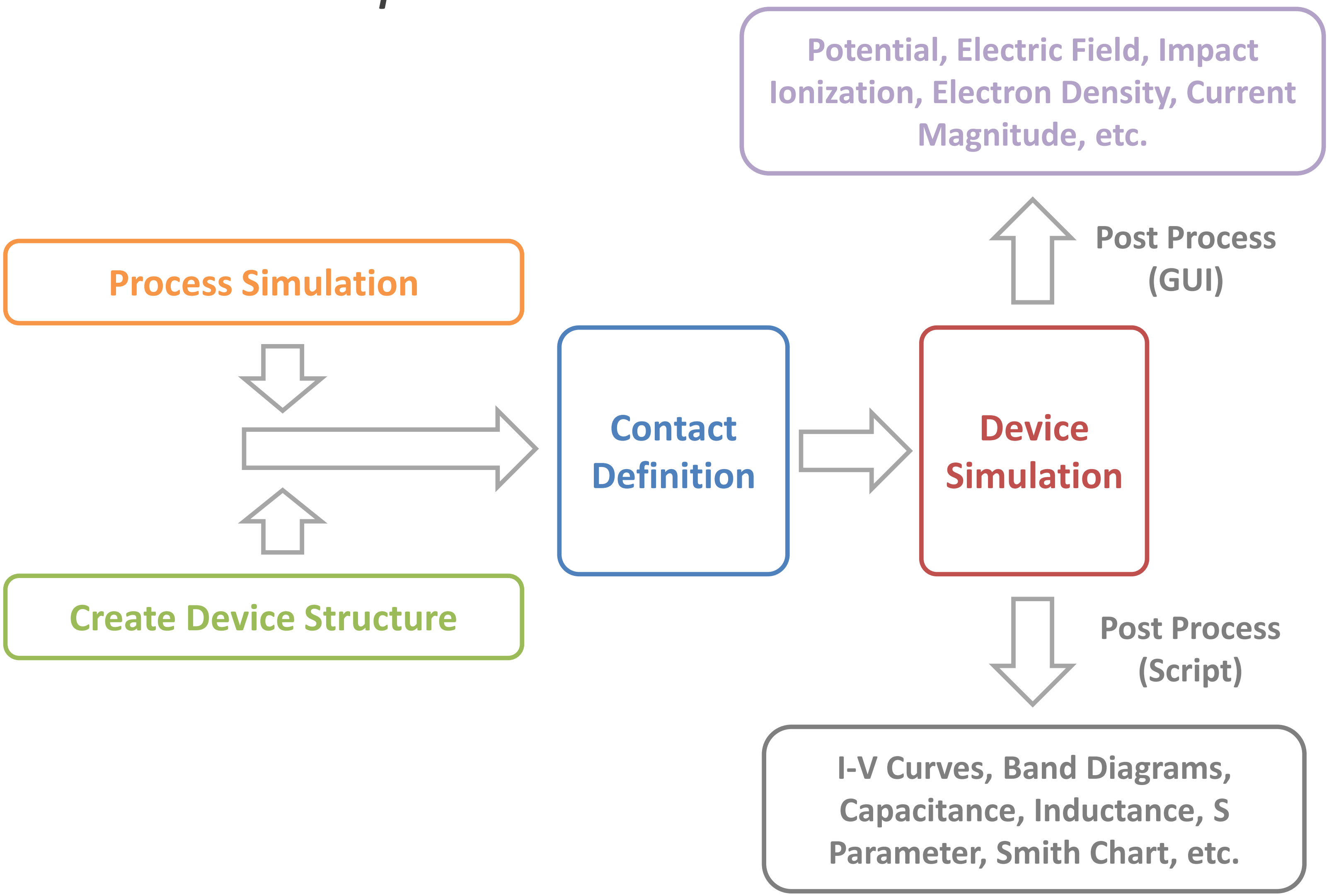
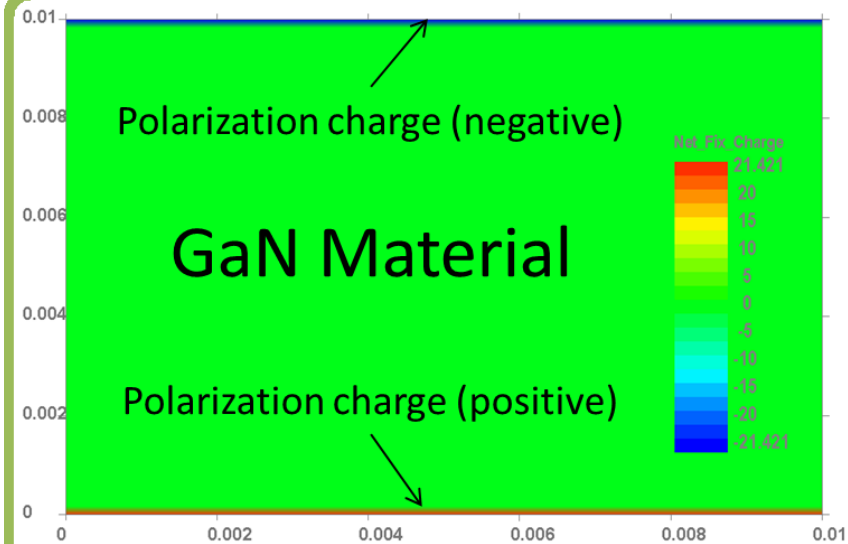
Simulation Steps

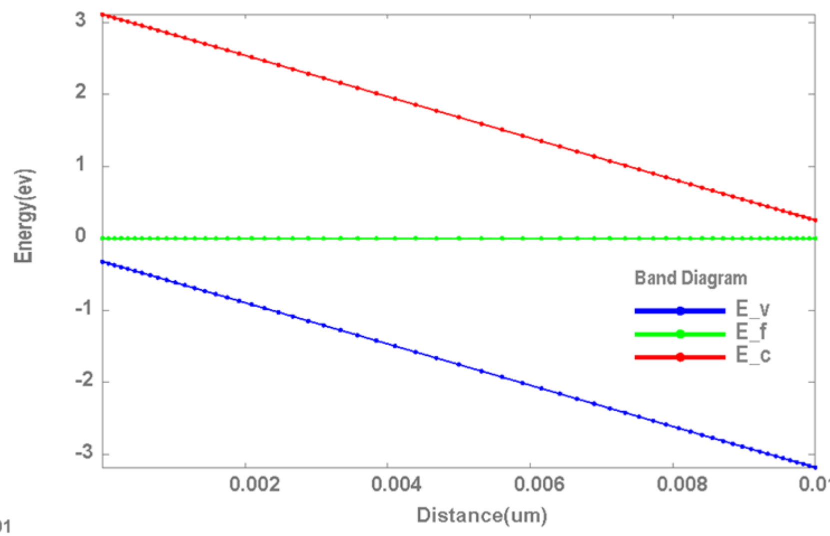


GaN Single Layer

Single GaN layer simulation with polarization and band diagram plots



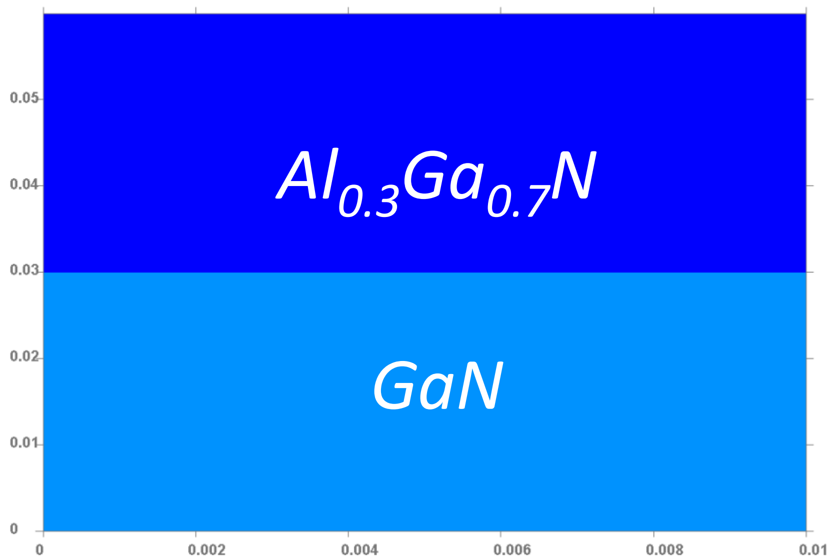
(a) Simulated GaN material polarization effect

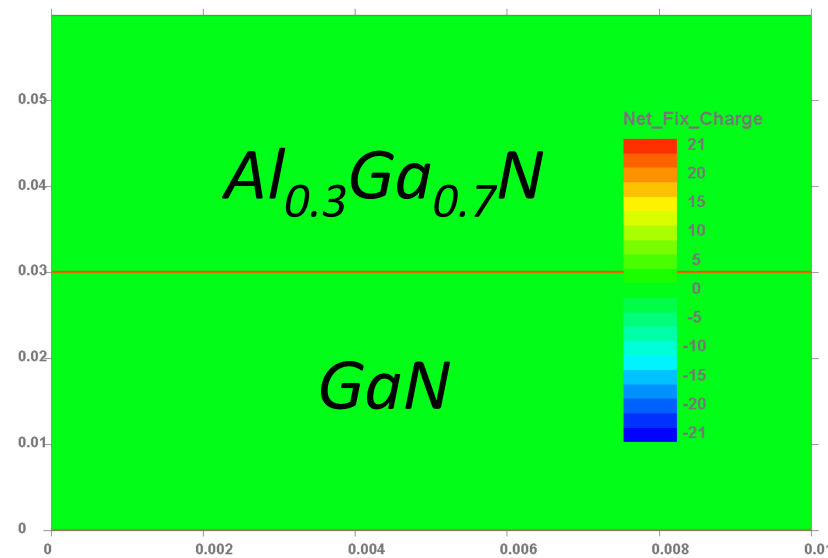


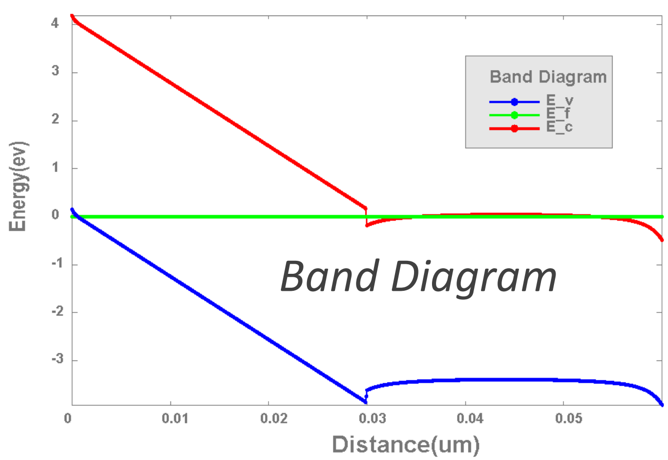
(b) Band diagram plot of GaN material (cut line from top to bottom)

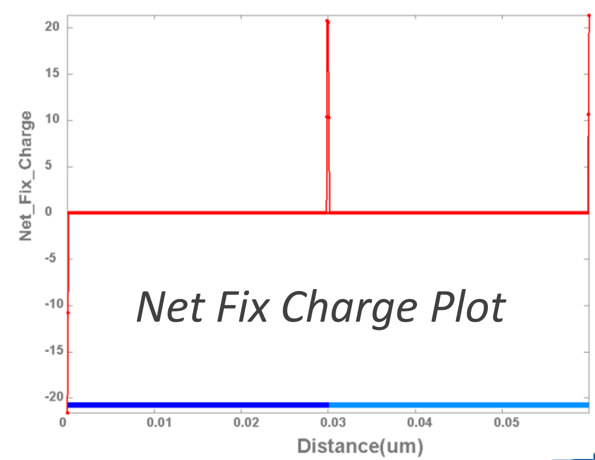
Polarization model should be activated, otherwise the band diagram will be flat

GaN + AlGaN Layers



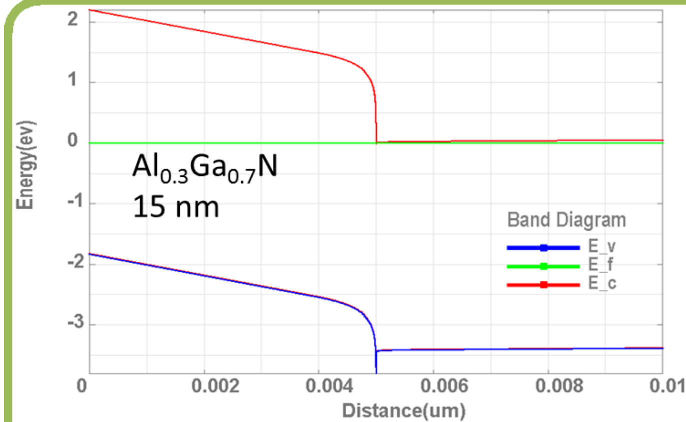




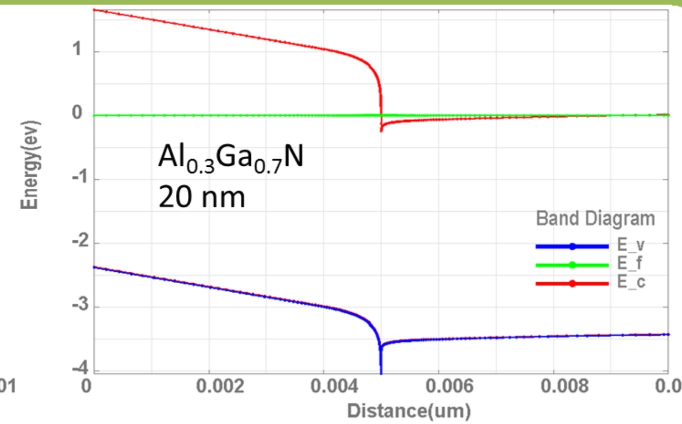


GaN + AlGaN Layers: AlGaN Layer Thickness

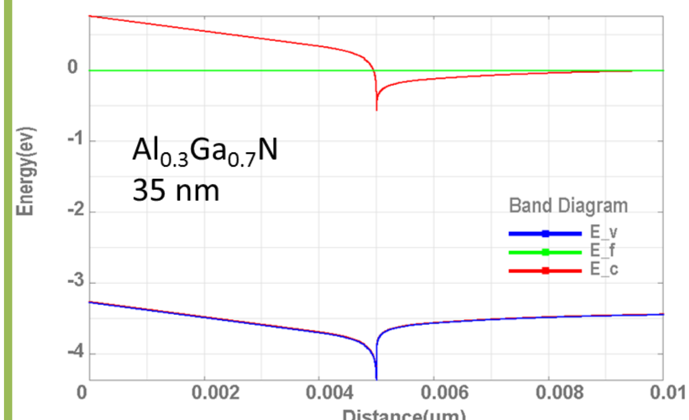
Band diagram at equilibrium of GaN-AlGaN structure with various AlGaN layer thickness



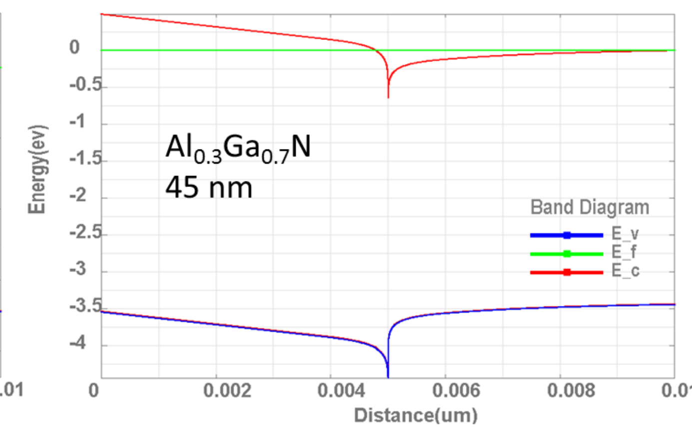
(a) Band diagram plot of GaN-AlGaN structure with $Al_{0.3}Ga_{0.7}N$ layer thickness of 15 nm



(b) Band diagram plot of GaN-AlGaN structure with $Al_{0.3}Ga_{0.7}N$ layer thickness of 20 nm



(c) Band diagram plot of GaN-AlGaN structure with $Al_{0.3}Ga_{0.7}N$ layer thickness of 35 nm



(d) Band diagram plot of GaN-AlGaN structure with $Al_{0.3}Ga_{0.7}N$ layer thickness of 45 nm

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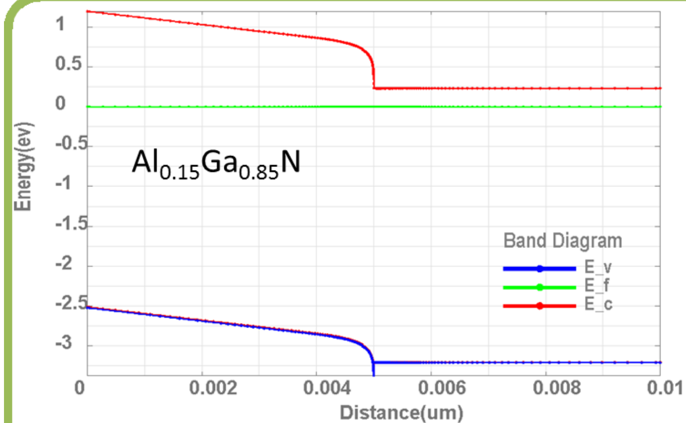
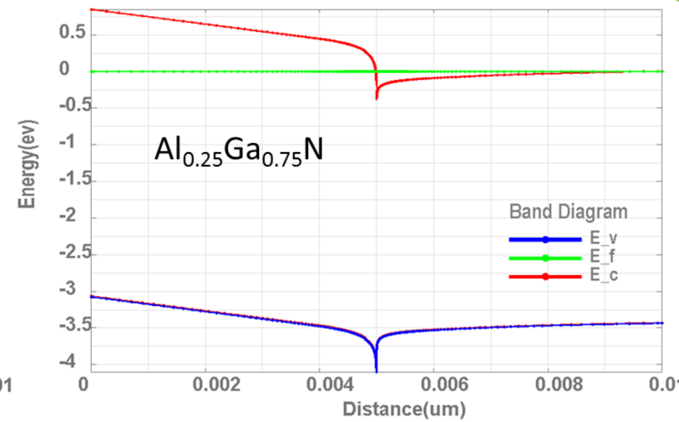
GaN + AlGaN Layers: *Al Mole Fraction in AlGaN*

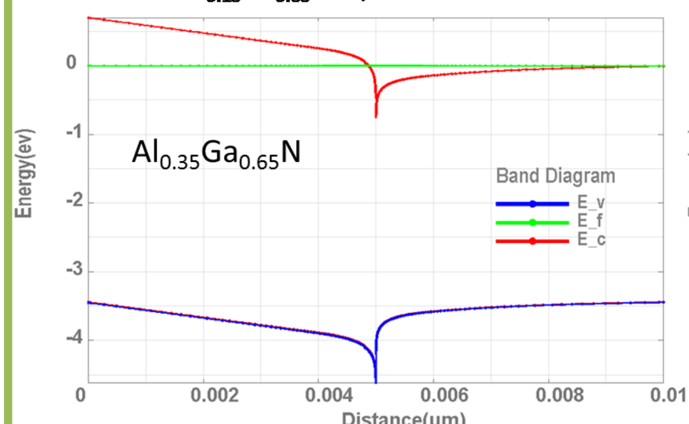
Band diagram at equilibrium of GaN-AlGaN structure with various Al mole fraction



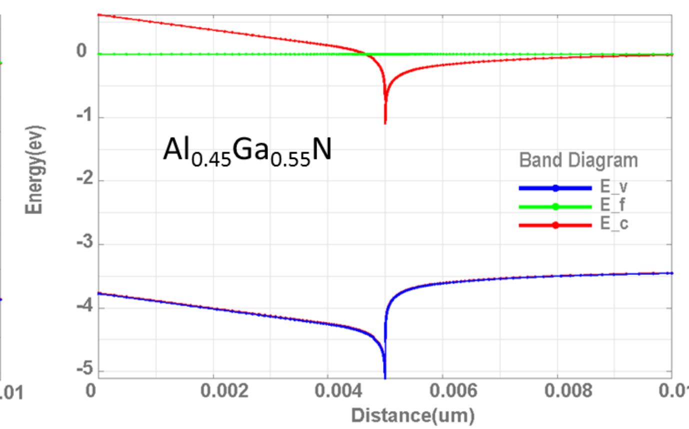
(a) Band diagram plot of GaN-AlGaN structure with $Al_{0.15}Ga_{0.85}N$ layer thickness of 30 nm



(b) Band diagram plot of GaN-AlGaN structure with $Al_{0.25}Ga_{0.75}N$ layer thickness of 30 nm



(c) Band diagram plot of GaN-AlGaN structure with $Al_{0.35}Ga_{0.65}N$ layer thickness of 30 nm



(d) Band diagram plot of GaN-AlGaN structure with $Al_{0.45}Ga_{0.55}N$ layer thickness of 30 nm

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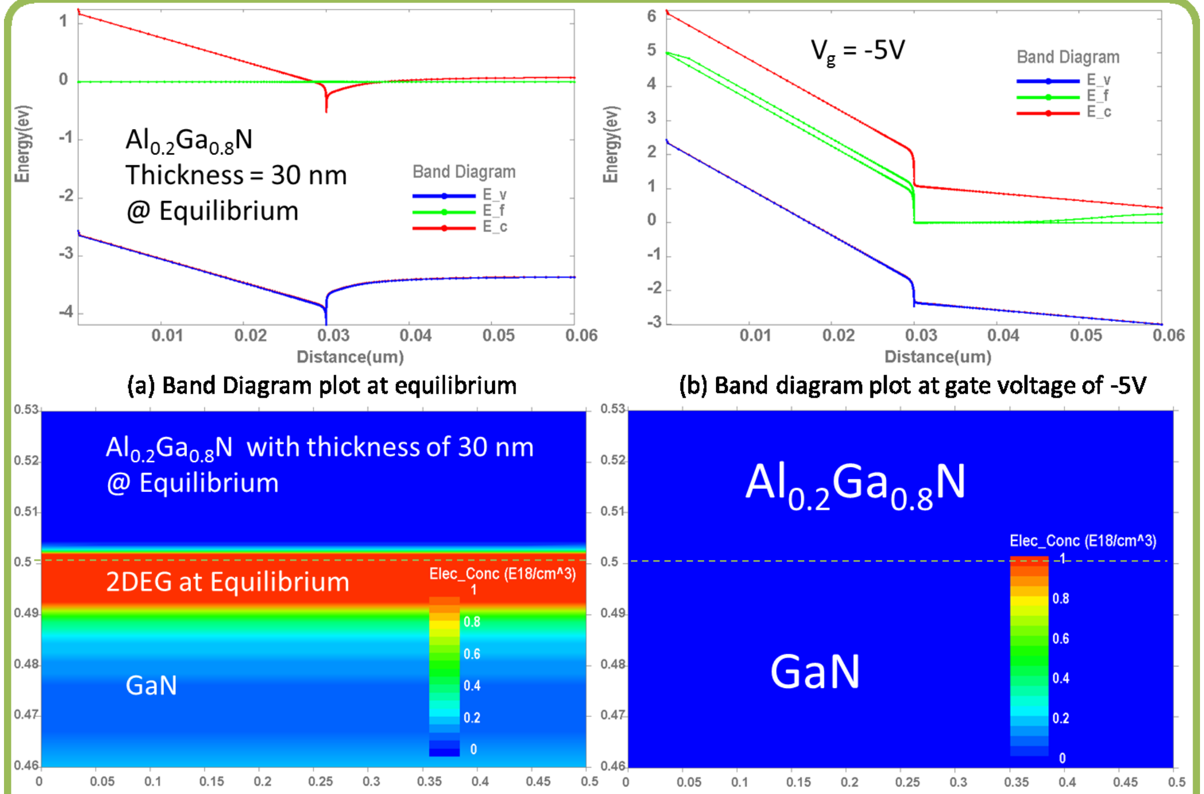
GaN + AlGaN + Contacts

Band diagram and electron concentration plots at equilibrium and at V_g = -5V



(a) Band Diagram plot at equilibrium

(b) Band diagram plot at gate voltage of -5V

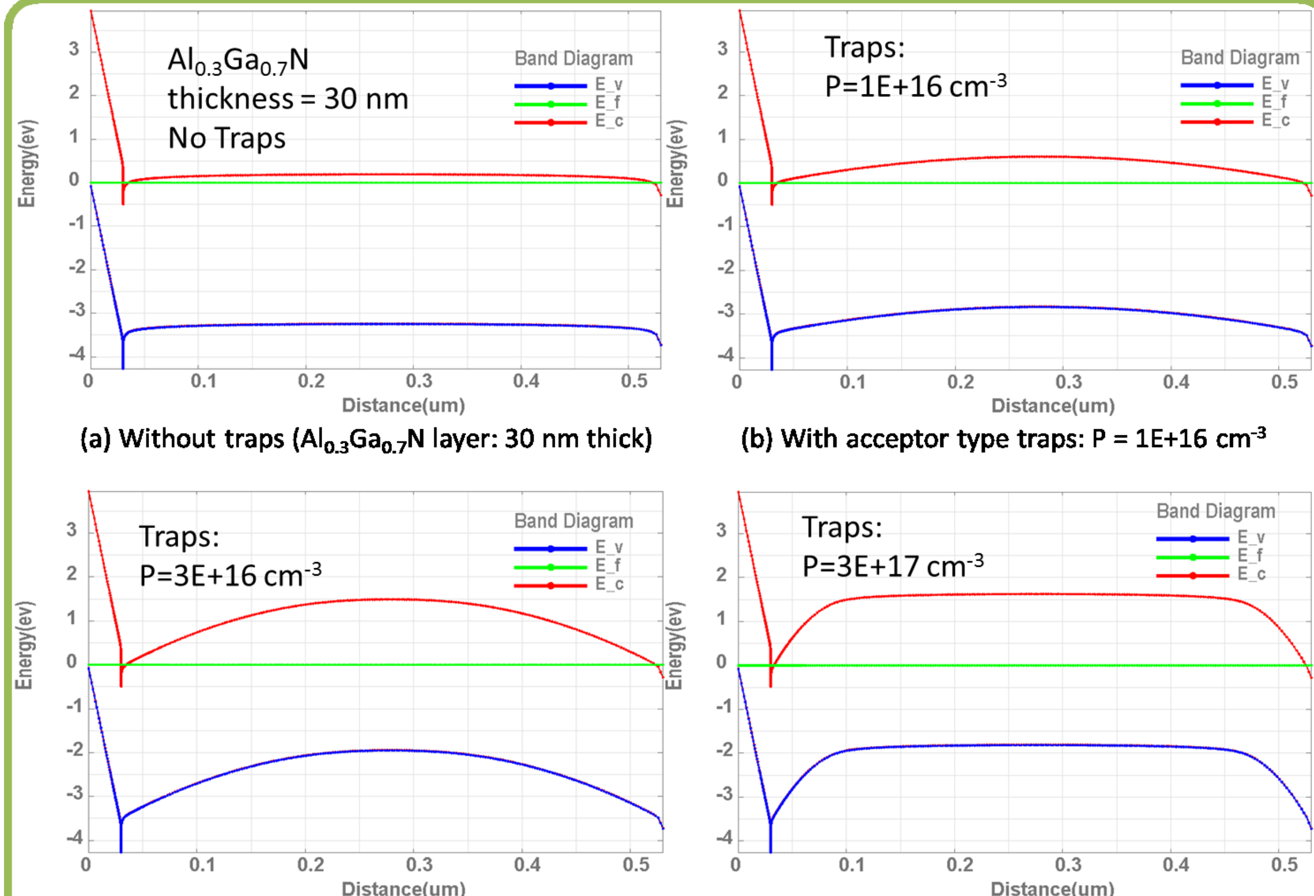
(c) Electron concentration at equilibrium

(d) Electron concentration at gate voltage of -5V

A Schottky contact (work function = 5.1 eV) is applied to the top of AlGaN layer while an Ohmic contact is applied to the bottom of GaN layer. -5V is applied to the top Schottky contact with bottom Ohmic contact grounded.

P Type of Traps in the GaN Layer

Band diagram at equilibrium of GaN-AlGaN structure with different trap placement



(a) Without traps ($Al_{0.3}Ga_{0.7}N$ layer: 30 nm thick)

(b) With acceptor type traps: P = 1E+16 cm^{-3}

(c) With acceptor type traps: P = 3E+16 cm^{-3}

(d) With acceptor type traps: P = 3E+17 cm^{-3}

Traps are placed in the GaN layer to model a semi-insulating substrate and prevent leakage current under the 2DEG channel

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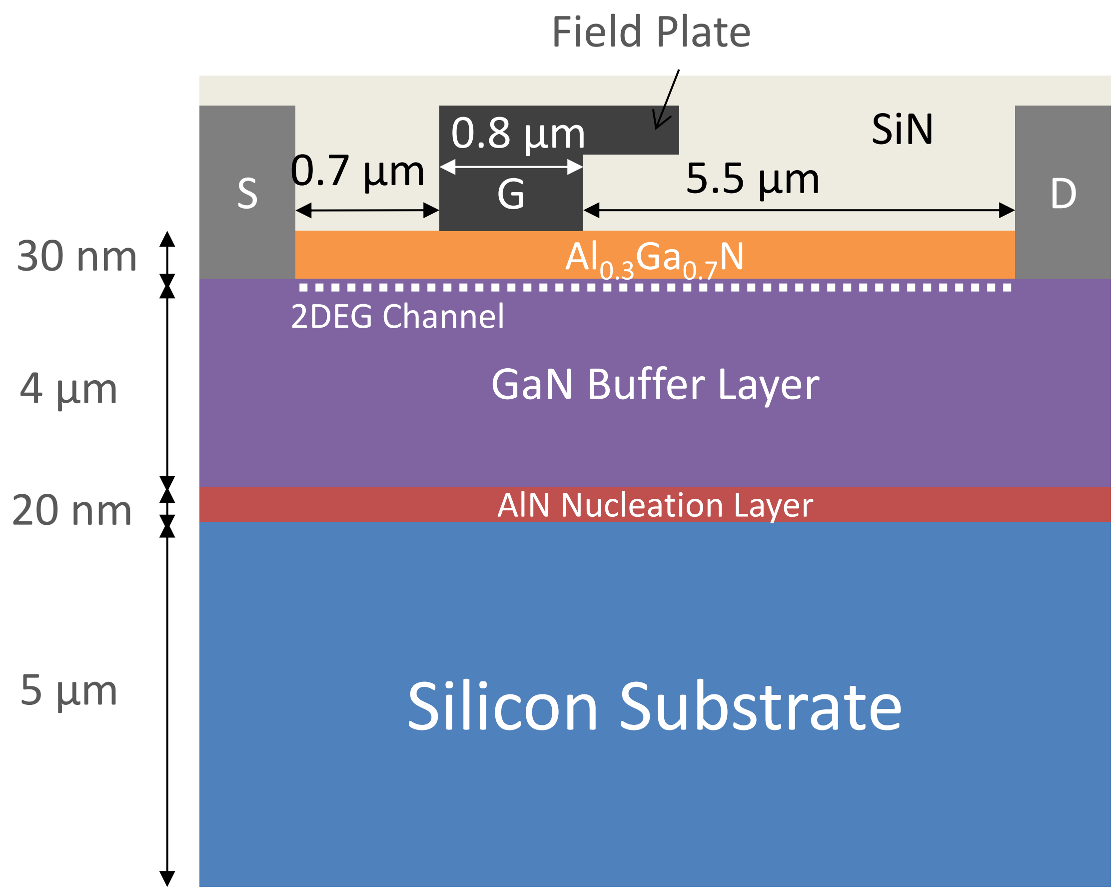
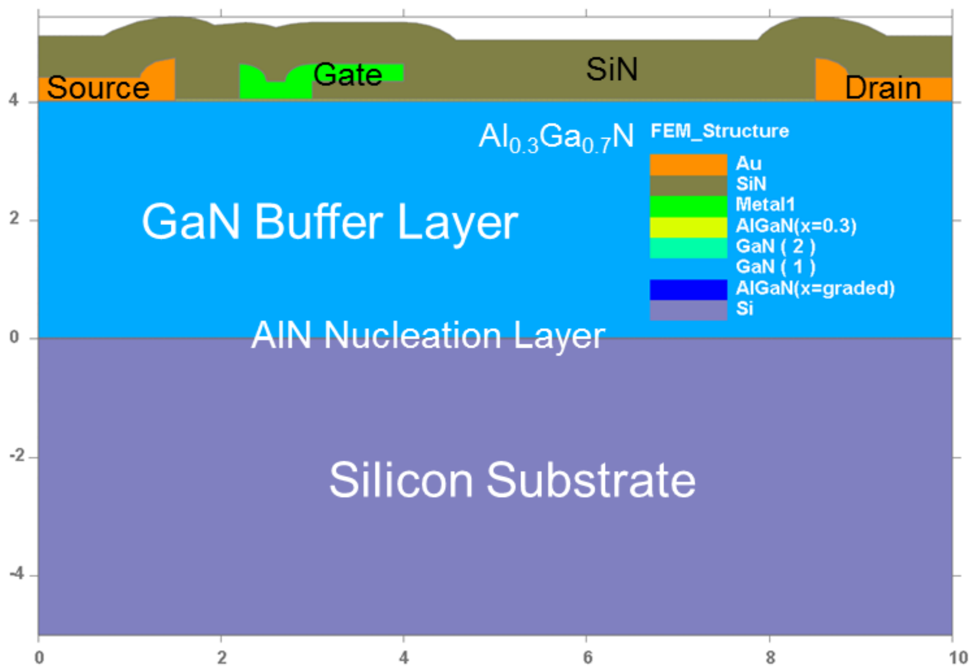
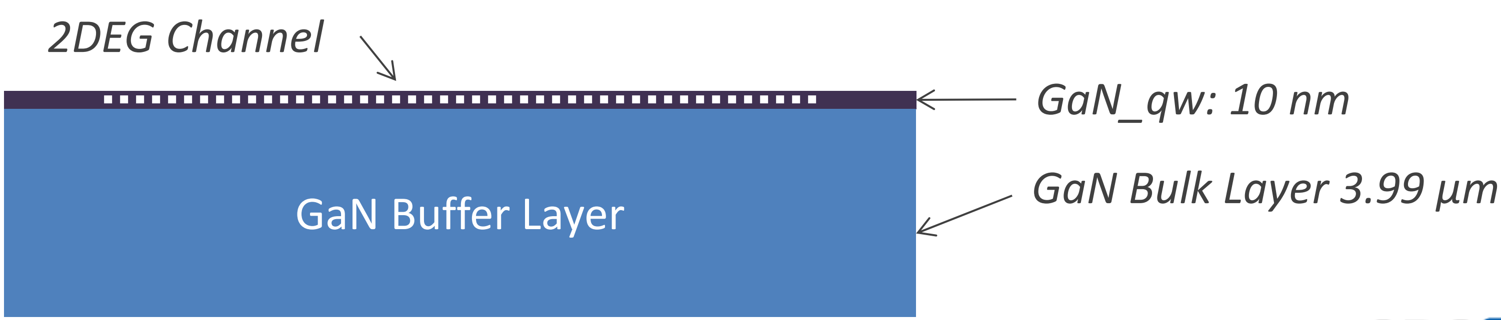
A Simple GaN Power HEMT Example



Simulation Setup:



- Intrinsic stress can be applied in the SiN layer to simulate the stress effect
- Polarization charge model is applied with a screening factor
- Interface charges / traps can be placed to simulate the surface states
- P type traps are placed in the GaN buffer layer to make it semi-insulating



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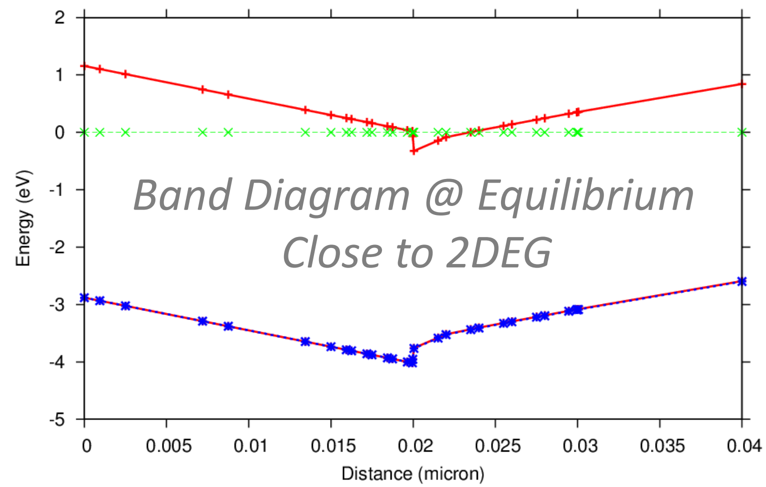
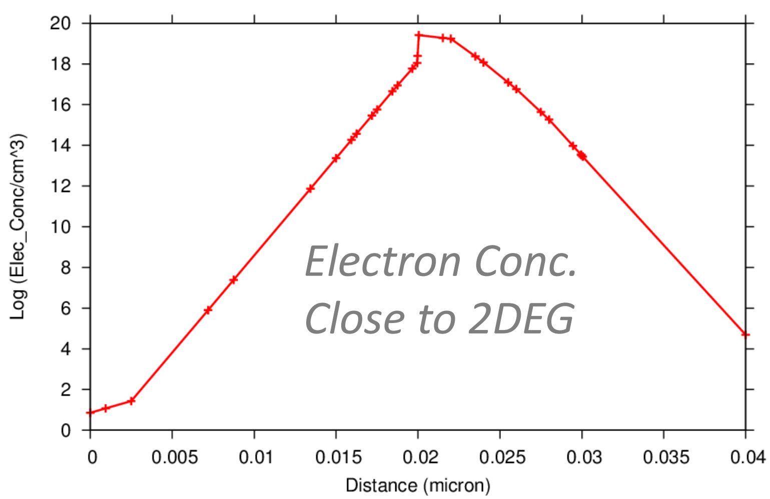
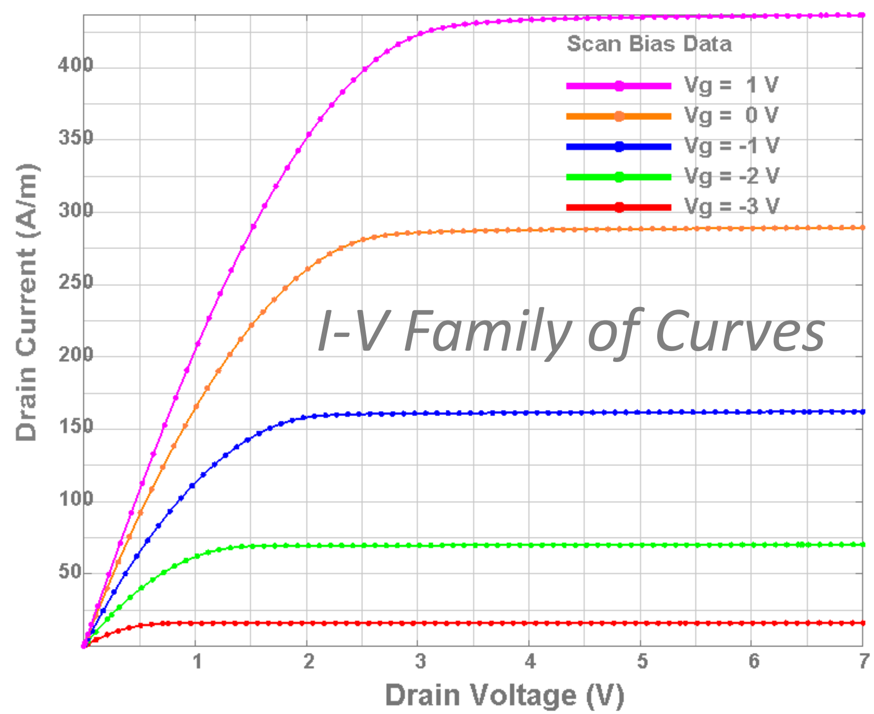
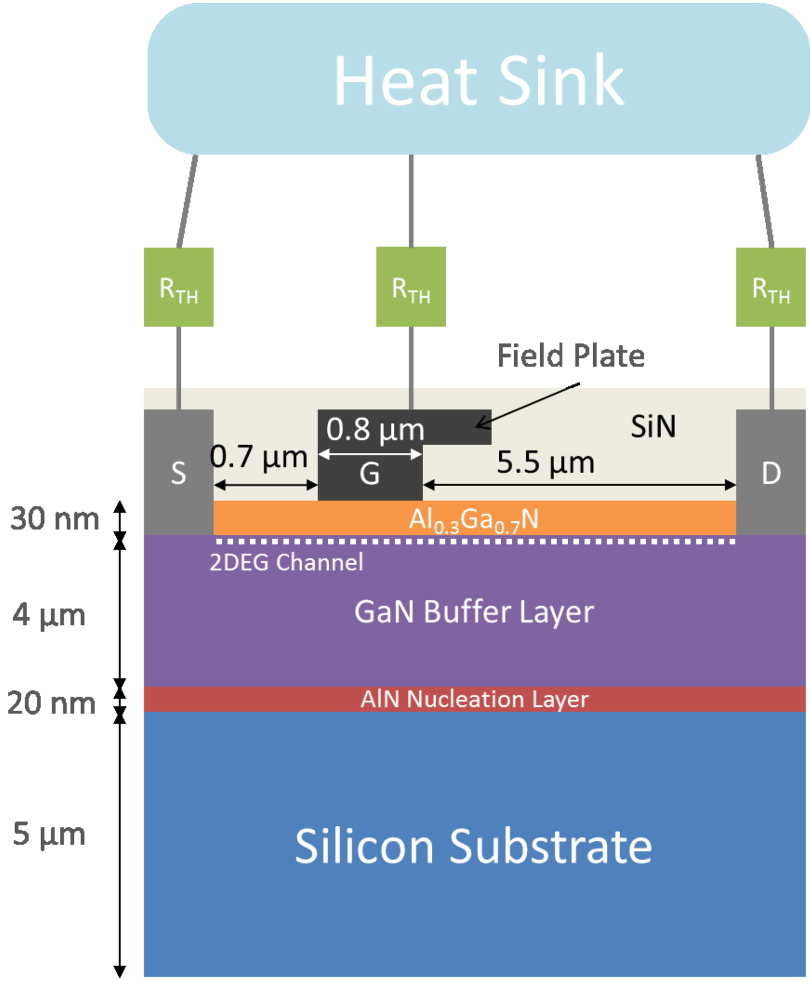
Device Simulation: Band Diagram and I_d-V_d Curves

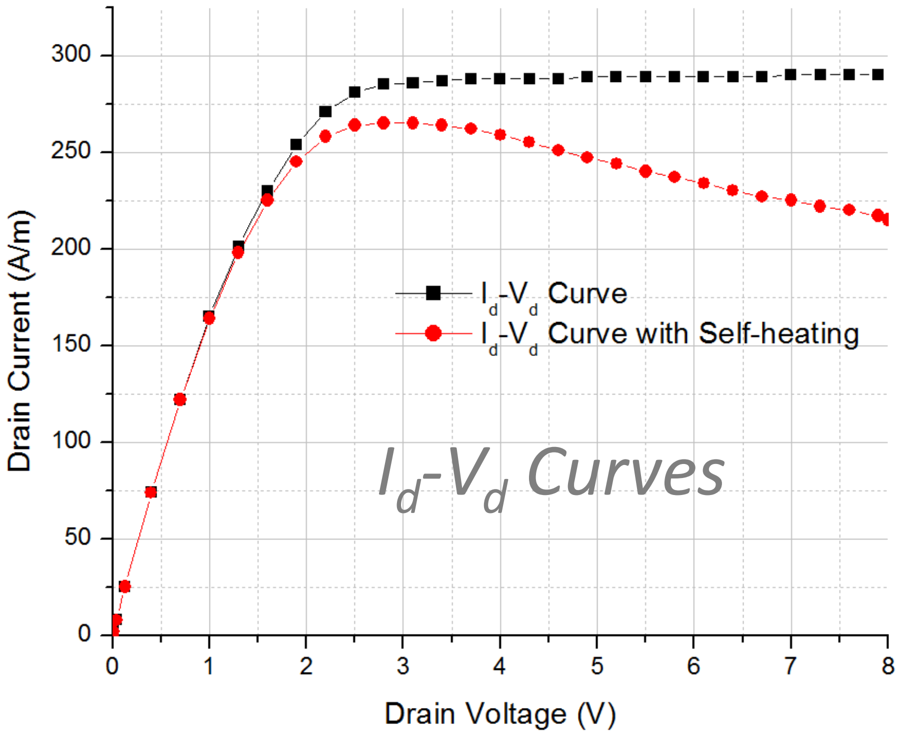






Device Simulation: Self-Heating





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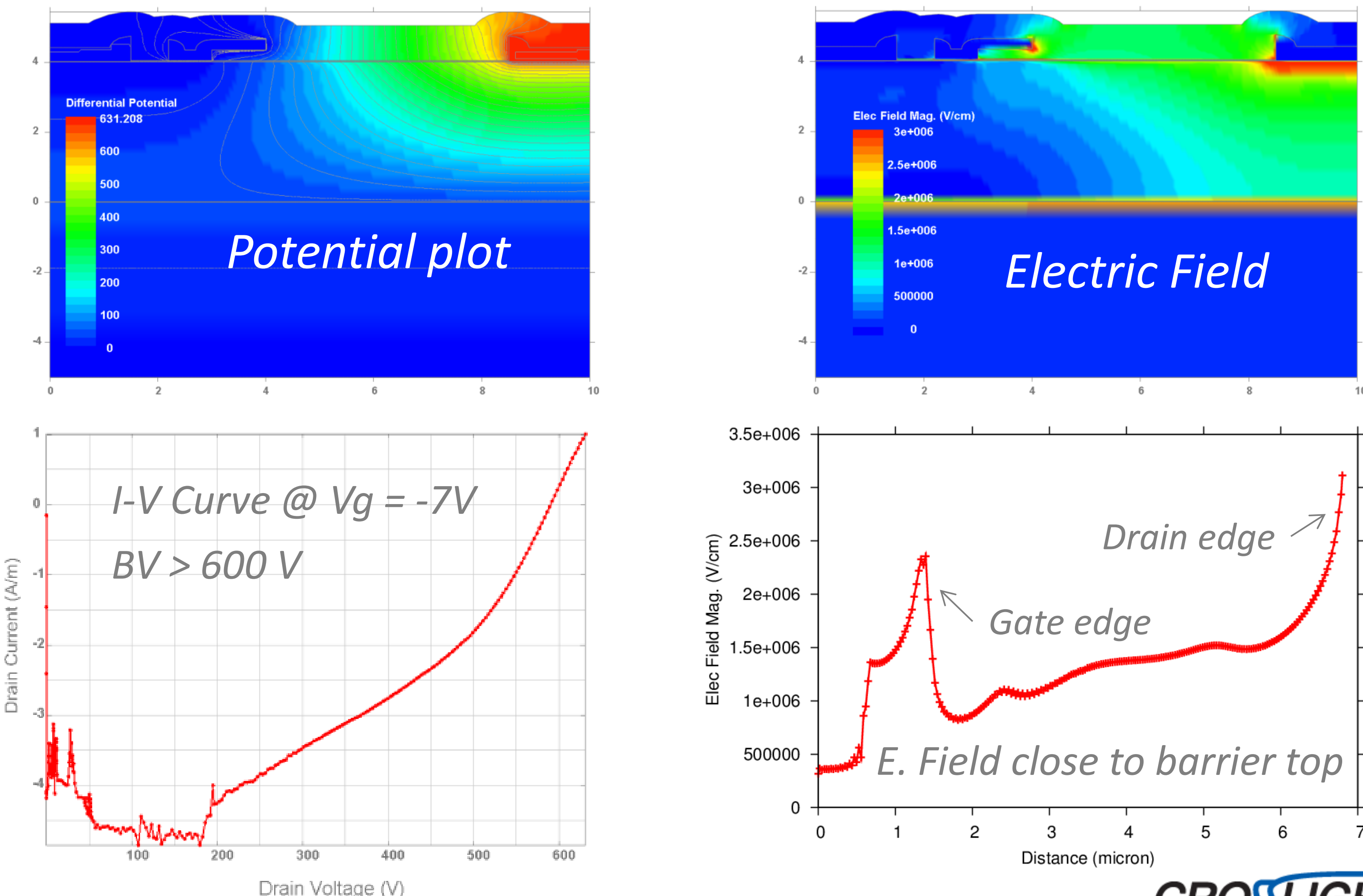
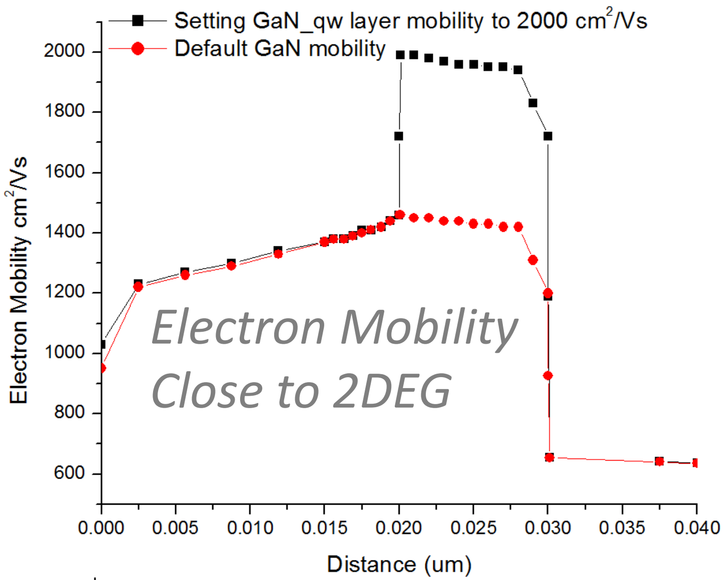
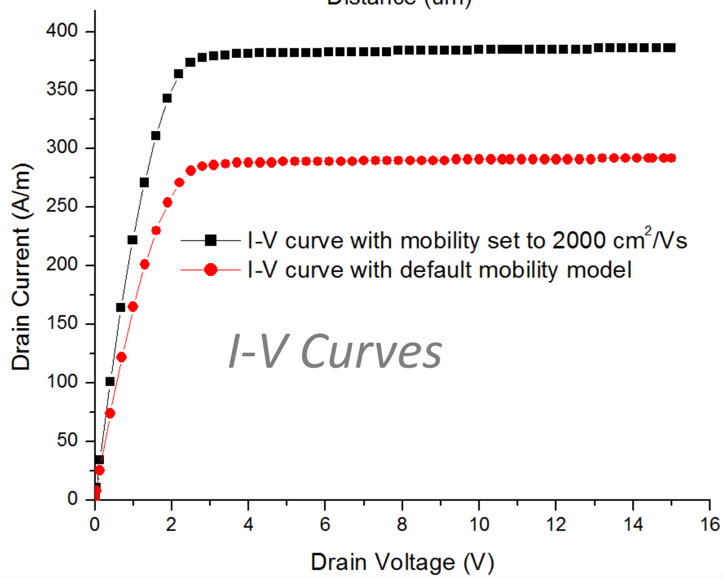
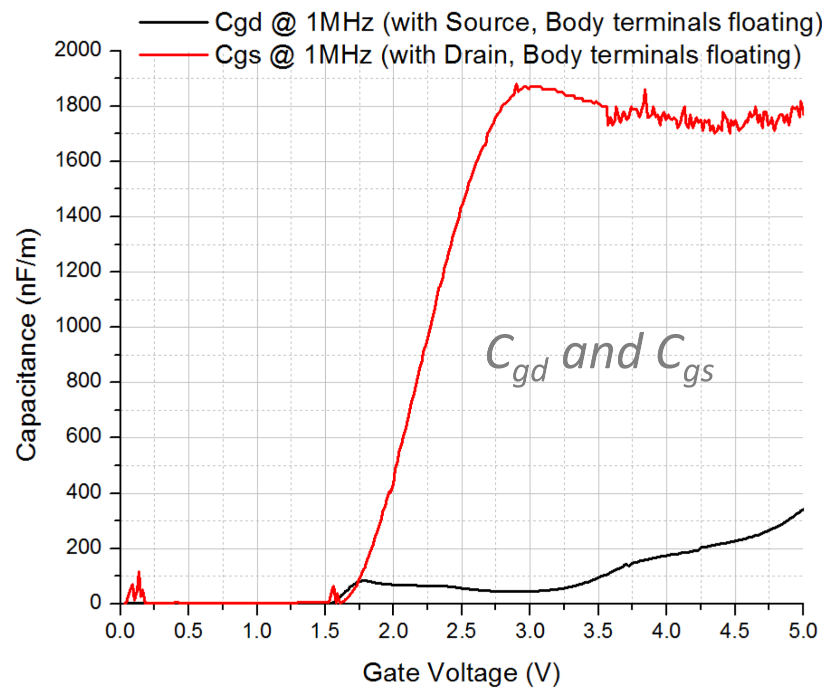
Device Simulation: Breakdown



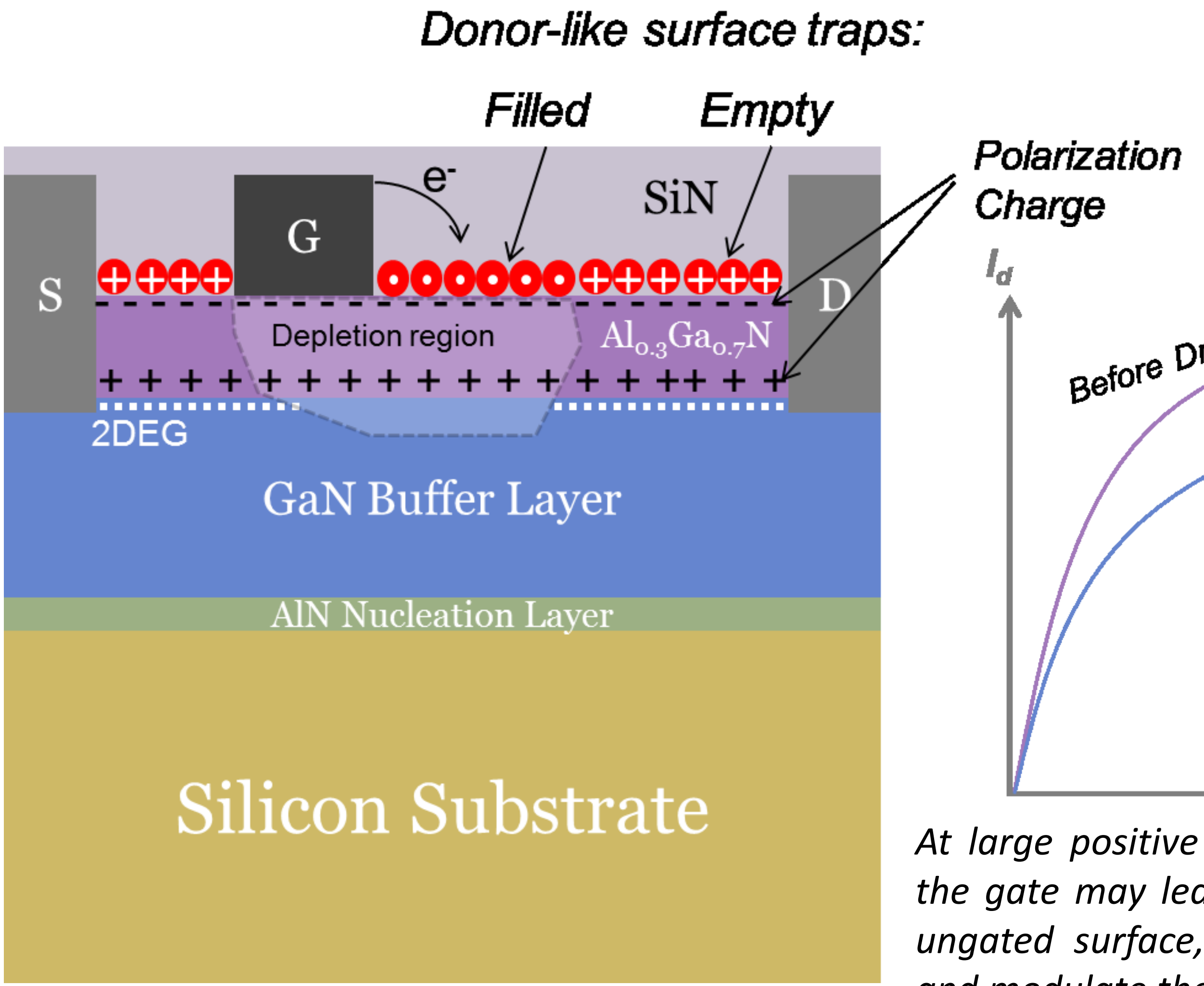
2DEG Mobility and AC Simulation

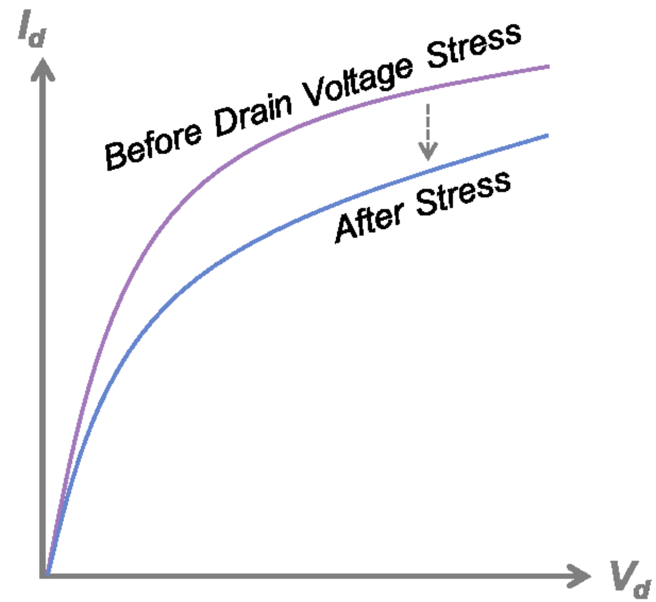






Current Collapse Phenomenon





At large positive drain bias, electrons from the gate may leak to the trap states in the ungated surface, creating a "virtual gate" and modulate the depletion region

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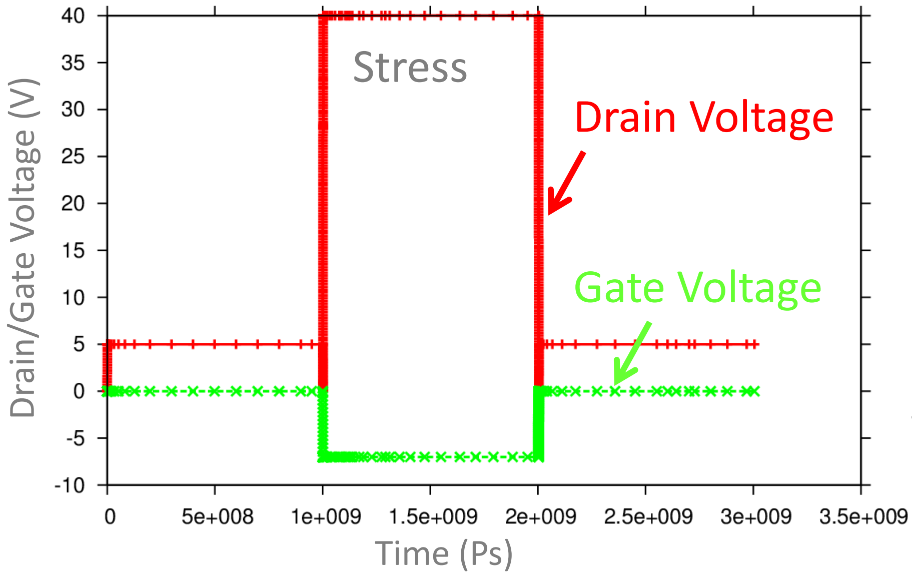
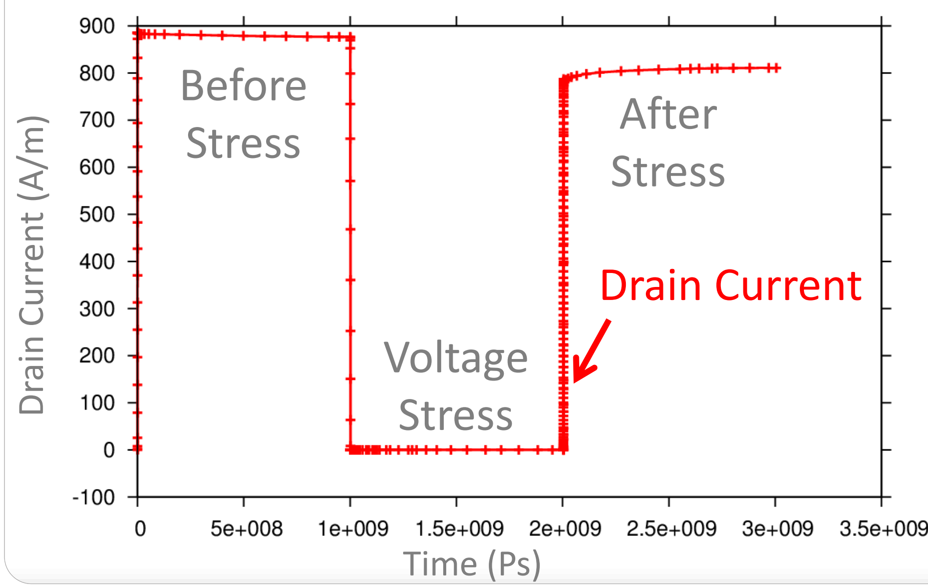
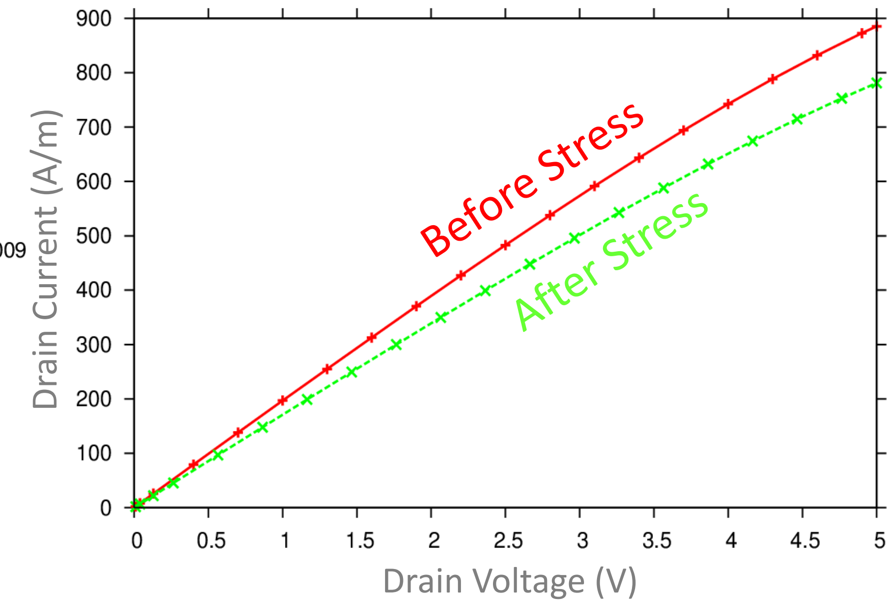
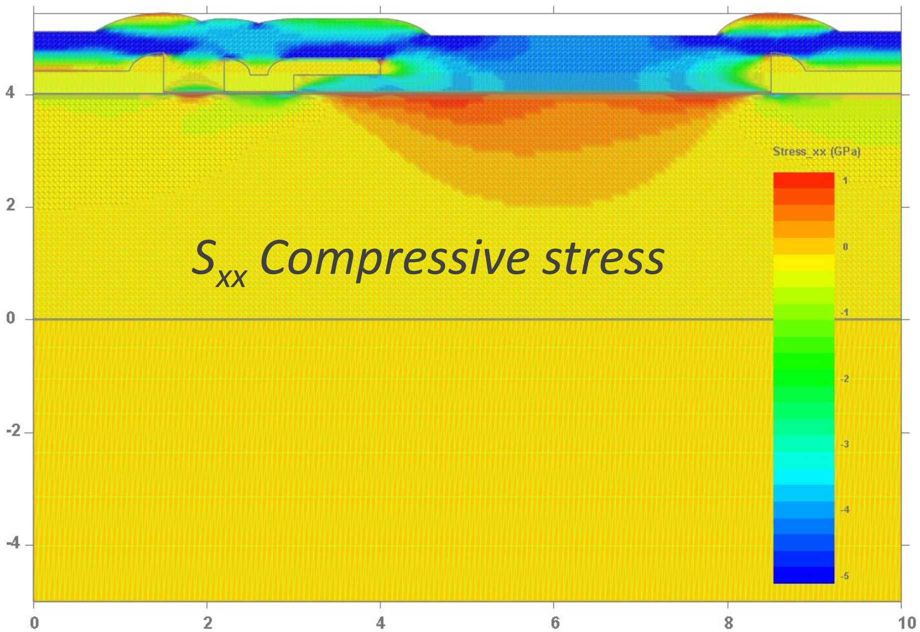
Current Collapse: *Transient Simulation*

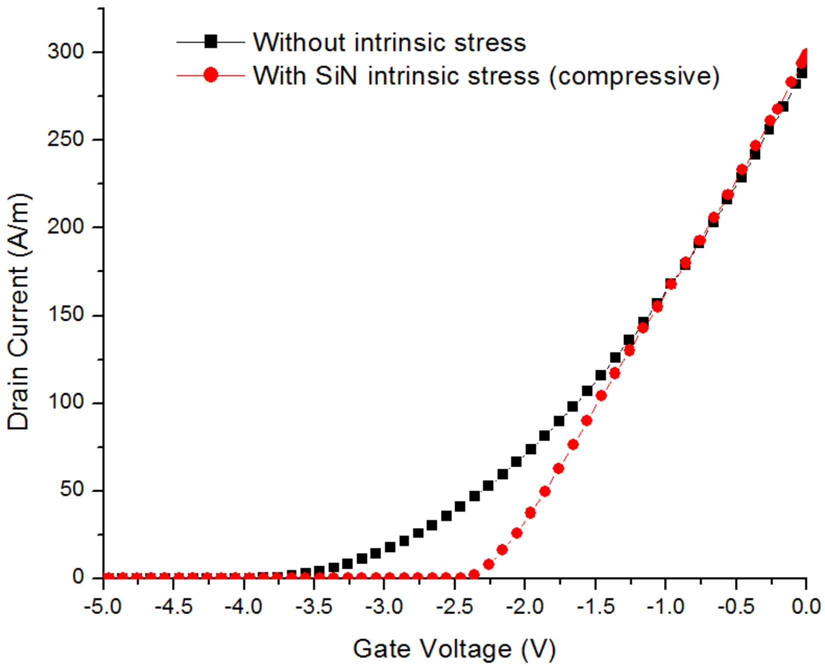






Threshold Voltage and Stress Simulation





- *In addition to stress caused by material lattice mismatch, the intrinsic stress from SiN layer can be defined in the process simulation. The stress profile can be used by the device simulator to calculate the piezoelectric polarization.*

- *Stress engineering may help to achieve enhancement mode?*

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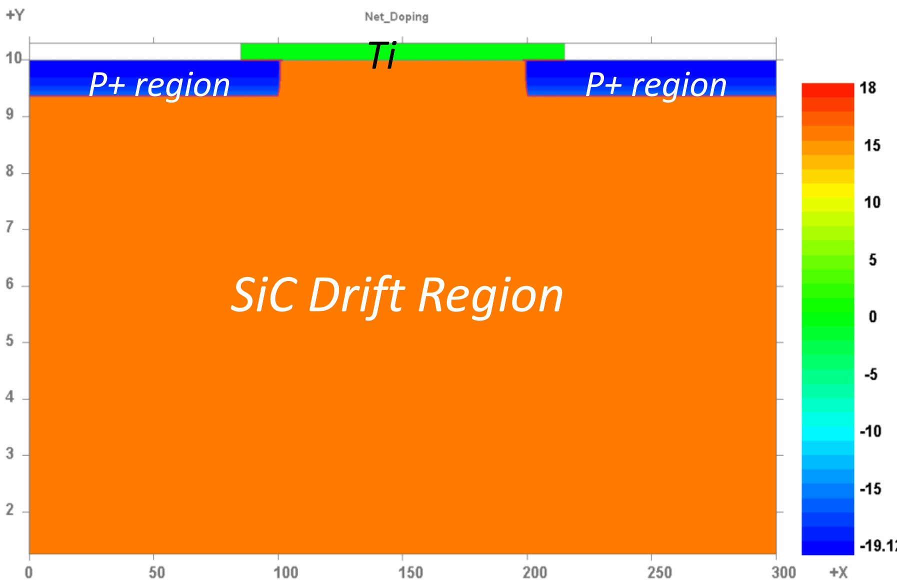
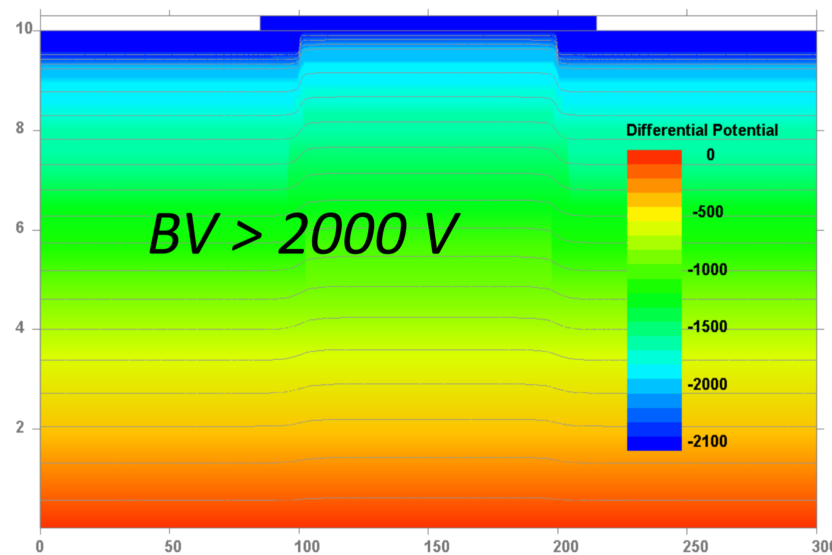
A Simple SiC Power SBD Example

- Substrate: 200 um SiC, N type with Dop. Con.= 1E+18 cm^{-3}
- Drift region: 10 um SiC, N type with Dop. Con.= 7E+15 cm^{-3}
- Titanium / SiC Schottky contact (Ti thickness: 1.3 um)





Note: Substrate is not shown in this plot to enlarge the top portion

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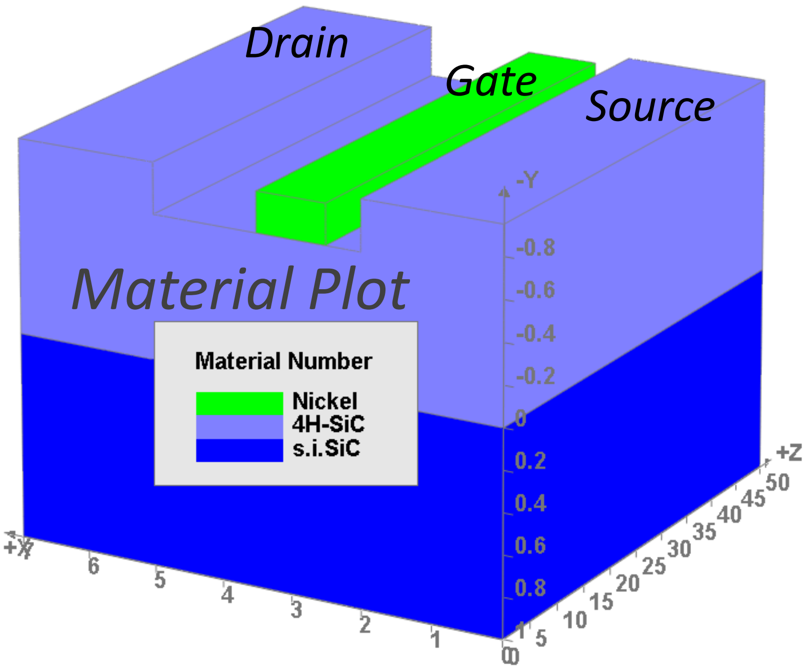
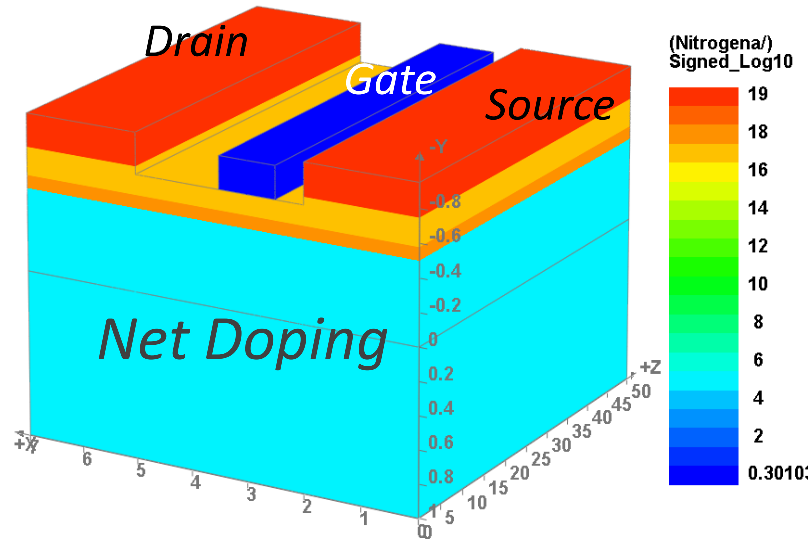
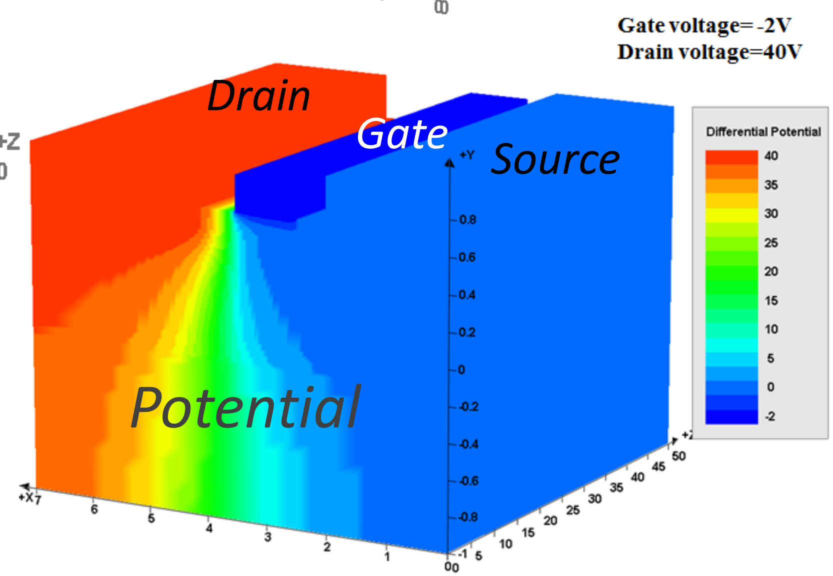
A Simple SiC Power MESFET Example







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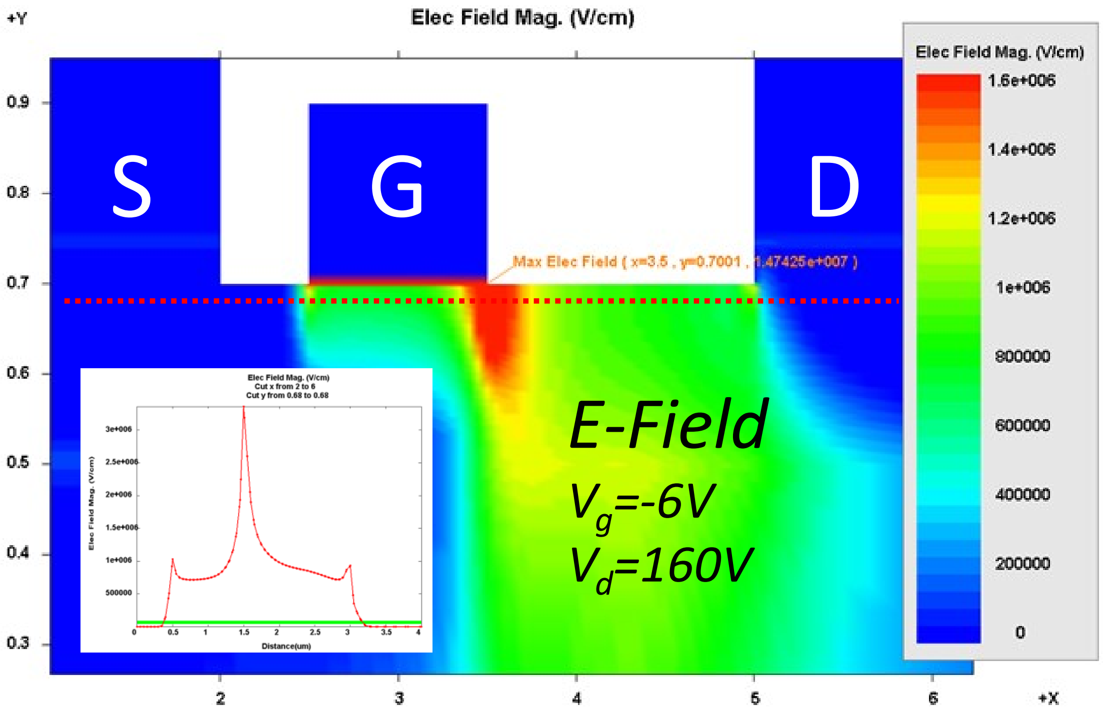
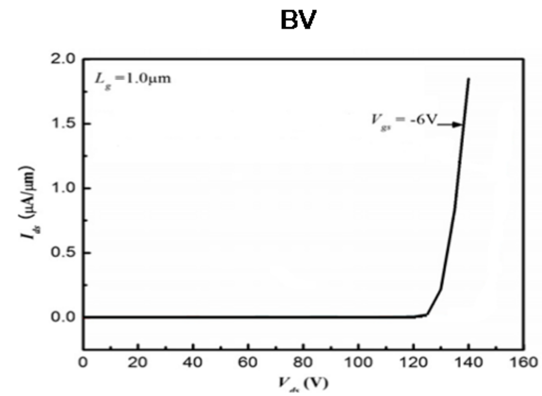
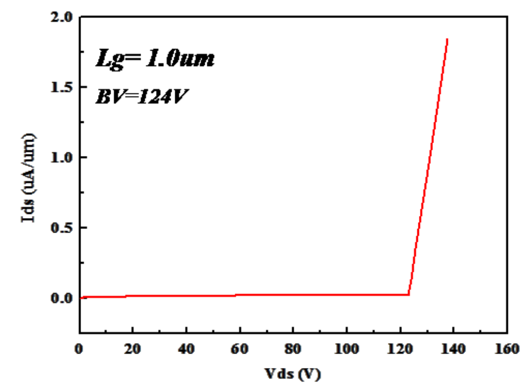
SiC MESFET Breakdown





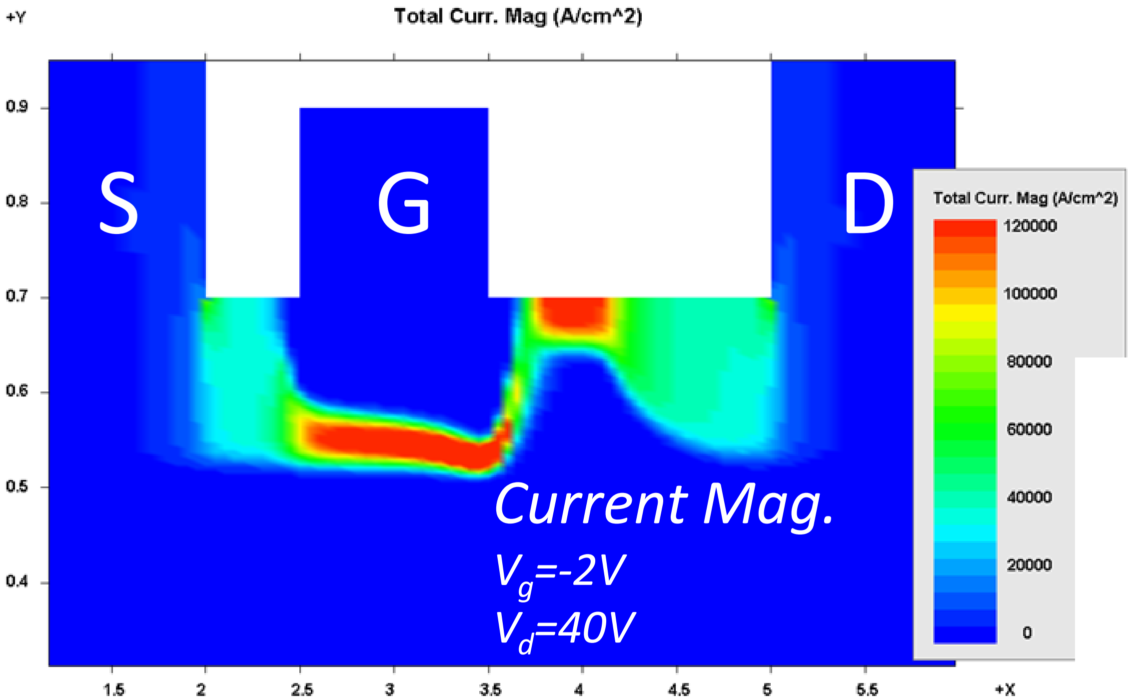
Experimental Result

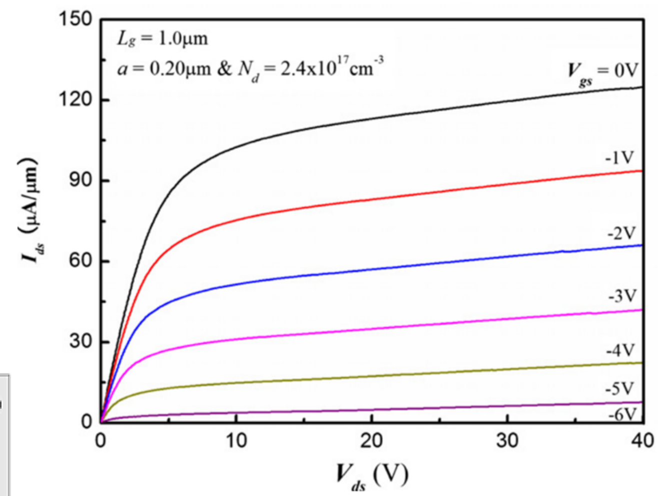


Simulation Result

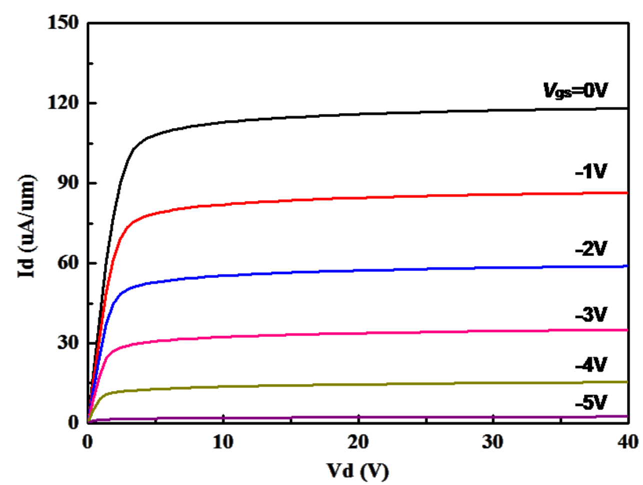
Reference: *C. L. Zhu et al. Solid-State Electronics 51 (2007) 343-346*

SiC MESFET I-V Curves





Experimental Result



Simulation Result

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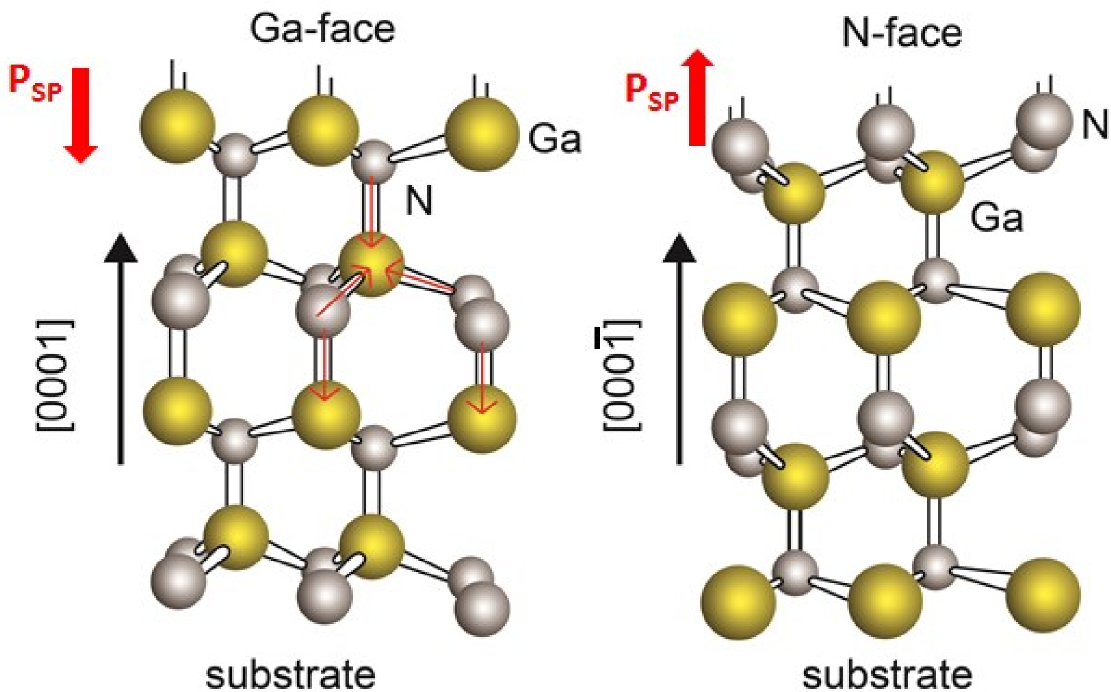
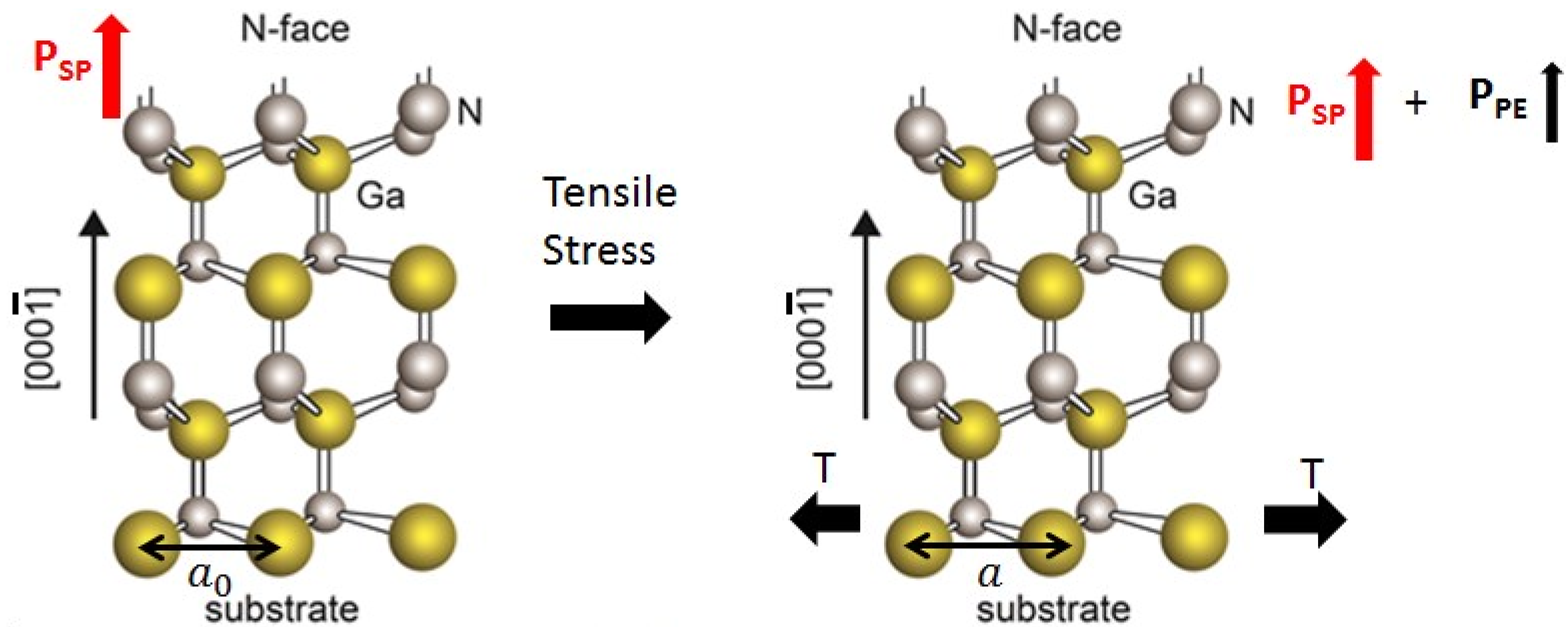
Contents

Polarization: Spontaneous Polarization



- *The bond between Ga atom and N atom is polar*
- *Direction of the polarization is from N atom to Ga atom*
- *Intrinsic asymmetry of the bonding in the equilibrium crystal structure*
- *Integrate all the micro dipoles -> spontaneous polarization*

Polarization: Piezoelectric Polarization



Besides spontaneous polarization, applying mechanical stress to the material distorts the crystal structure, resulting in further polarization: ***Piezoelectric Polarization P_{PE}***

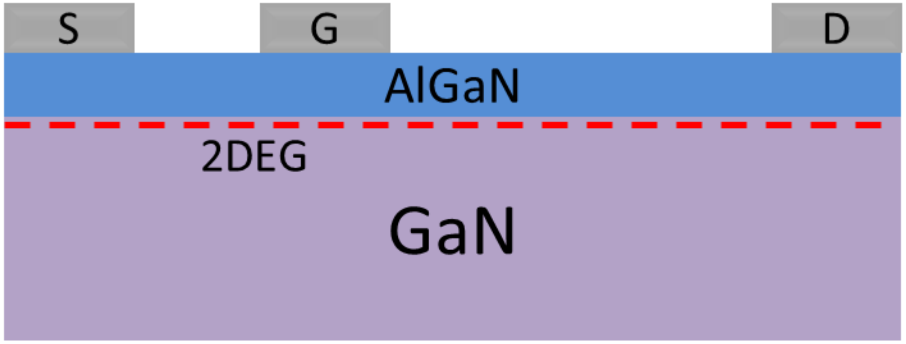
$$P_{PE} = 2\frac{a - a_0}{a_0}\left(e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right)$$

Two-Dimensional Electron Gas (2DEG)

The Origin of 2DEG

- *Due to polarization of AlGaN and GaN, there is large negative bound charge at the AlGaN surface.*

- *Nowadays, it is widely accepted that surface donor-like traps, could be the source of both the channel electrons (2DEG) and the positive charge screening the large negative polarization-induced bound charge.*



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Electron Mobility Models for GaN

- **FMCT Model:**

Proposed by Farahmand etc. in 2001, but fail at high temperature

$$v = \frac{\mu_0 F + v_{sat}(F/F_C)^{n_1}}{1 + a(F/F_C)^{n_2} + (F/F_C)^{n_1}}$$

- **YHT Model:**

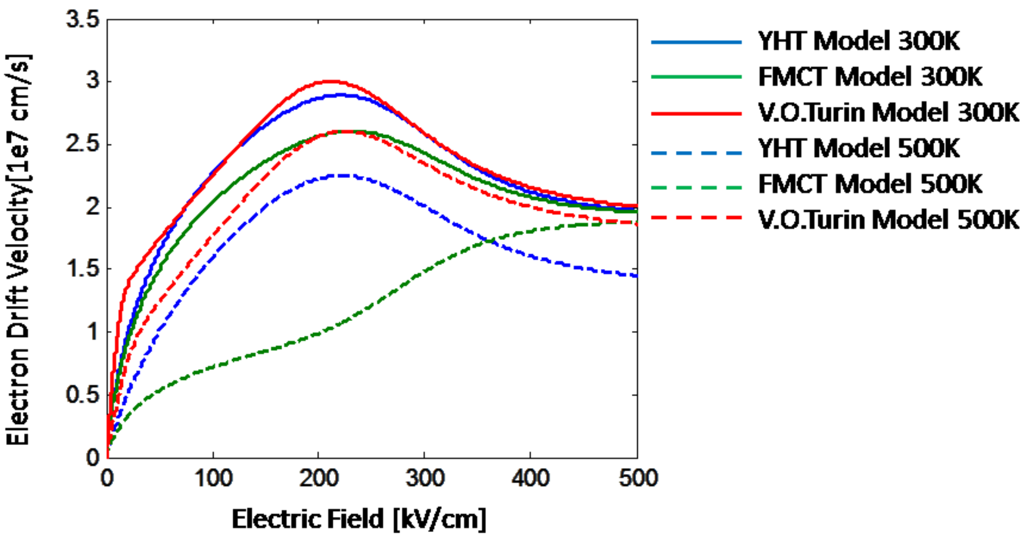
Proposed by Yang, etc., modified FMCT model with temperature effect.

$$\gamma = \gamma_0(\gamma_1 + \gamma_2(T/300) + \gamma_3(T/300)^2)$$

- **V. O. Turin Model:**

Proposed by V. O. Turin, etc., considered the kink effect in low field region.

$$v_{MTE} = \frac{F(E) + v_{sat}(E/E_{MT})^{\beta_T}}{1 + (E/E_{MT})^{\beta_T}}$$



Different electron mobility models for GaN at T=300K and doping concentration=$10^{17}cm^{-3}$

References:

Turin, Valentin O., Solid-State Electronics 49, no. 10 2005: 1678–82.
Yang, etc., IEEE Transactions on Electron Devices 58, no. 4 2011: 1076–83.
Farahmand, M., etc., IEEE Transactions on Electron Devices 48, no. 3 2001: 535–42.

Impact Ionization Parameters for GaN

Chynoweth's Law *is generally used in TCAD simulation. For electrons, the impact ionization coefficient* $\alpha_n(E)$*:*

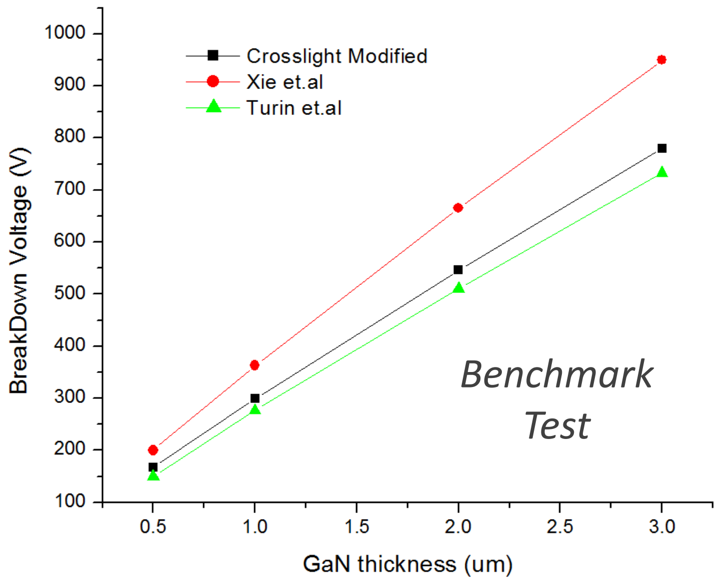
$$\alpha_n(E) = a_n \cdot e^{(-\frac{b_n}{E})}$$

where a_n *and* b_n *are fitting parameters for electrons,* E *is the electric field strength. For holes,* $\alpha_p(E)$*:*

$$\alpha_p(E) = a_p \cdot e^{(-\frac{b_p}{E})}$$

Parameters	Crosslight*	Xie [2]	Turin [3]
a_n for electrons	2.00E+6 cm^{-1}	2.6E+8 cm^{-1}	2.90E+8 cm^{-1}
b_n for electrons	3.00E+7 V/cm	3.40E+7 V/cm	3.40E+7 V/cm
a_p for holes	1.34E+8 cm^{-1}	4.98E+6 cm^{-1}	1.34E+8 cm^{-1}
b_p for holes	2.03E+7 V/cm	2.03E+7 V/cm	2.03E+7 V/cm

**Note that Crosslight's parameter has two ranges, the parameter shown here is the first range*



Impact Ionization Parameters for SiC

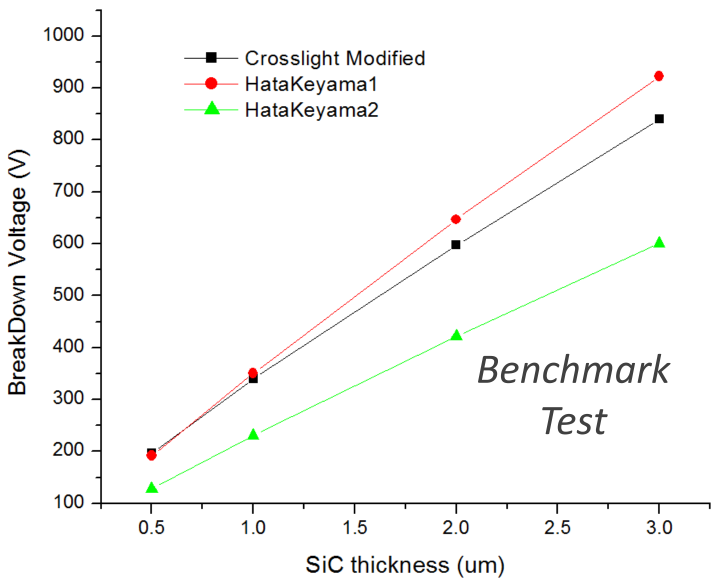
***Chynoweth's Law** is generally used in TCAD simulation. For electrons, the impact ionization coefficient $\alpha_n(E)$:*

$$\alpha_n(E) = a_n \cdot e^{(-\frac{b_n}{E})}$$

where a_n and b_n are fitting parameters for electrons, E is the electric field strength. For holes, $\alpha_p(E)$:

$$\alpha_p(E) = a_p \cdot e^{(-\frac{b_p}{E})}$$

Parameters	Crosslight	Hatakeyama <0001>[5]	Hatakeyama <11$\overline{20}$>[5]
a_n for electrons	4.60E+5 cm^{-1}	1.76E+8 cm^{-1}	2.10E+7 cm^{-1}
b_n for electrons	1.78E+9 V/cm	3.30E+7 V/cm	1.70E+7 V/cm
a_p for holes	1.16E+7 cm^{-1}	3.41E+7 cm^{-1}	2.96E+7 cm^{-1}
b_p for holes	1.72E+7 V/cm	2.50E+7 V/cm	1.60E+7 V/cm



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Convergence: Tips and Tricks

- *The choice of voltage or current bias affects the convergence and stability of the Newton solver.*

- *In order to guarantee convergence, small changes in the applied bias should always result in small changes in the overall solution. Here are two typical examples:*

    - *For BV simulation where the total amount of current flowing in the device is very small, the actual current amount may fluctuate due to lack of numerical precision, making it difficult to use current bias. This situation can be detected by observing the net current over all the electrodes: if the sum is not zero, then Kirchhoff's Current Law is violated and the current is too low to use as a control variable.*

    - *In a forward-biased diode example, the solver can enter a non-convergent state if the applied (anode) voltage bias is much higher than the turn-on voltage. Since the conductivity increases exponentially with bias in a typical diode, seemingly small changes in voltage can result in very large changes of the solution.*

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Convergence: *Tips and Tricks*

This leads us to a simple general rule:

- *Use voltage bias for devices with high resistance*
- *Use current bias for devices with low resistance*

For example, a typical diode under forward bias has low resistance past its turn-on point but high resistance at lower bias or under reverse bias conditions. With these two extremes in mind, the following general strategy is recommended when setting up a simulation under forward bias:

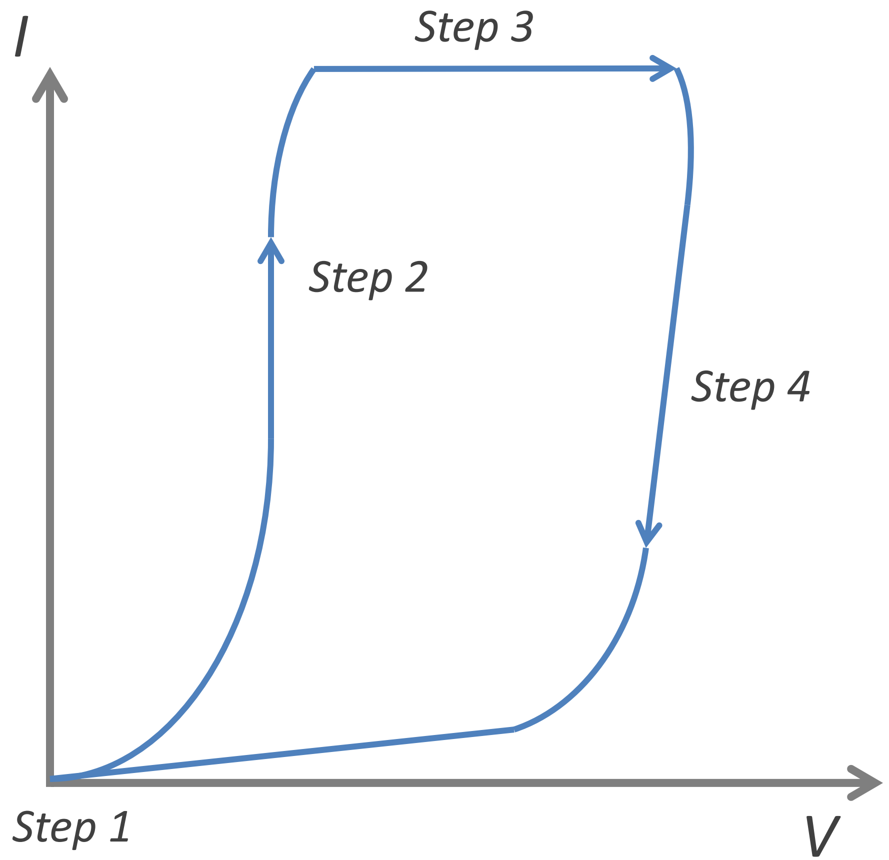
1. *Solve for equilibrium solution*
2. *Apply voltage until 80-90% of the built-in bias value is reached. Some software tools also allow the possibility of terminating the voltage increase once certain current conditions have been met*
3. *Verify that Kirchhoff's Current Law is satisfied at this bias point*
4. *Apply current bias until desired value is reached*

Convergence: Parameter Scan

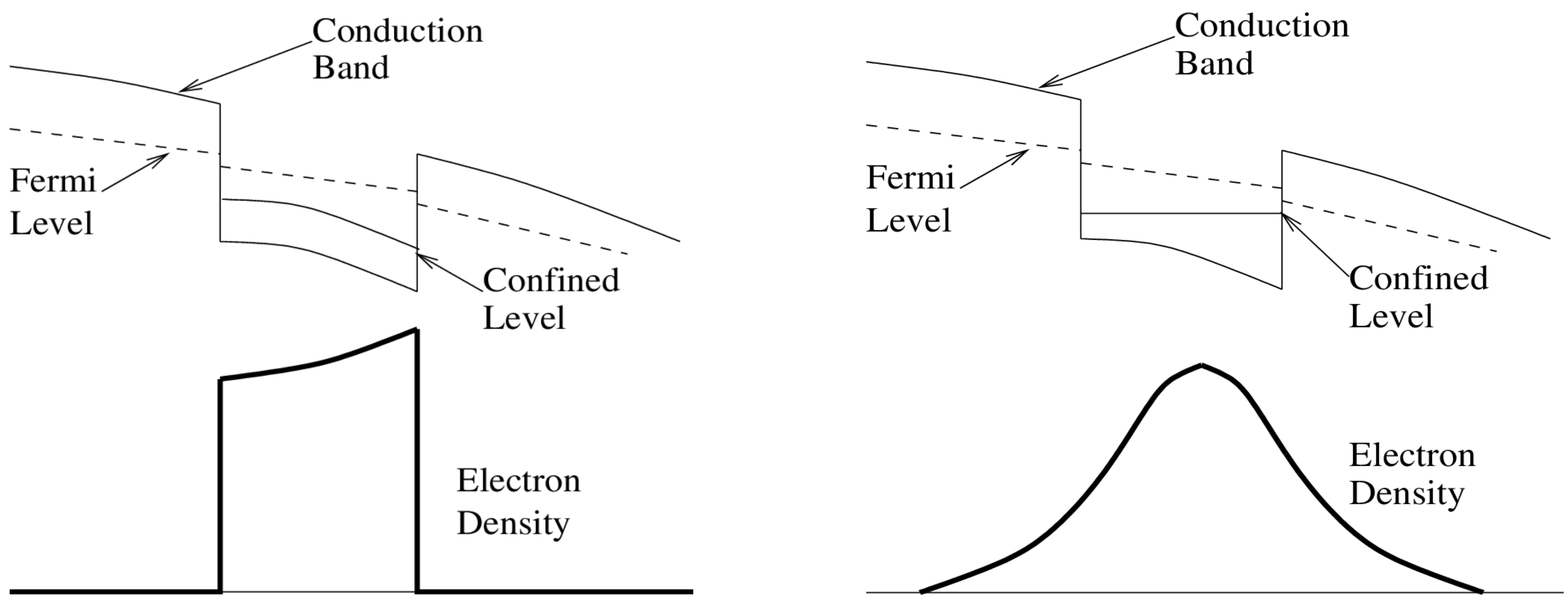
- *Convergence is usually easy at high current.*
- *Basic idea is to artificially change a parameter, such as bandgap, temperature, polarization charge, near equilibrium to make it easier to converge.*

Steps:

1. *Change a parameter.*
2. *Ramp up the voltage until desired value (such as break down)*
3. *Hold the high current while recovering the changed parameter (bandgap, etc.)*
4. *Ramp down the voltage to get desired I-V*



Self-consistent Carrier Density Model



$$n_{2D}(x,y) = \sum_j g_n^j(y)\rho_j^0\, kTln\left[1 + \exp[\frac{E_{fn}(x,y) - E_j(x,y)}{kT}]\right]$$

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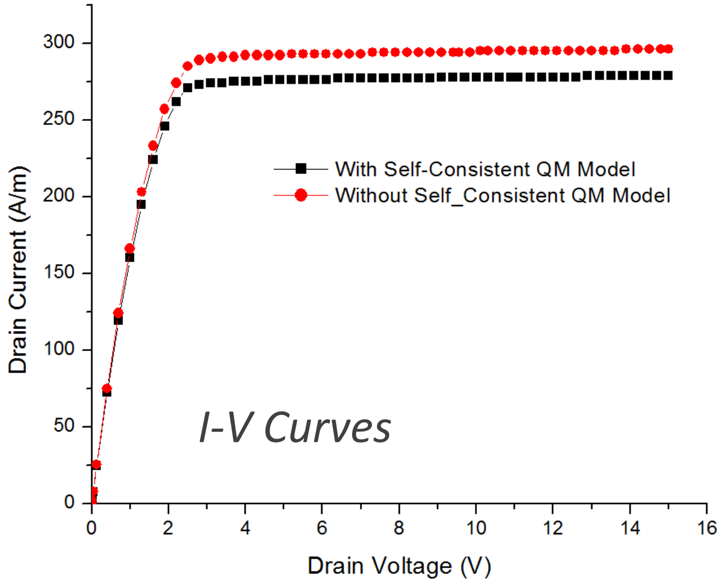
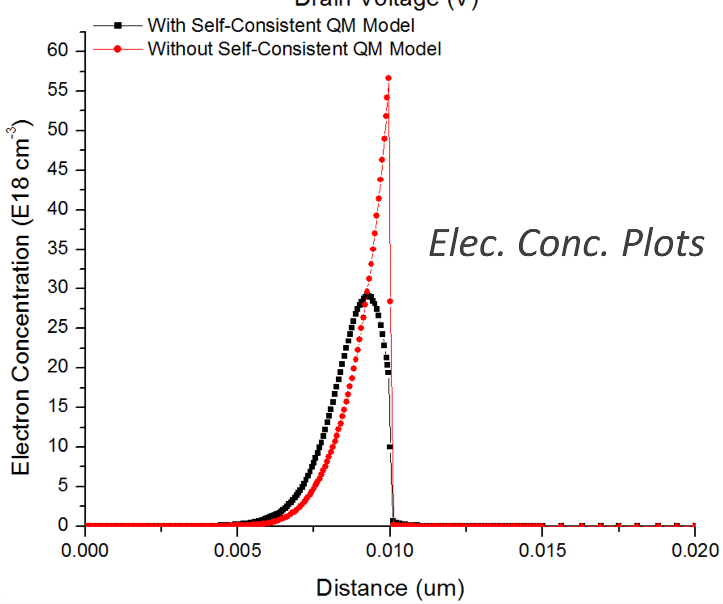
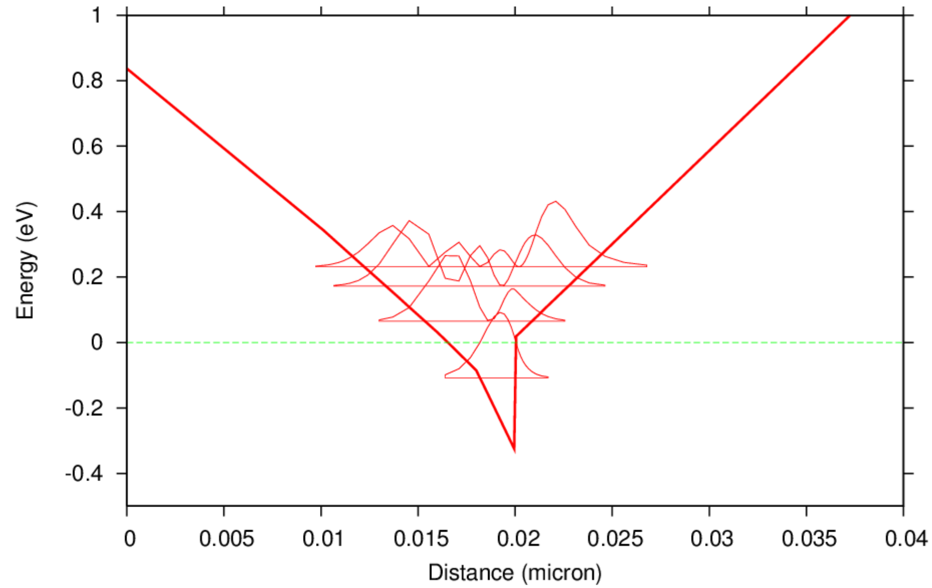
Self-consistent Carrier Density Model



I-V Curves



Elec. Conc. Plots



Band-Diagram Plot with Self-Consistent QM Model

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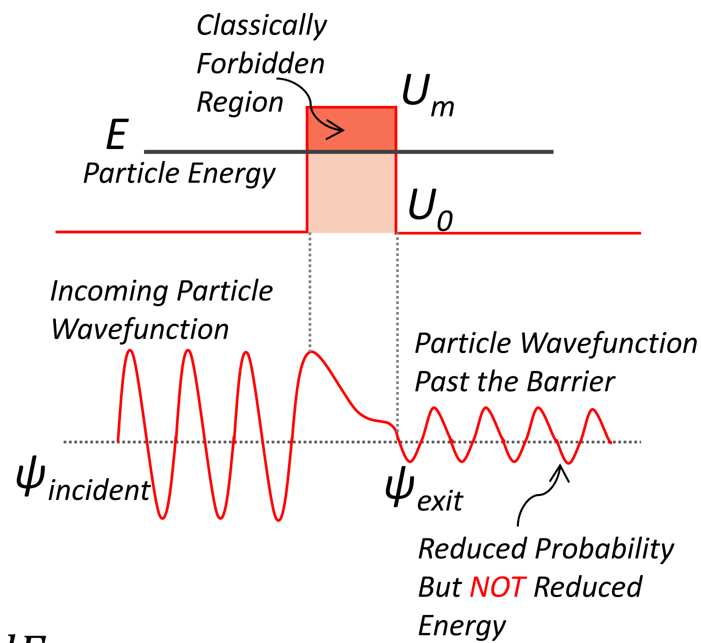
Incorporating QM Tunneling in TCAD



A. Tunneling current at top of barrier

$$J = J_{dd,m} + J_{tun} = (1 + \alpha_m) J_{dd,m}$$

$$J_{tun} = qvn_m (kT)^{-1} \int_{U_0}^{U_m} exp\left(\frac{U_m - E}{kT}\right) D_T(E) dE$$

$(1 + \alpha_m)$ = *Barrier-Peak tunneling enhancement factor*

Incorporating QM Tunneling in TCAD

B. Tunneling current at an arbitrary point

- *Distribution function:*

$$n_E(x) = n_{Ex}\exp(\frac{U(x)-E}{kT})$$

- *Tunneling current may be used to compute local current (local current model)*

$$J_{tun} = qvn(x)(kT)^{-1}\exp(\frac{U(x)-U_m}{kT})\int_{U_0}^{U_m} exp\left(\frac{U_m-E}{kT}\right)D_T(E)dE$$

- *Mesh points away from the barrier-peak have lower tunneling current*
- *Basis for local transport model*

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Incorporating QM Tunneling in TCAD

C. Total or average tunneling current

- *At the edge of the tunneling region,* $U(x) = U_0$

$$J_{tun} = f_{aT} J_{dd} = J_{dd}(kT)^{-1} \int_{U_0}^{U_m} exp\left(\frac{U_0 - E}{kT}\right) D_T(E) dE$$

- *A simple average with a Boltzmann distribution function*
- f_{aT} = *average tunneling factor, or total tunneling coefficient*
- *Basis for non-local transport model*

Incorporating QM Tunneling in TCAD

D. Local vs. non-local transport model

Local model:

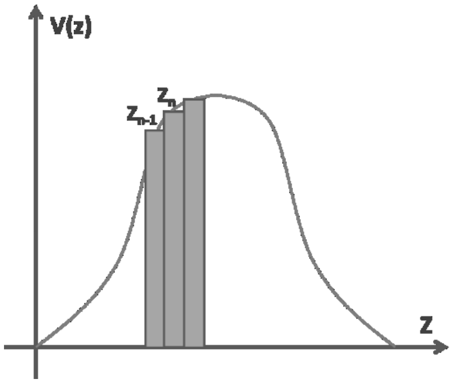
- *Pros: better self-consistency, smooth distribution of current and densities.*
- *Cons: convergence maybe difficult. Cannot handle pure insulator regions (lack of local current).*

Non-local model:

- *Pros: better convergence, suitable for wide bandgap and insulators.*
- *Cons: inconsistency with local model, may cause unphysical back-diffusion*

Propagation Matrix For QM Tunneling

The purpose is to compute tunneling transparency for tunneling transmission



For QM wave propagating in z-direction:

$$\frac{-h^2 d}{2dz}\left[\frac{1}{m(z)}\frac{d}{dz}\phi(z)\right] + V(z)\phi(z) = E\phi(z)$$

Make Piece-wise constant assumption for V(z) and m(z) to obtain general solution:

$$\phi_n\,(z) = A_n e^{ik_n(z-z_n)} + B_n e^{-ik_n(z-z_n)} \;\; \textit{for} \;\; z_{n-1} \le z \le z_n$$

where

$$k_z = \sqrt{\frac{2m_n}{\hbar^2}(E - V_n)}$$

which can take real or imaginary value depending on the sign of $(E - V_n)$

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Propagation Matrix For QM Tunneling

We apply continuity boundary condition for $\phi(z)$ *and* $(1/m(z))d\phi(z)/dz$ *(continuity in probability and probability flux) at* $z = z_n$ *to obtain propagation matrix:*

$$\begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix} = T_{n+1,n} \begin{bmatrix} A_n \\ B_n \end{bmatrix}$$

define

$$P_{n+1,n} = \frac{m_n k_{n+1}}{m_{n+1} k_n}$$

where the propagation matrix is given by:

$$T_{n+1,n} = \frac{1}{2} \begin{bmatrix} (1 + P_{n+1,n}) e^{ik_{n+1} h_{n+1,n}} & (1 - P_{n+1,n}) e^{ik_{n+1} h_{n+1,n}} \\ (1 - P_{n+1,n}) e^{-ik_{n+1} h_{n+1,n}} & (1 + P_{n+1,n}) e^{-ik_{n+1} h_{n+1,n}} \end{bmatrix}$$

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Propagation Matrix For QM Tunneling

Repeating the matrix equation to relate the incident and transmitting waves:

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = G_{N,0} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}$$

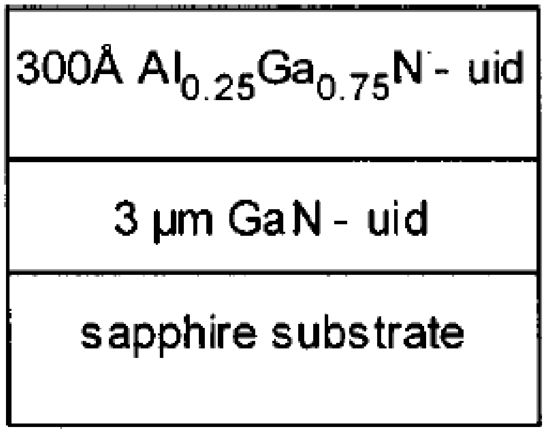
QM transmittance ($|t|^2$) and reflectivity ($|r|^2$) can be obtained by setting:

$$\begin{bmatrix} A_0 \\ B_0 \end{bmatrix} = \begin{bmatrix} 1 \\ r \end{bmatrix}$$

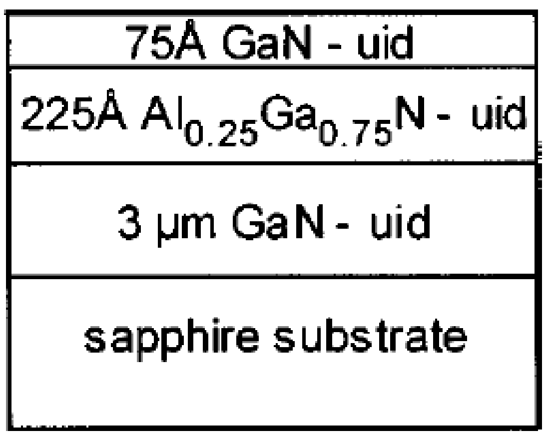
And

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = \begin{bmatrix} t \\ 0 \end{bmatrix}$$

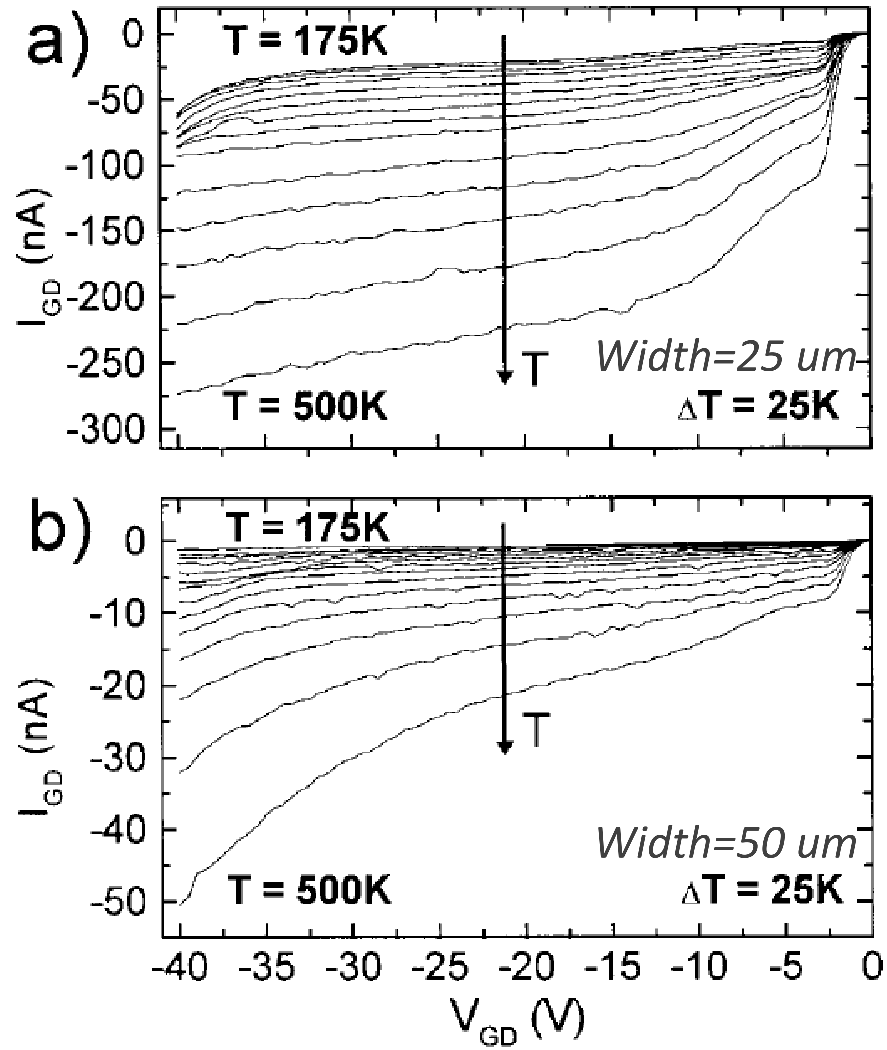
QM Tunneling Model for HEMT Gate Leakage



Standard Barrier HEMT



Enhanced-Barrier HEMT



E.J. Miller et.al., JAP, v.88, p5951(2000)

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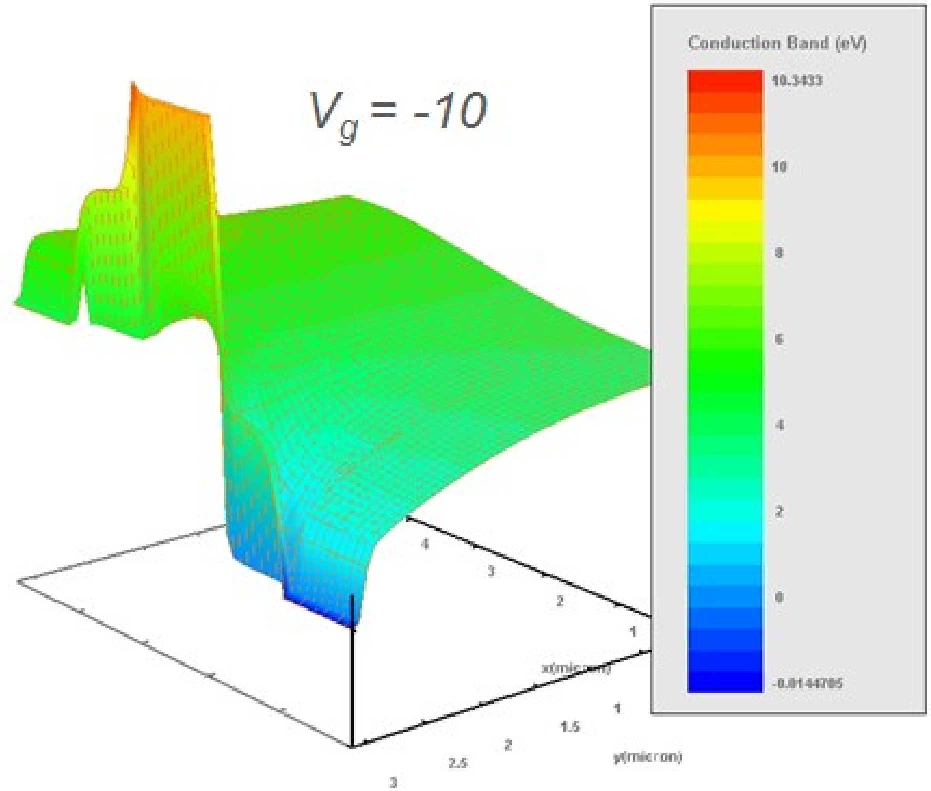
QM Tunneling Model for HEMT Gate Leakage

A 2D Problem



For reverse gate bias:

1) *Depletion of 2DEG under gate. No change in barrier shape*

2) *Lateral voltage pull-down by the S/D contact, causing thinning of barrier and increase of I_g*

3) *Further S/D voltage pull down causing voltage drop between G and S/D, I_g increase slows down*

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QM Tunneling Model for HEMT Gate Leakage

Critical Modeling Parameters

- *Polarization fraction at 2DEG and AlGaN/GaN interface. (0.7-1)*
- *Polarization fraction on top (passivated) surface (< 0.1)*
- *Gate metal work function (5.2-5.4).*
- *Deep donor traps for UID barriers (1.e17-1.e18/cm^3)*
- *Deep acceptor traps for substrate GaN (1.e17/cm^3)*

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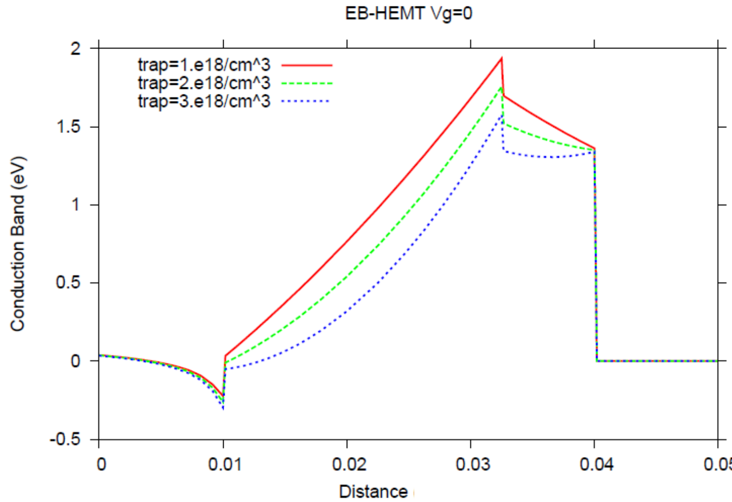
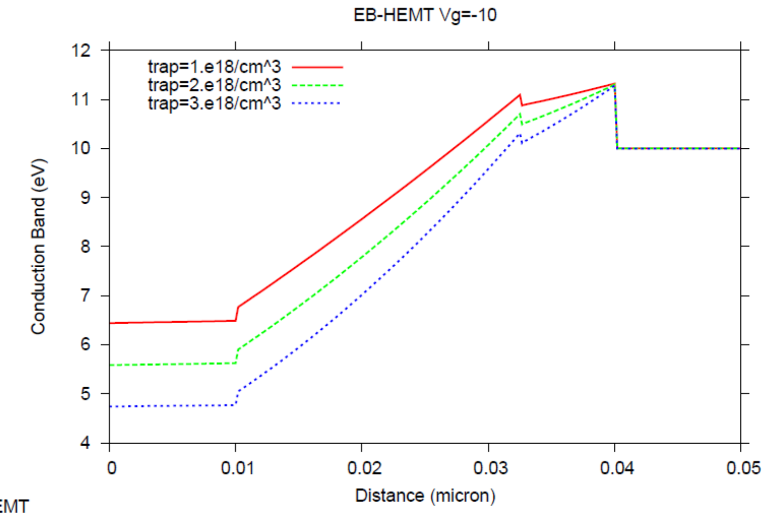
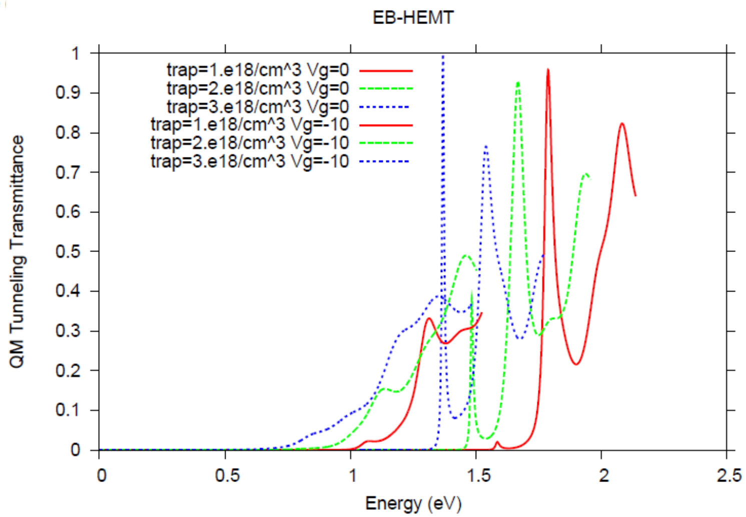
QM Tunneling Model for HEMT Gate Leakage

Traps Affect Barrier Height







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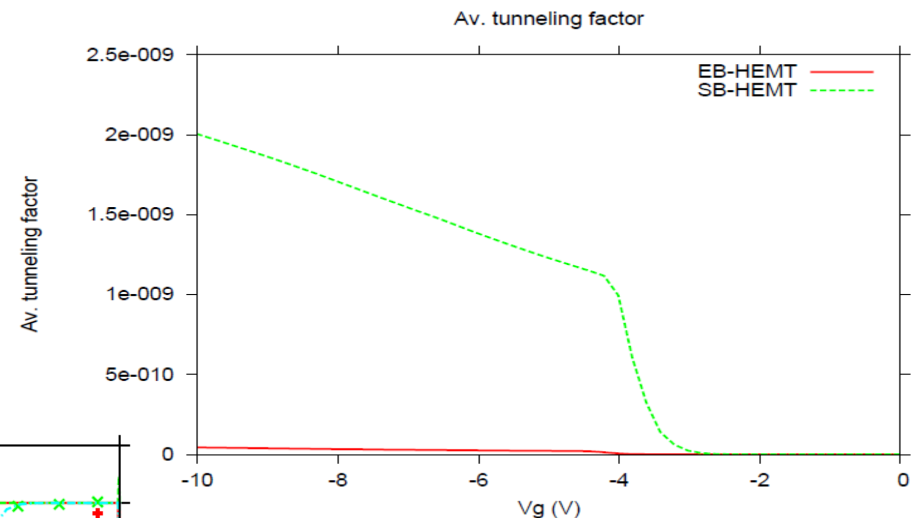
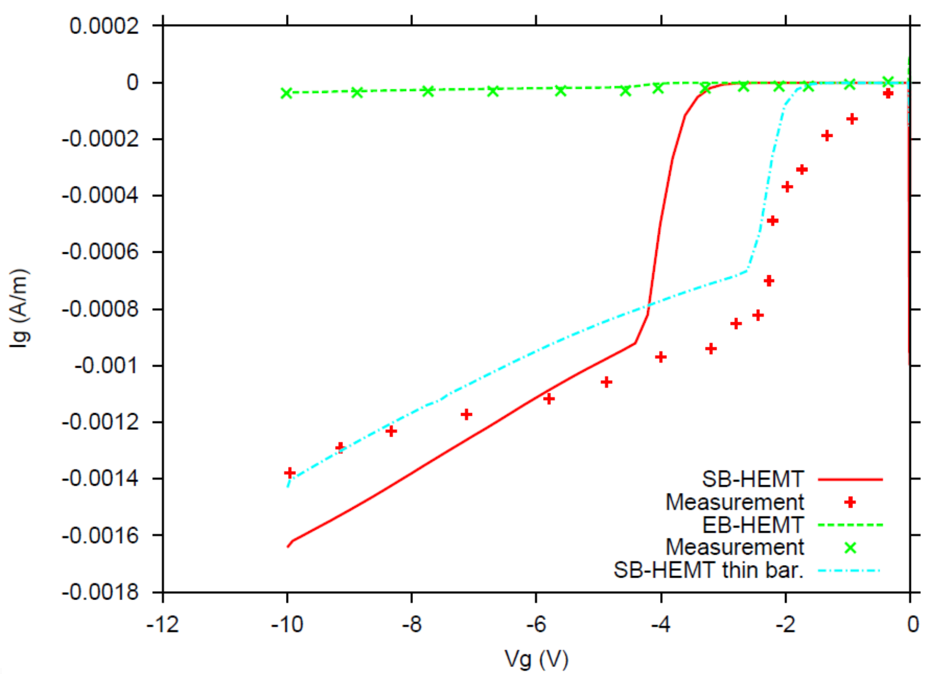
QM Tunneling Model for HEMT Gate Leakage

SB-HEMT vs. EB-HEMT





Compact Trap Assisted Tunneling Model

Trap Assisted Tunneling (TAT) assumes current from trap emission

$$J = q\int_0^{t_{bar}} \frac{N_{trap}}{\tau} dx$$

Field dependent rate with temperature dependent factor:

$$\frac{1}{\tau} = S_{tat}(F) f_{temp}$$

$$f_{temp} = \exp\left(\frac{E_{t0}}{k300} - \frac{E_t}{kT}\right)$$

A. Linear model

$$S_{tat}(F) = S_{tat}(0) + \left(\frac{dS_{tat}}{dF}\right) F$$

$$J = qN_{trap} f_{temp}\left(\frac{dS_{tat}}{dF}\right)\Delta V$$

Ref. Dissertation, Andreas Gehring, 2003

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Compact Trap Assisted Tunneling Model

B. Poole-Frenkel Model

Field dependence comes from factor $\exp(\frac{E_t}{k300})$ *with* E_t *shifted by field within a Coulomb potential:*

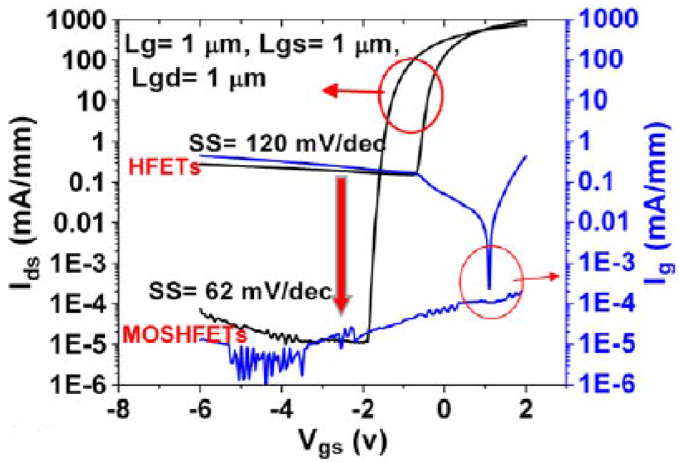
$$\Delta E_t = \sqrt{\frac{qF}{\pi\epsilon_0\epsilon}}$$

C. Hopping model

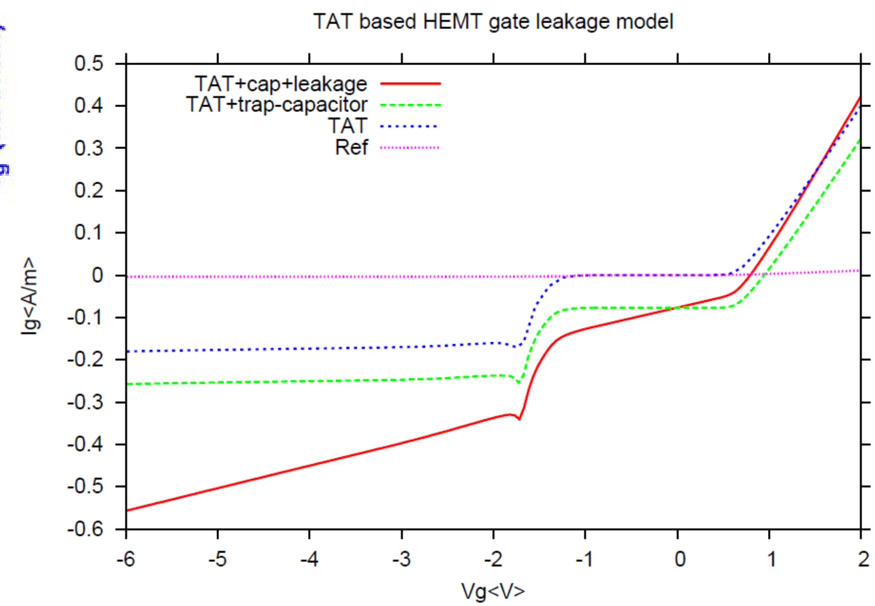
Trap level E_t *shifted by field in a rectangle potential well of size* d_{hop}*:*

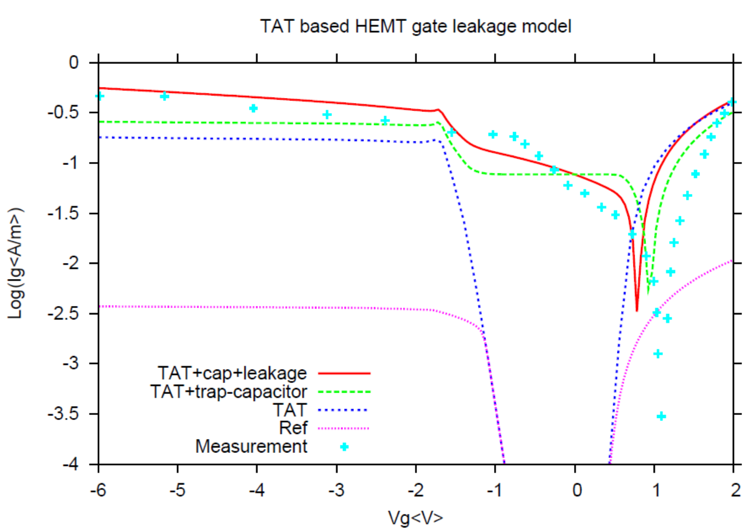
$$\Delta E_t = F d_{hop}$$

Compact Trap Assisted Tunneling Model



T. Huang et.al, IEEE EDL Vol.33 Issue 8





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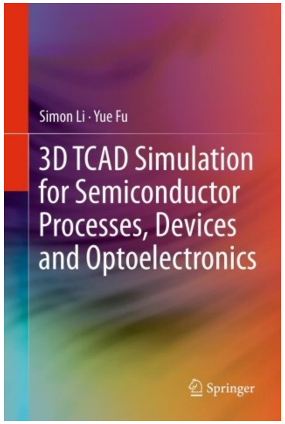
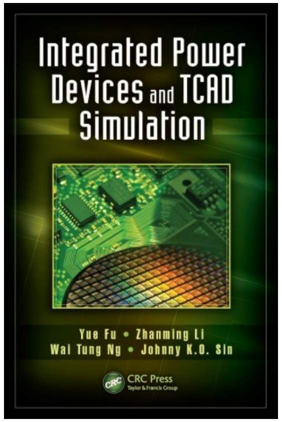
[7] E.J. Miller et.al., JAP, v.88, p5951(2000)

[8] C. L. Zhu et al. Solid-State Electronics 51 (2007) 343-346

[9] T. Huang et.al, IEEE EDL Vol.33 Issue 8





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