Modelling of Schottky-Barrier Diodes Operating under Strong Reverse-Bias Conditions

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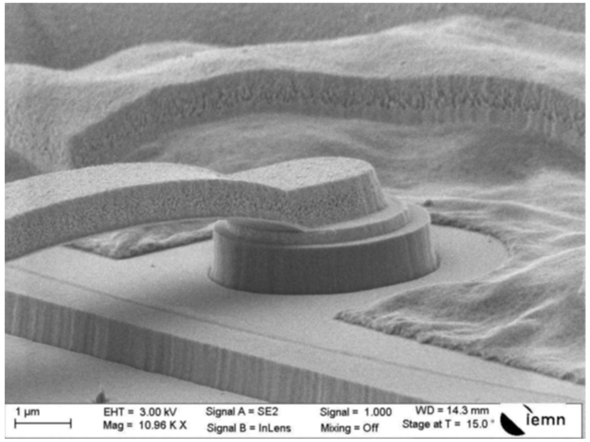
Universidad de Salamanca, Spain



OUTLINE

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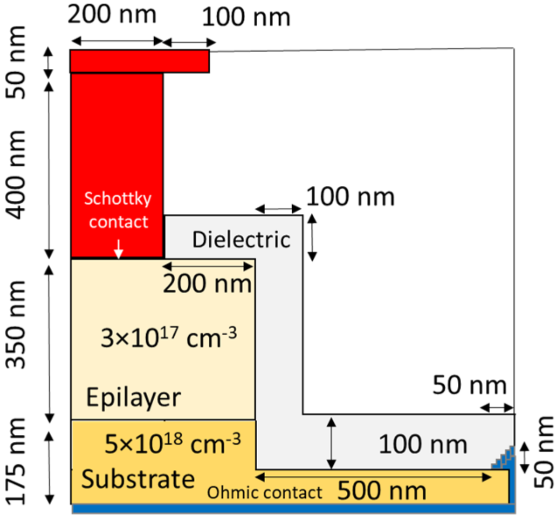
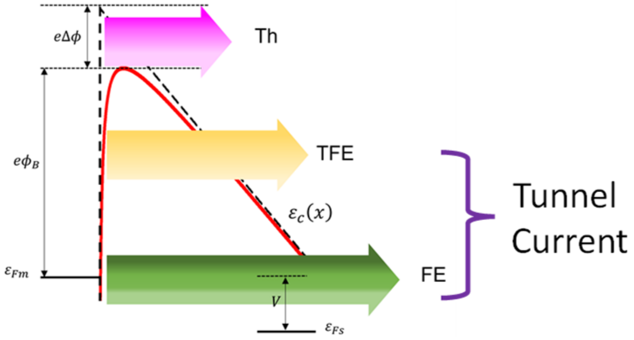
- Ideal full-depletion leakage current model
- Monte Carlo model
- Results
  - ⇨ 1D simulations
  - ⇨ 2D simulations
- Conclusions



Introduction

THz frequency multipliers based on Schottky-barrier diodes (SBDs): **GaAs → GaN**

Correct modelling of reverse current → essential to predict their breakdown



Low-injection conditions (low voltage, low doping)

Full Depletion (FD) approximation valid → analytical estimation of the barrier profile

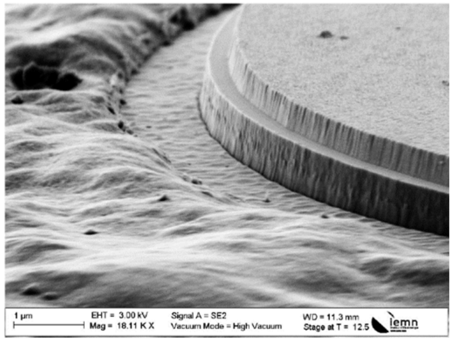
↓

Ideal current components: thermionic emission and tunneling currents

High-injection conditions (strong reverse bias, contact edge, inhomogeneities)

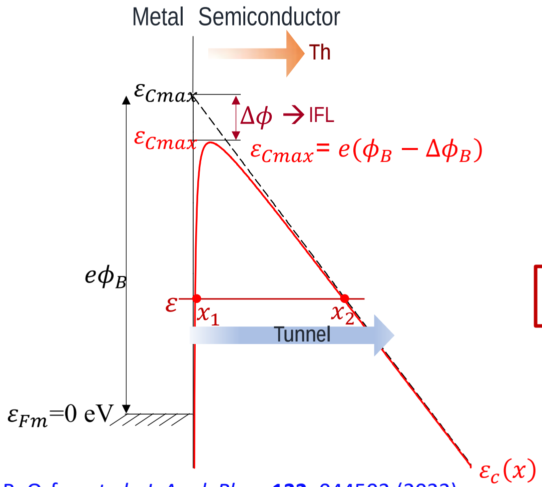
barrier profile → self-consistently calculated with carrier concentration

simulation of carrier transport → electron and hole impact ionization



This work: analysis of **GaN SBDs** by means of Monte Carlo simulations where all the involved physical effects are taken into account

Ideal full-depletion leakage current model



B. Orfao *et al.*, *J. Appl. Phys.* **132**, 044502 (2022)

$$\varepsilon_c(x) = e\phi_B - e\underbrace{\left[\frac{2eN_D}{\varepsilon_S}(V_B - V)\right]^{1/2}}_{E_{max}} x + \frac{e^2 N_D x^2}{2\varepsilon_S} - \frac{e^2}{16\pi\varepsilon_S x}$$

doping effect

image-charge effect

Parameters: ϕ_B, ε_s, N_D and m^*

$$\boxed{J(\varepsilon)d\varepsilon = -eN(\varepsilon)T_C(\varepsilon)d\varepsilon}$$

WKB approximation

$$N(\varepsilon) = \frac{A^*T}{ek_B}\ln\left[1 + exp\left(-\frac{\varepsilon - \varepsilon_F}{k_BT}\right)\right] \Longrightarrow \cong \exp\left(-\frac{\varepsilon - \varepsilon_{Fm}}{k_BT}\right) \quad \text{for } \varepsilon - \varepsilon_F \gg k_BT$$

$$T_C(\varepsilon) = exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2}\sqrt{2m^*[\varepsilon_C(x) - \varepsilon]}dx\right)$$

$N(\varepsilon)$: number of electrons per unit area per unit time incident on the barrier per unit energy normal to the barrier

Thermionic emission

$$\varepsilon > \varepsilon_{Cmax} \Longrightarrow T_C(\varepsilon) = 1$$

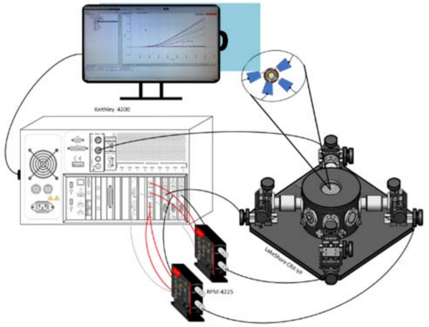
$$J_{Th} = A^*T^2 \exp\left(-\frac{\varepsilon_{Cmax}}{k_BT}\right)\left[\exp\left(\frac{e(V - J_{th}SR_s)}{\eta k_BT}\right) - 1\right]$$

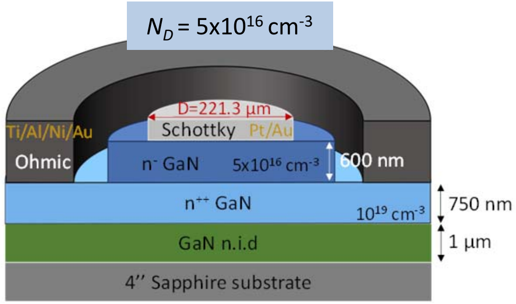
Tunneling current

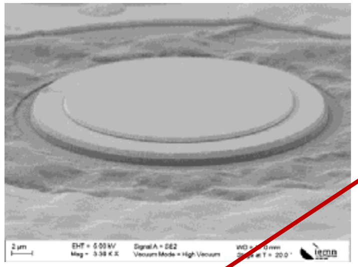
$$\varepsilon < \varepsilon_{Cmax} \Longrightarrow 0 < T_C(\varepsilon) < 1$$

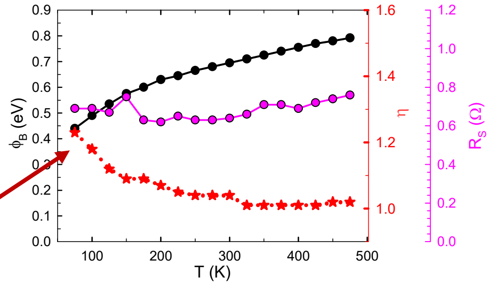
$$J_{tunnel} = e\int_{\varepsilon_{min}}^{\varepsilon_{Cmax}} N(\varepsilon) \cdot T_c(\varepsilon)d\varepsilon$$

Ideal full-depletion leakage current model: experimental validation







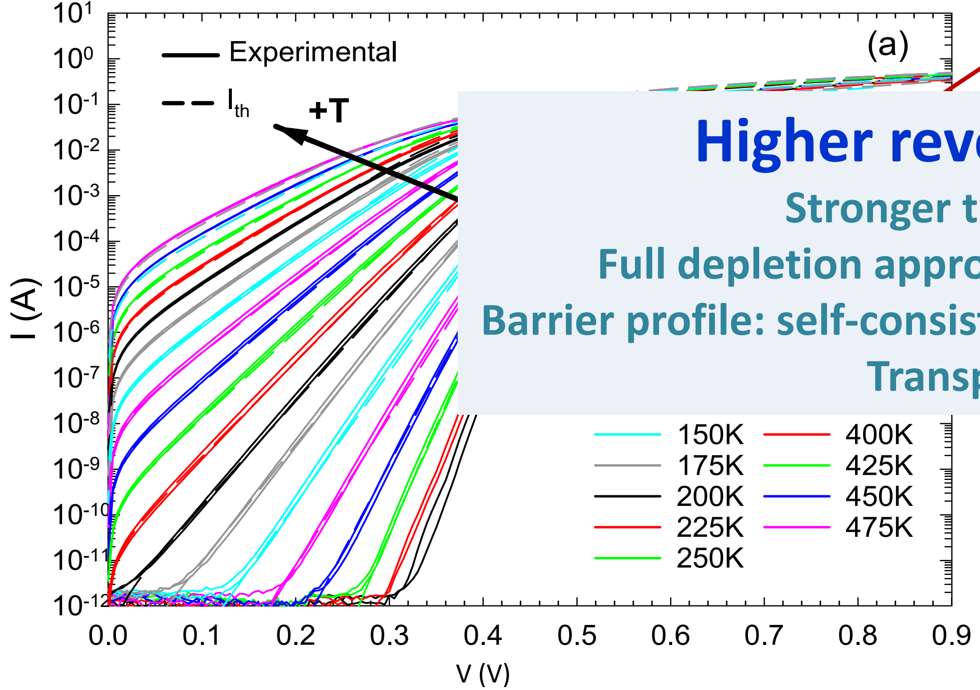


$\eta \approx 1.05$

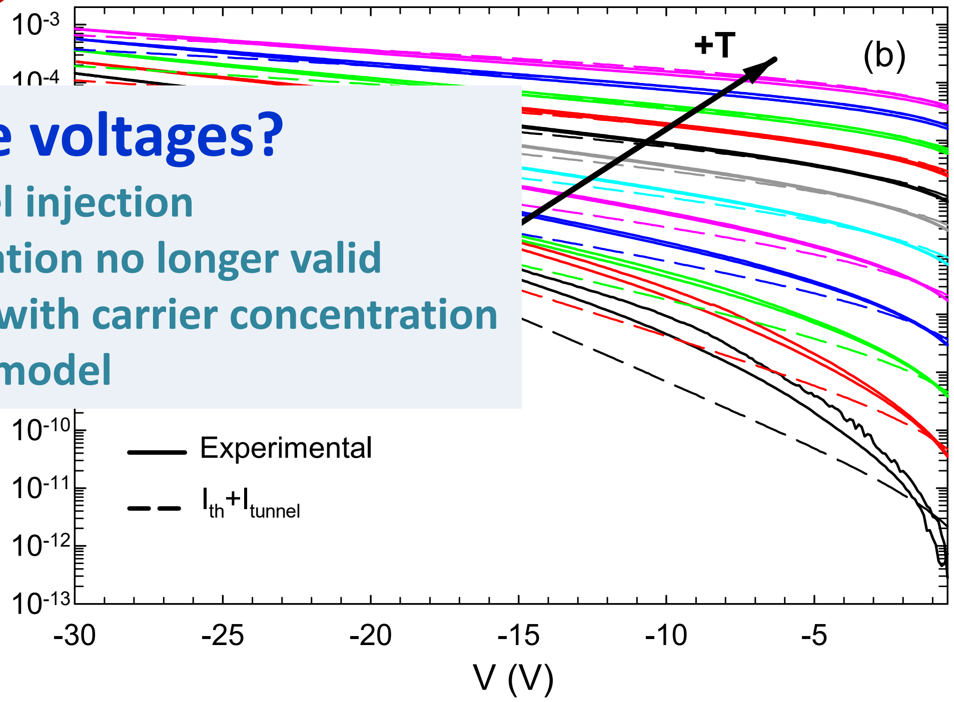
$R_S \approx 1\ \Omega$

$\phi_B \approx 0.7$ - 0.8 eV

Forward bias



Reverse bias



Higher reverse voltages?

Stronger tunnel injection

Full depletion approximation no longer valid

Barrier profile: self-consistent with carrier concentration

Transport model

Monte Carlo model: transport

Electrons

Γ_1-U-Γ_3 non-parabolic spherical valleys

ionized impurities, polar and nonpolar optical phonons, acoustic phonons, intervalley

S. García et. al. , *J. Appl. Phys.* **115**. 044510 (2014)

Time step: 0.2 - 2.5 fs
Mesh size: 0.5 - 5 nm

Holes

heavy, light and split-off bands

ionized impurities, nonpolar optical and acoustic phonons, and polar optical phonons; all including inter-valley transitions

S. Chen and G. Wang, *J. Appl. Phys*. **103**, 023703 (2008)

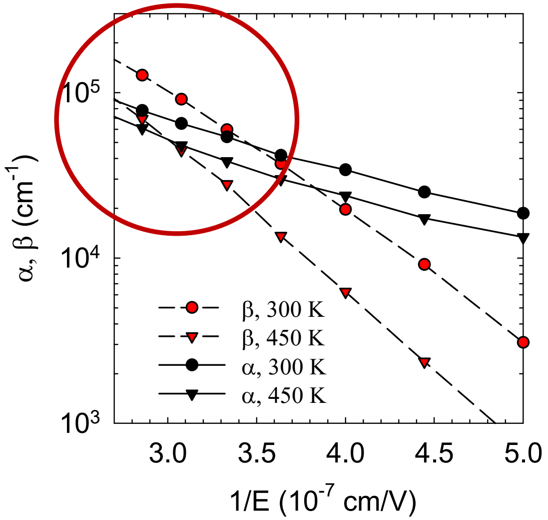
Impact Ionization

Keldysh approach

$$P(\varepsilon) = S\left(\frac{\varepsilon - \varepsilon_{th}}{\varepsilon_{th}}\right)^2 \qquad \varepsilon > \varepsilon_{th}$$

$$P(\varepsilon) = 0 \qquad \varepsilon < \varepsilon_{th}$$

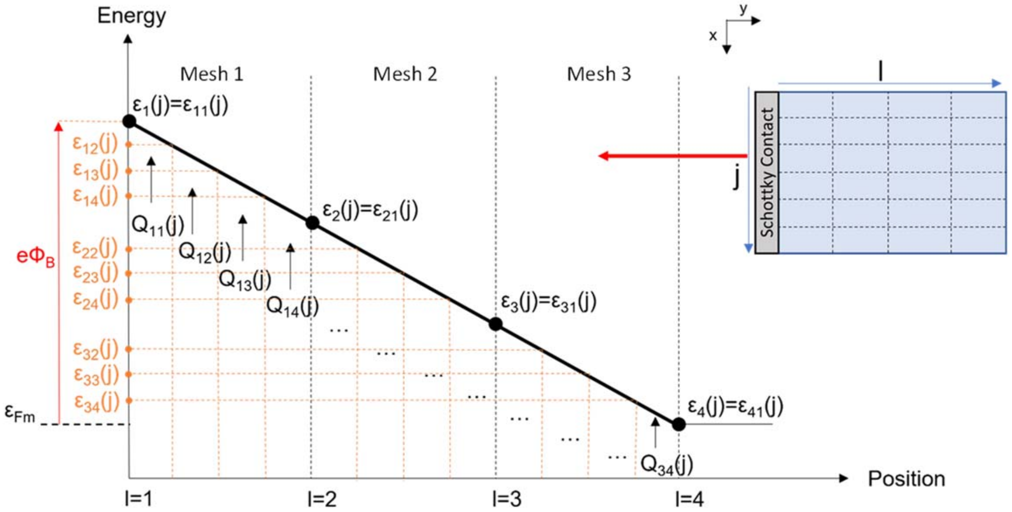
	Electrons	Holes
ε_{th} (eV)	3.0	3.0
S (10^{12} s^{-1})	5.0	25.0



Monte Carlo model: tunnel injection

Self consistency Barrier profile obtained from the self-consistent solution of Poisson’s equation

MC 2-D Energy discretization linked to the spatial mesh used to solve Poisson’s equation



$$J(\varepsilon)d\varepsilon = -eN(\varepsilon)T_C(\varepsilon)d\varepsilon$$

$$N(\varepsilon) = \frac{A^*T}{ek_B}\ln\left[1 + exp\left(-\frac{\varepsilon-\varepsilon_F}{k_BT}\right)\right]$$

$$T_C(\varepsilon) = exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2}\sqrt{2m^*[\varepsilon_C(x)-\varepsilon]}dx\right)$$

$$Q_{li}(j) = \Delta teN(\varepsilon_{li}(j))T_C\,(\varepsilon_{li}(j))\Delta\varepsilon_{li}(j)$$

MC
- Number of injected carriers
- Mesh and energy interval

MC 1-D Energy discretization independent of the spatial mesh. Barrier lowering taken into account

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Simulations
- Without tunnel injection
- With and without impact ionization (II)
- Estimation of the current with the FD approach

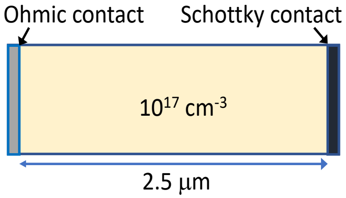
Current evaluated by counting particles at the Schottky contact

Electrons: tunnel injection **Holes:** impact ionization

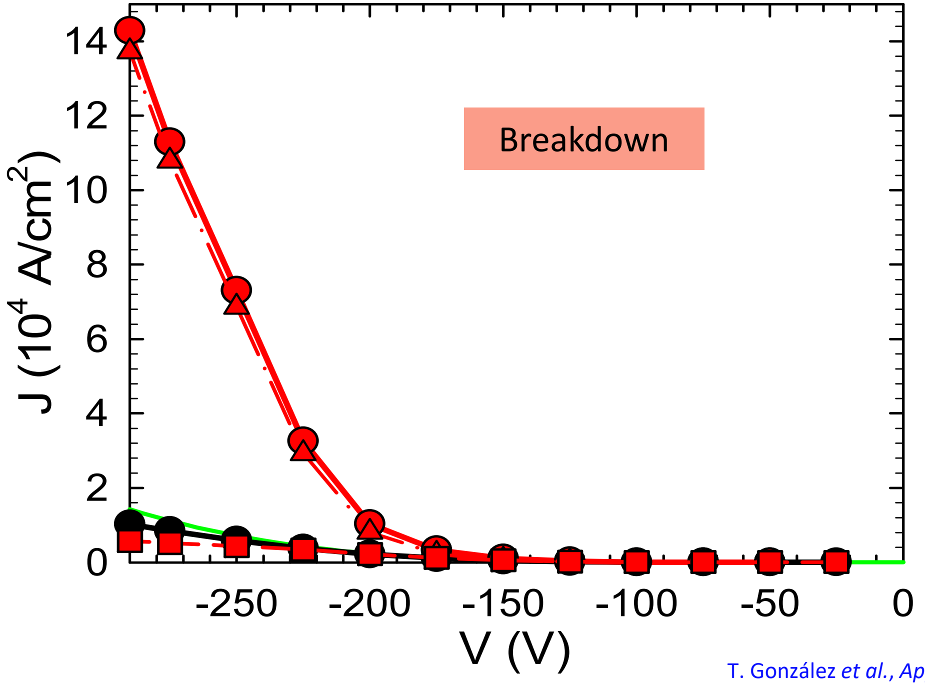
Results: 1D simulations (diode 1)

Low-doped diode

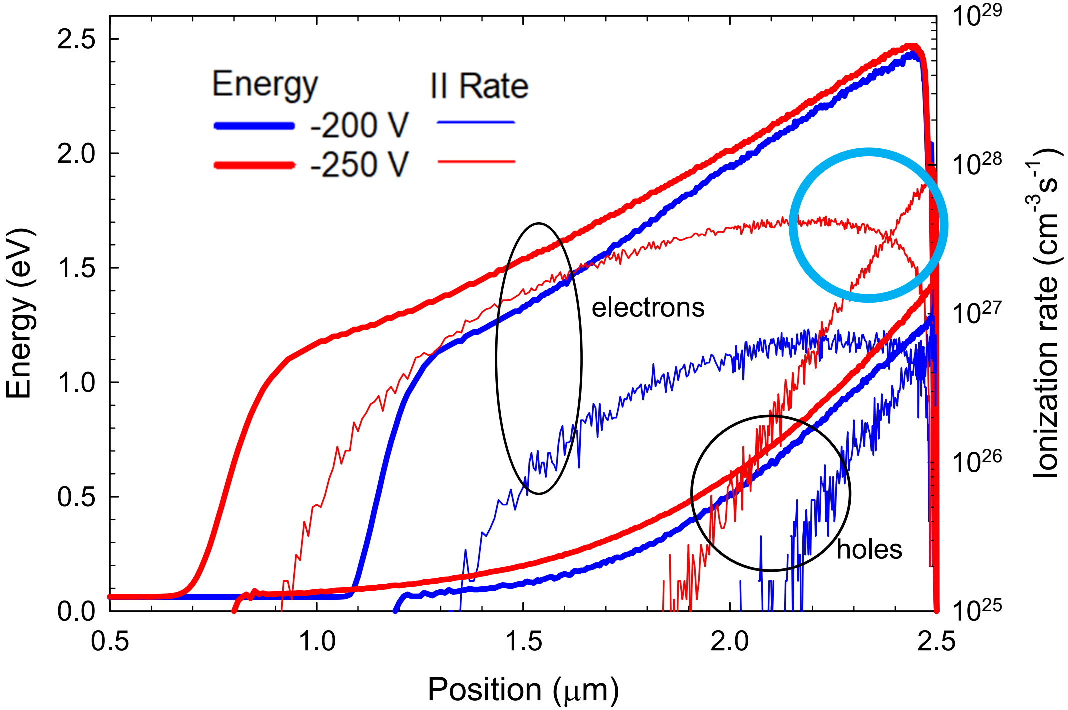
T=450K
$\phi_B = 0.935$ eV



low tunnel injection



Energy and ionization rate

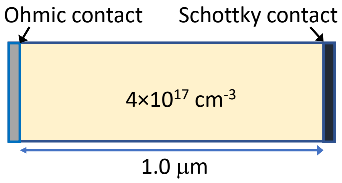


T. González *et al.*, *Appl. Phys. Express* **16**, 024003 (2023)

Results: 1D simulations (diode 2)

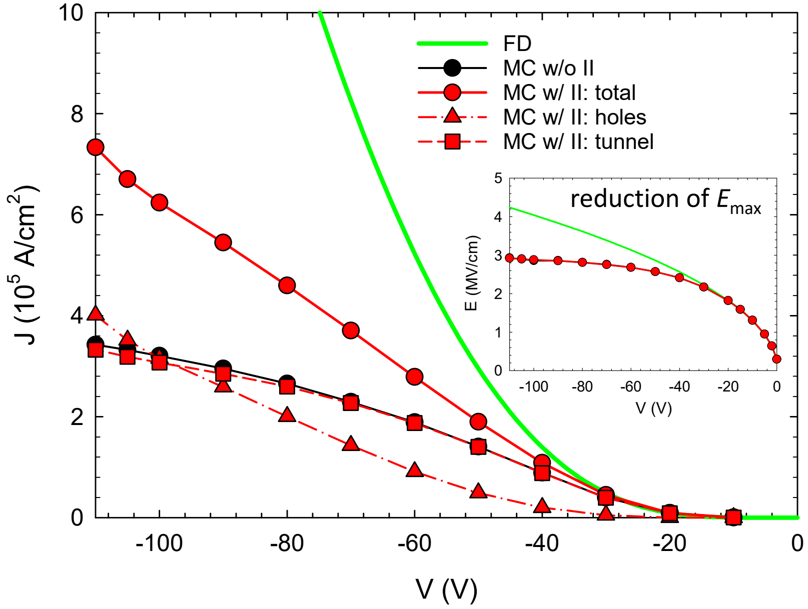
Highly-doped diode

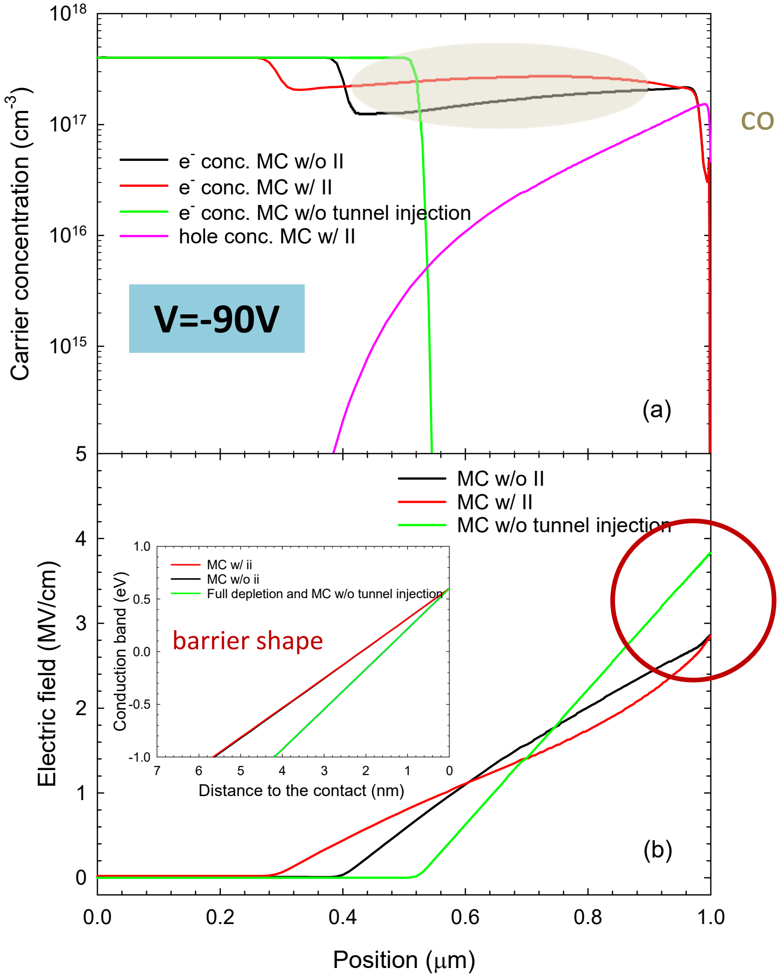
T=300K
$\phi_B = 0.6$ eV



strong tunnel injection

I-V

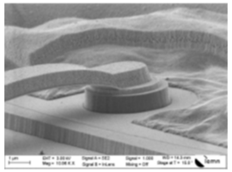




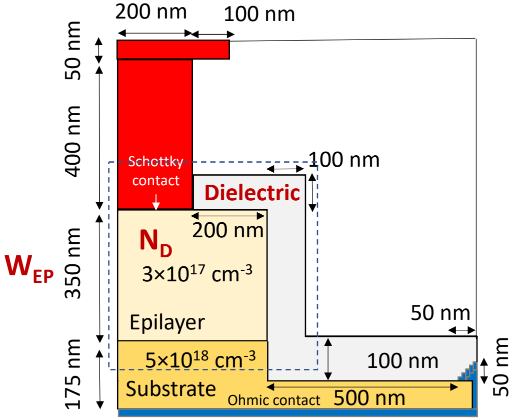
high e^- concentration

Results: 2D simulations (without impact ionization) - passivation dielectric

small-size diodes
for THz frequency multipliers

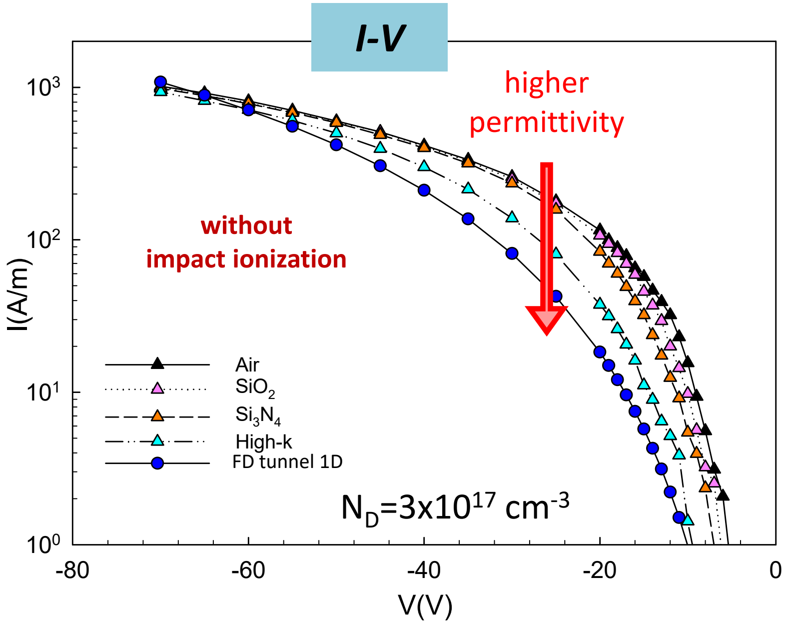


T=300K
ϕ_B= 0.5 eV

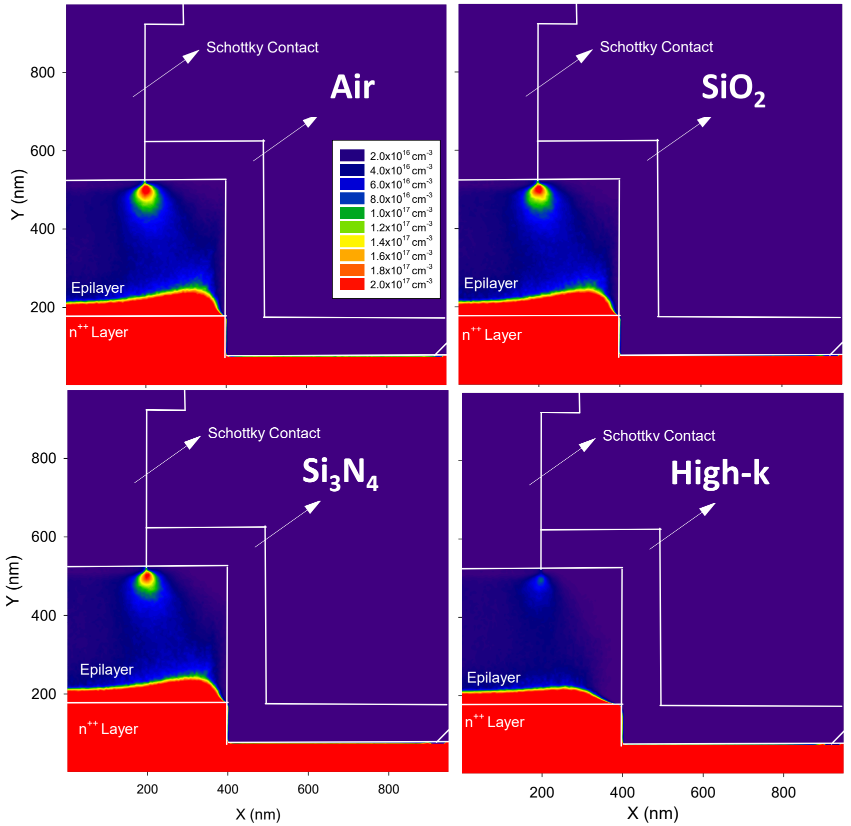


2D effects

higher electric field at the contact edge
↓
current crowding
smoothed by dielectrics with high-k

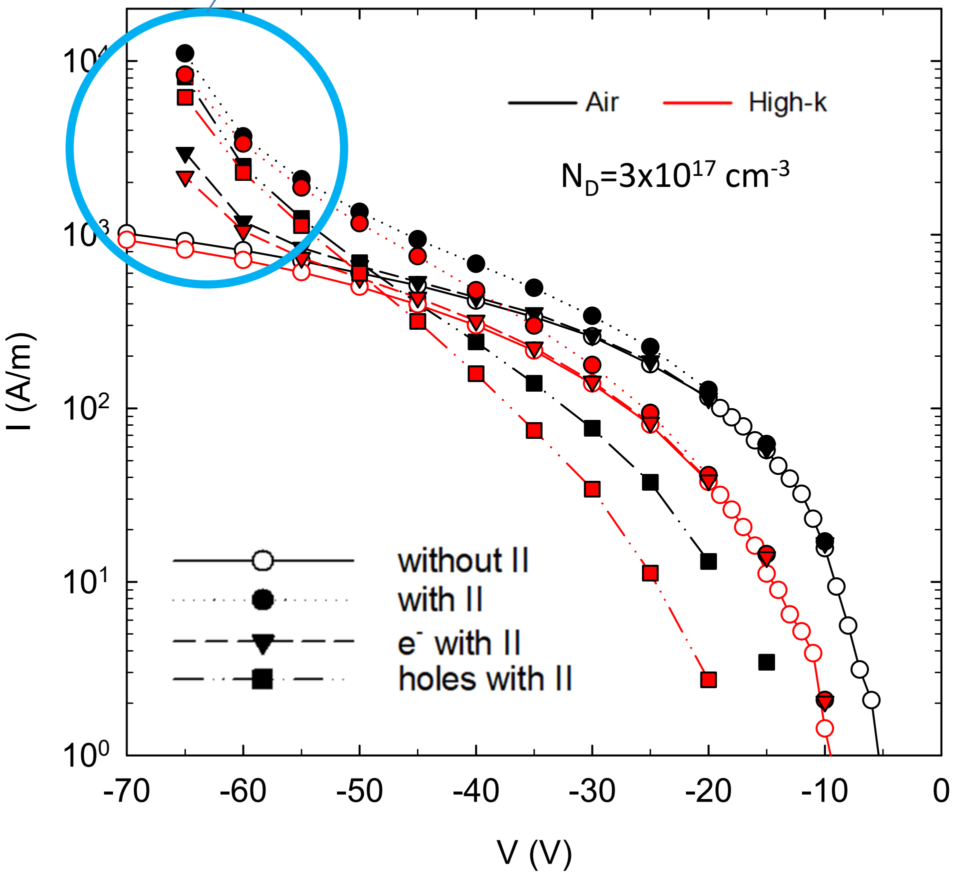


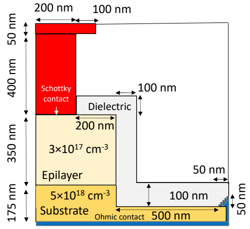
electron concentration *V*=-30V



Results: 2D simulations (with impact ionization) - breakdown

Breakdown → increase of both tunnel injection and impact ionization

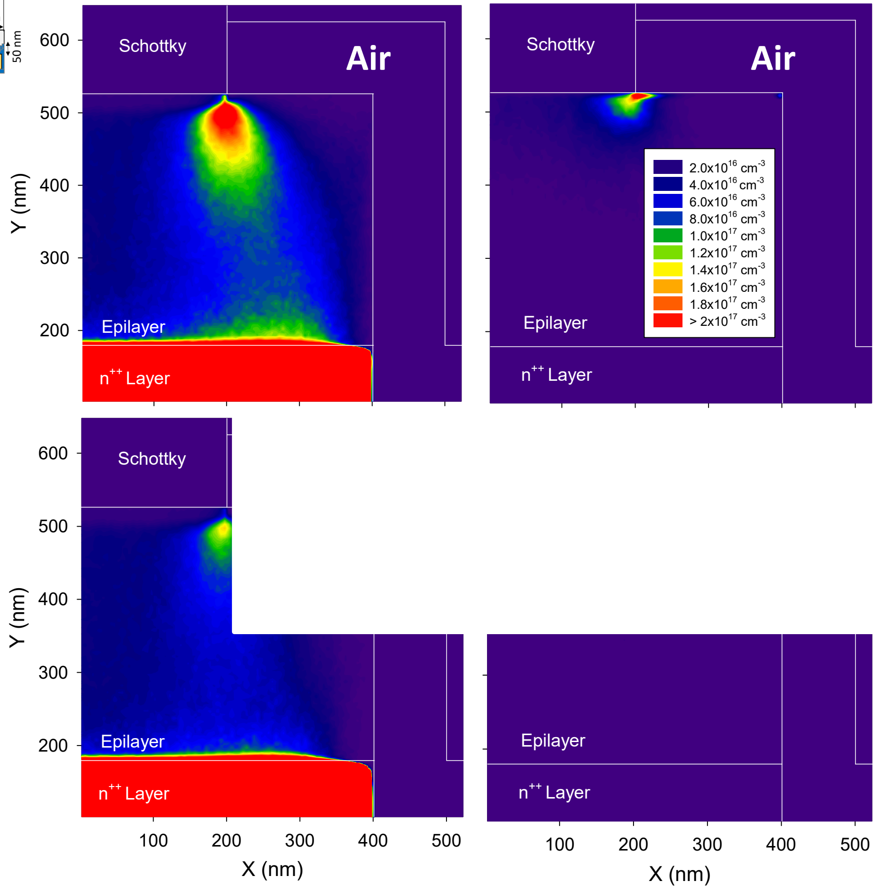




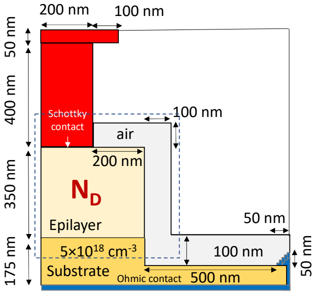
electron concentration

V=-35V

hole concentration



Results: 2D simulations (with impact ionization) - epilayer doping

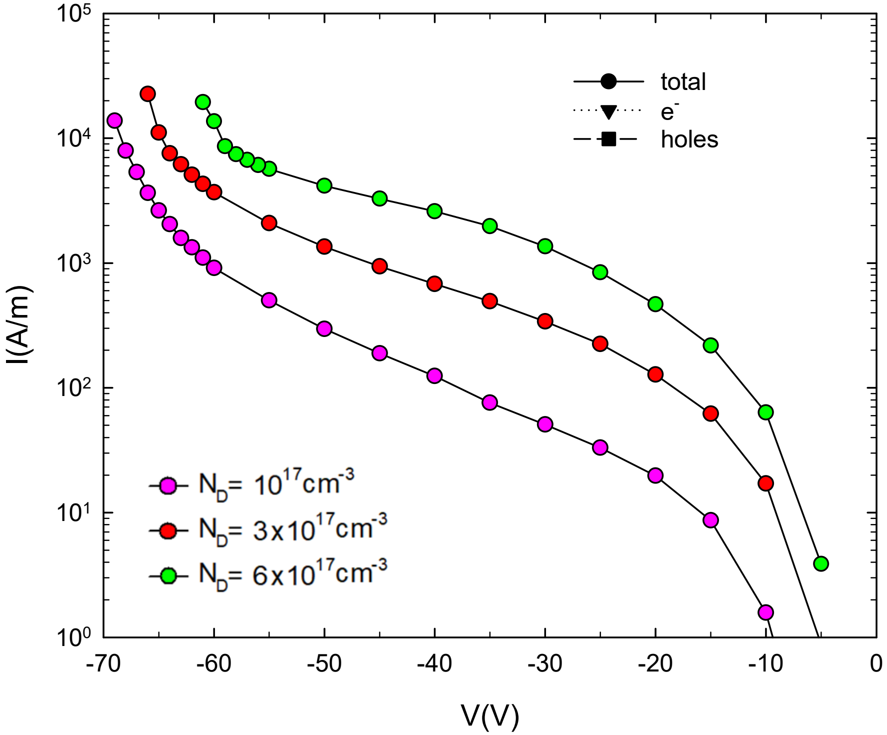


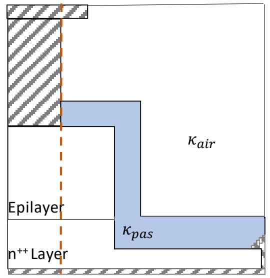
W_{EP}= 350 nm

higher doping

↓

lower breakdown voltage





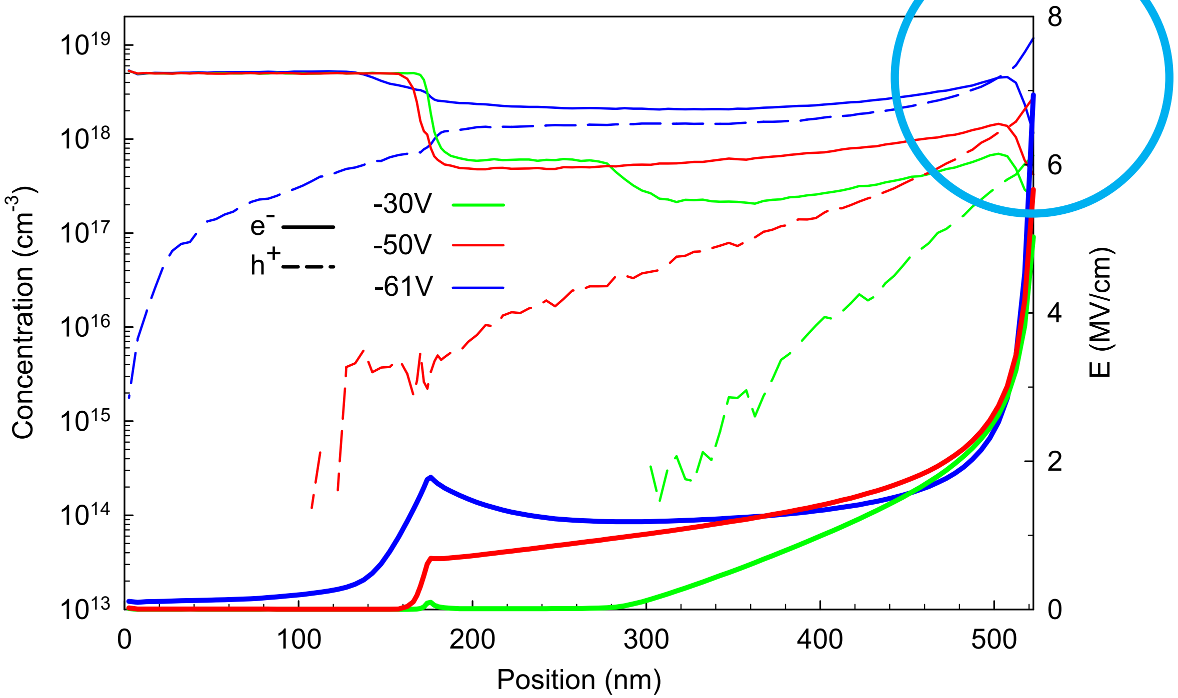
Breakdown

↓

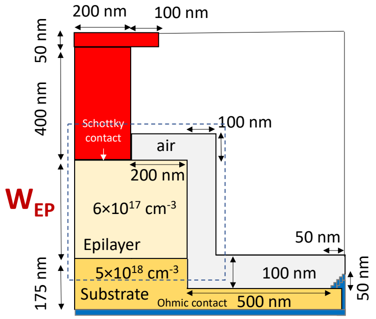
feedback impact ionization ⇔ tunneling

(more pronounced for higher N_D)

N_D=6x10^{17}cm^{-3}

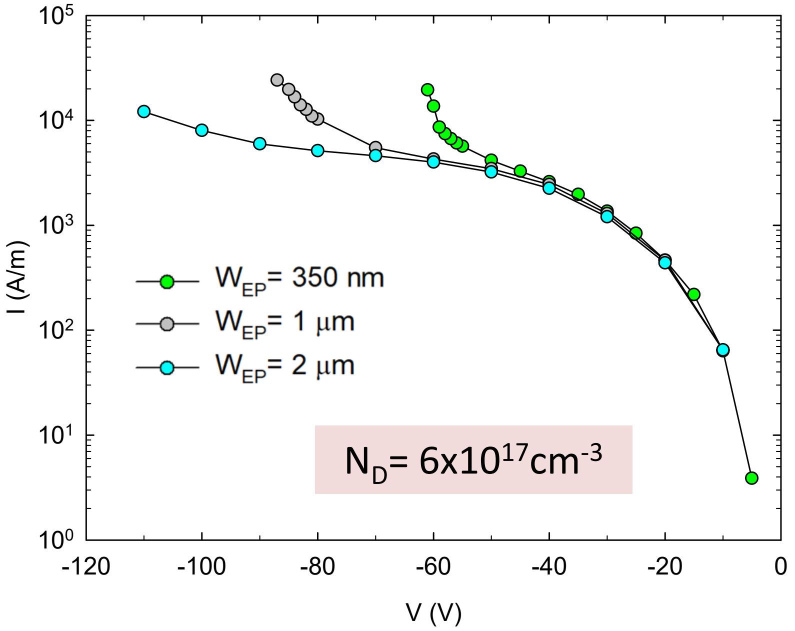


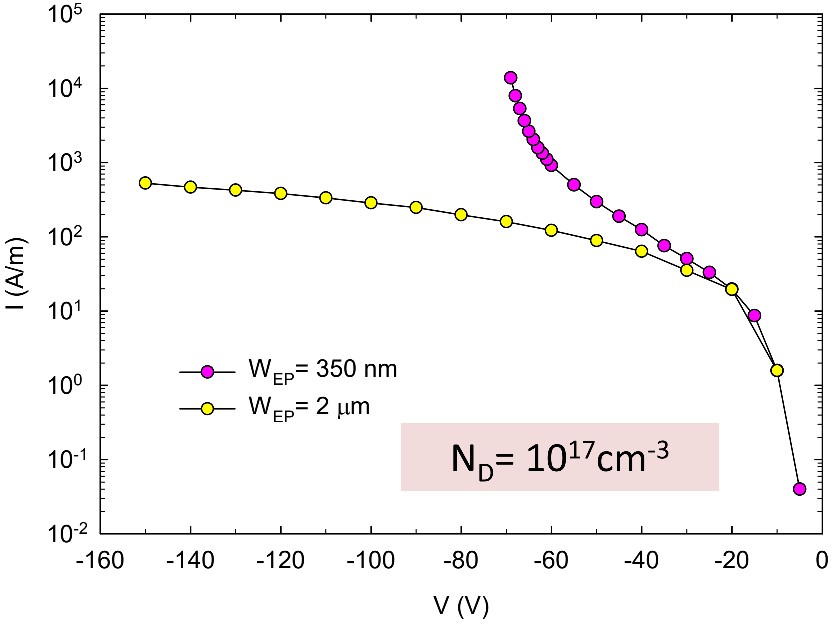
Results: 2D simulations (with impact ionization) - epilayer thickness



Thicker epilayer
↓
higher breakdown voltage
and softer breakdown

Breakdown
↓
impact ionization





Conclusions

- Correct prediction of the I-V curves of SBDs at high applied voltages in reverse bias → shape of the barrier and associated tunnel injection self-consistently calculated with carrier concentration in the depletion region → accounting for electrons and holes generated by impact ionization

- Voltage range at which these effects are relevant and relative influence of tunnel injection and impact ionization → thickness and doping of the epilayer, and barrier height

- Analyzed effects likely to be present in some specific regions of SBDs: contact edge or surface inhomogeneities (high current densities and/or electric fields are locally reached)

- Lower doping and higher thickness of the epilayer → higher breakdown voltage

Acknowledgements

Thank you!

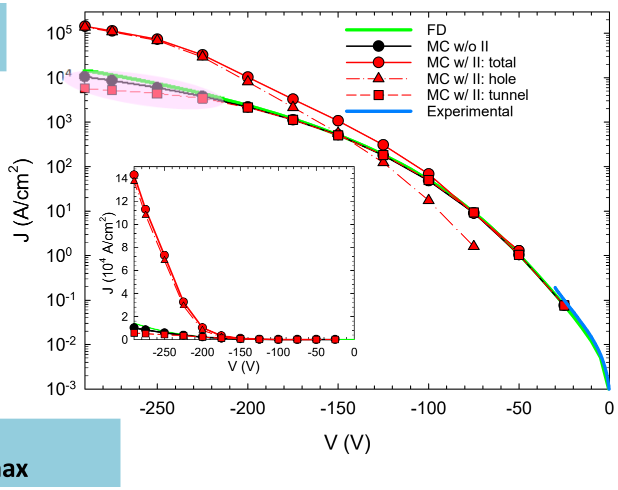
M. Zaknoune, Y. Cordier (GaN SBDs)

PID2020-115842RB-I00

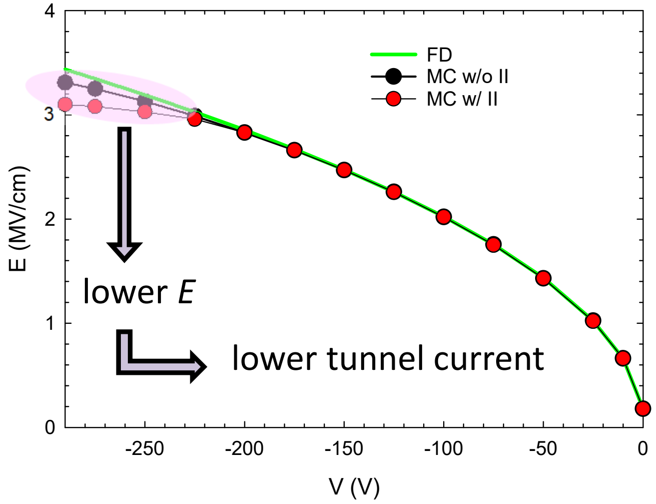
SA254P18

Results: 1D simulations (diode 1)

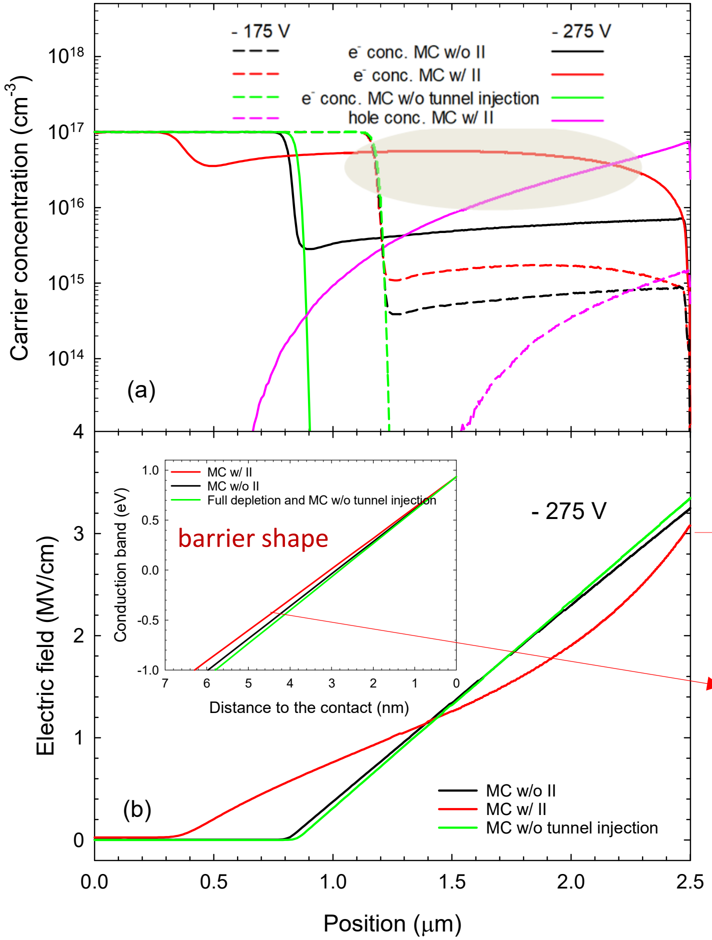
I-V



E_{max}



Spatial profiles

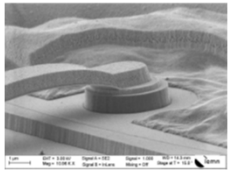


high e⁻ concentration

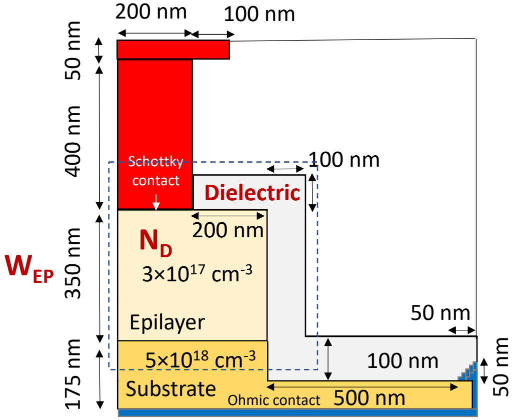
lower E_{max}

wider barrier

Results: 2D simulations (without impact ionization) - passivation dielectric



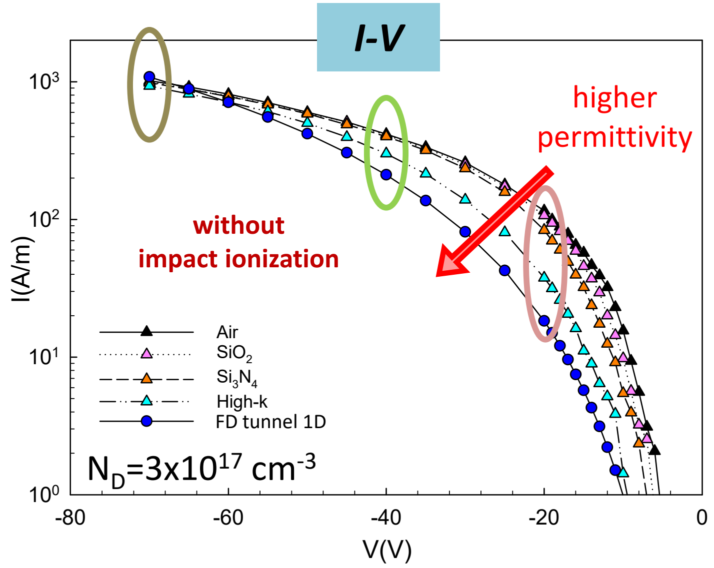
T=300K
ϕ_B= 0.5 eV

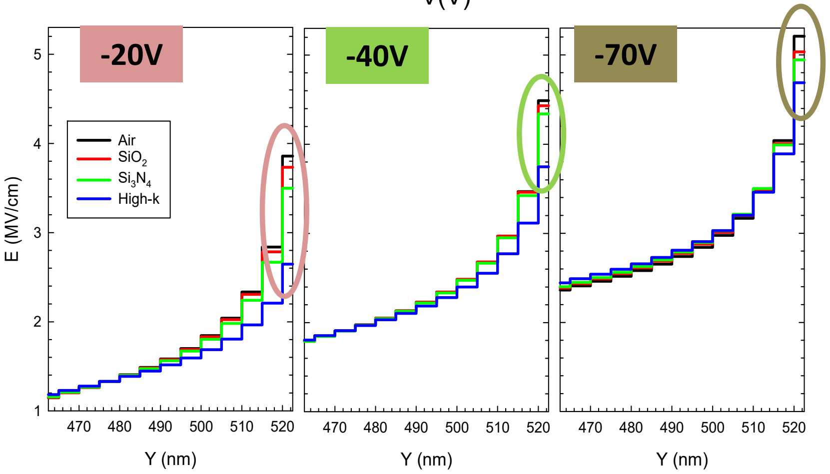


2D effects

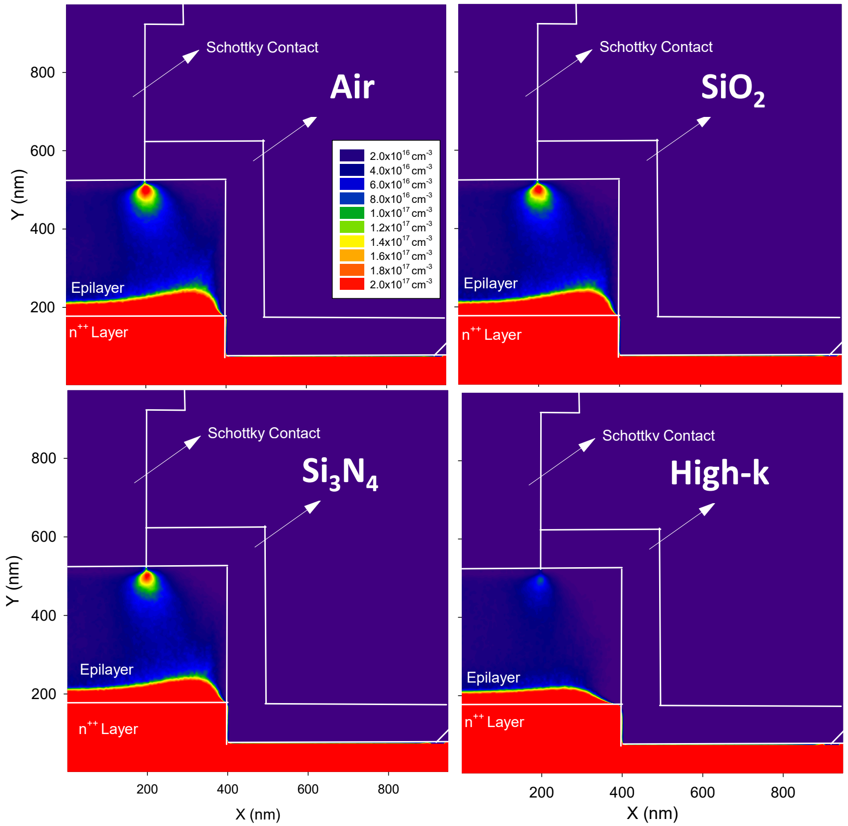
higher electric field at the contact edge
↓
current crowding
smoothed by dielectrics with high-k

I-V



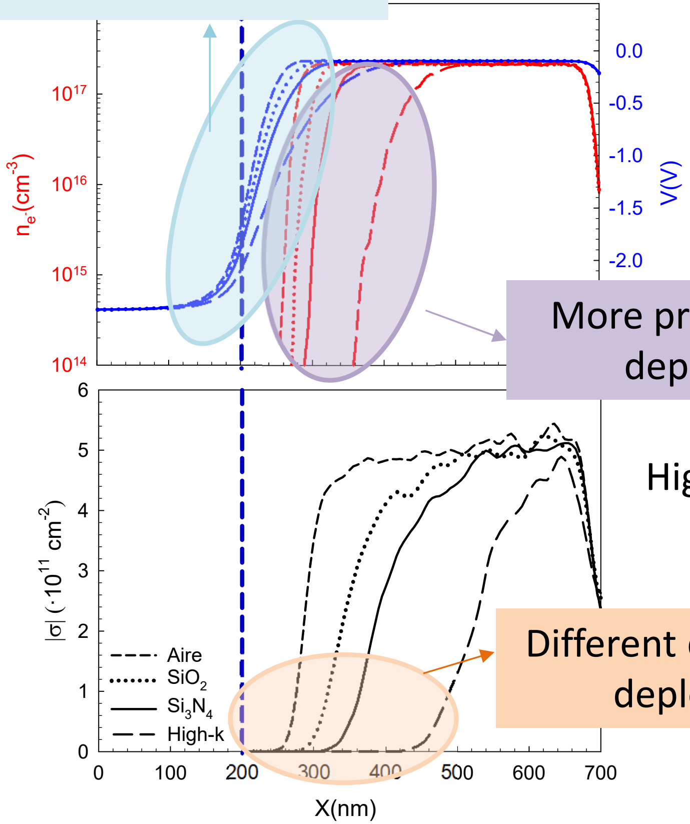


electron concentration V=-30V



Influence of Passivation

Stronger penetration of the electric field ➡ Higher κ_{pas}

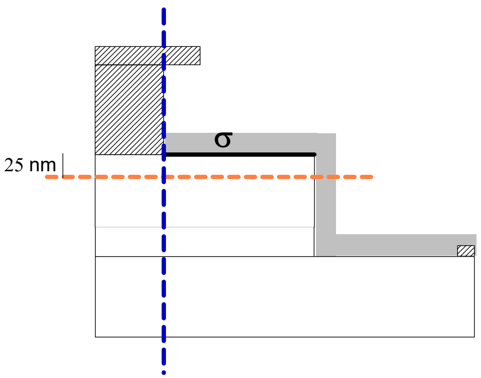


More pronounced depletion

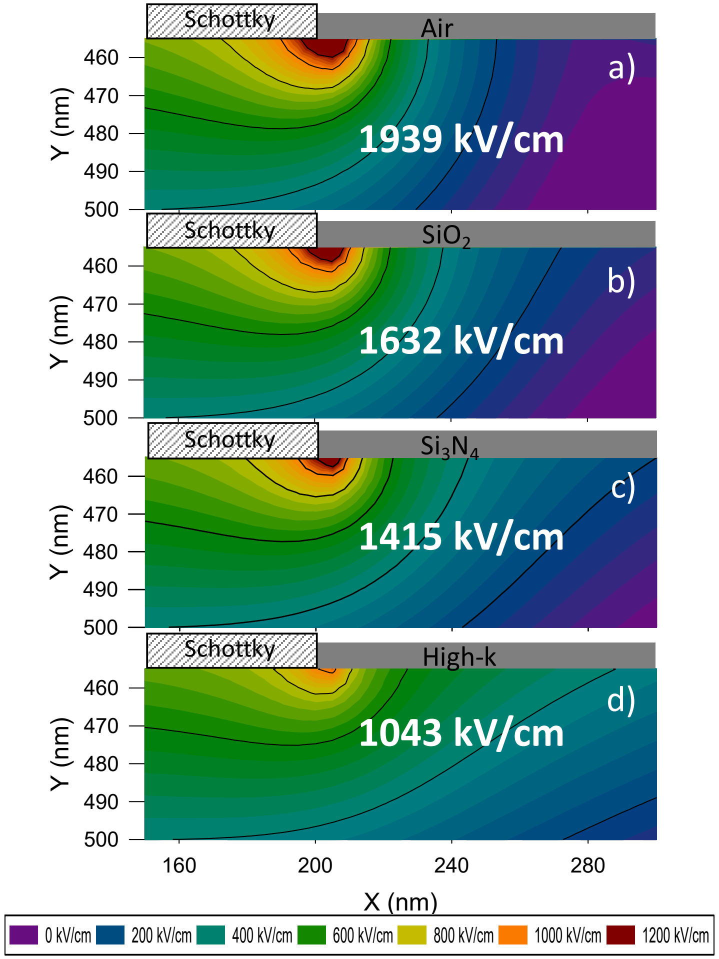
⇓ Higher κ_{pas}

Different due to the depletion

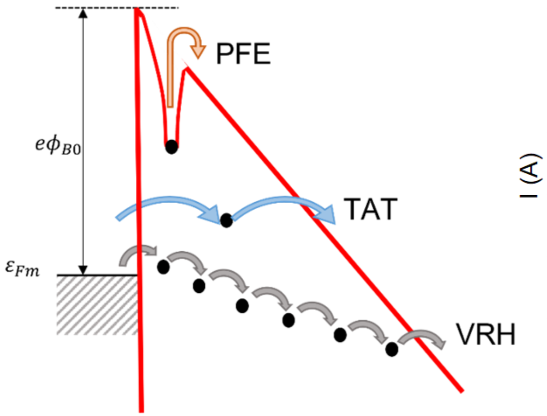
$V - V_B = -4.1V$

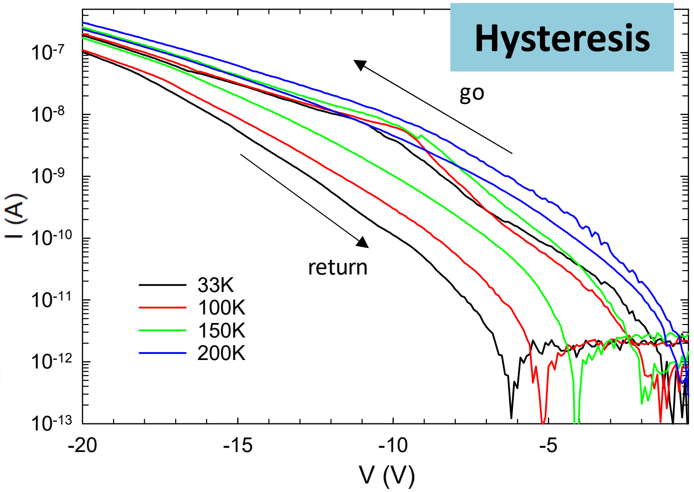


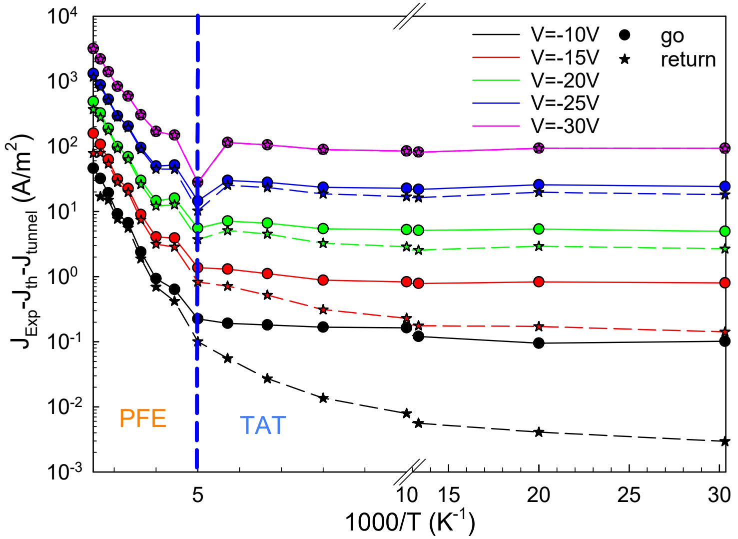
Electric Field

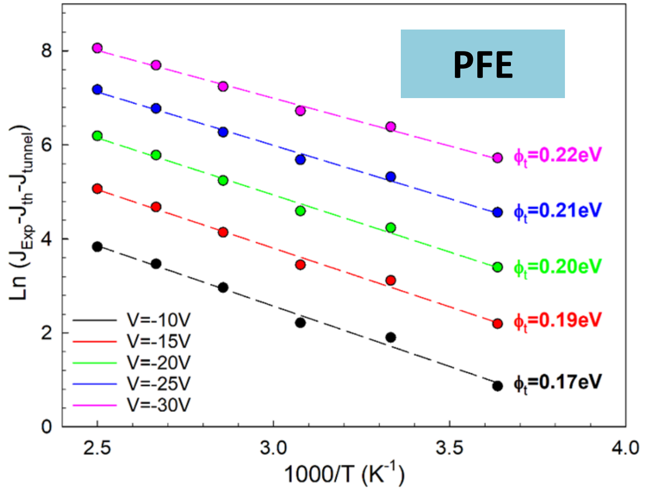


Leakage current



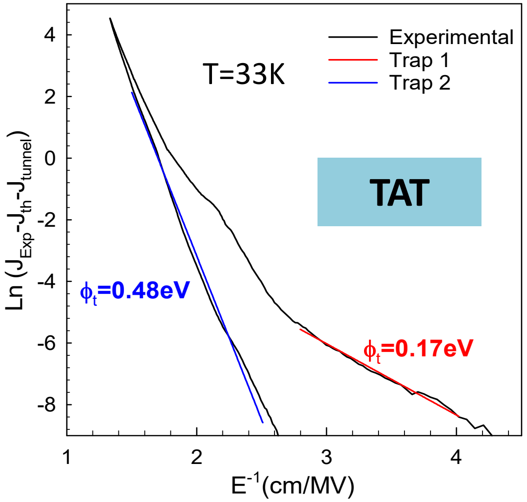






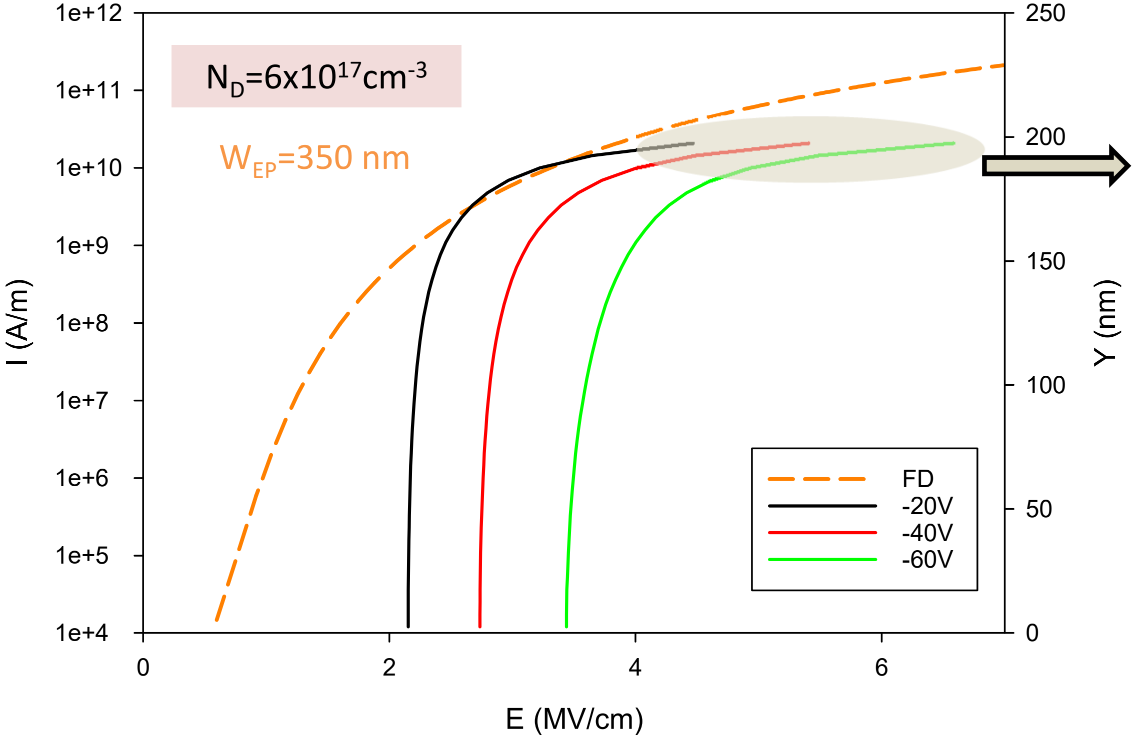
$$J_{TAT} \propto exp\left(\frac{-4\sqrt{2em^*}\phi_t^{3/2}}{3\hbar E}\right)$$

$$J_{PFE} \propto E exp\left(\frac{-e(\phi_t - \sqrt{eE/\pi\kappa_{SC}})}{k_B T}\right)$$



2-D effects

Lower *V* ⇨ Difference of E along the contact ⇨ Higher contribution to the current at the edge



Higher *E* at the edge of the contact

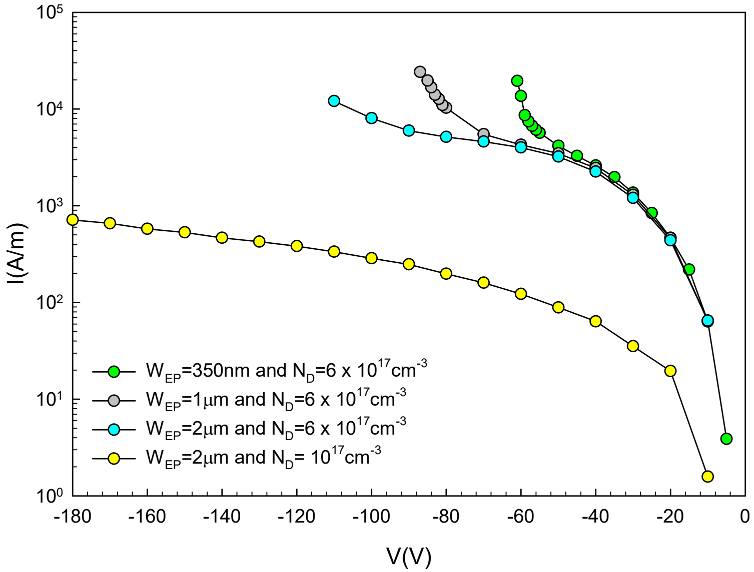
⇩

Higher *V*

Optimum design

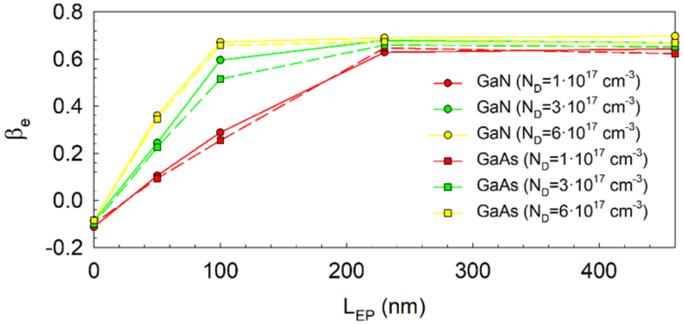
Improve breakdown

- Passivation material with **a high permittivity**
- Lower **doping**
- High **epilayer thickness** → Higher R_s



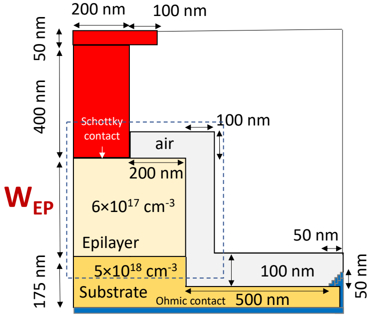
Reduce capacitance

- A reduction of **the epilayer lateral extension**
- A low **doping** of the epilayer



- Passivation material with **a low dielectric constant**
- A reduction of the dielectric **thickness**

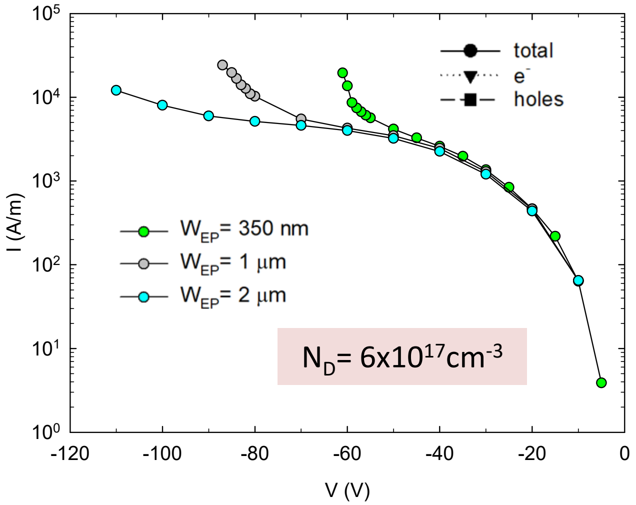
Results: 2D simulations (with impact ionization) - epilayer thickness

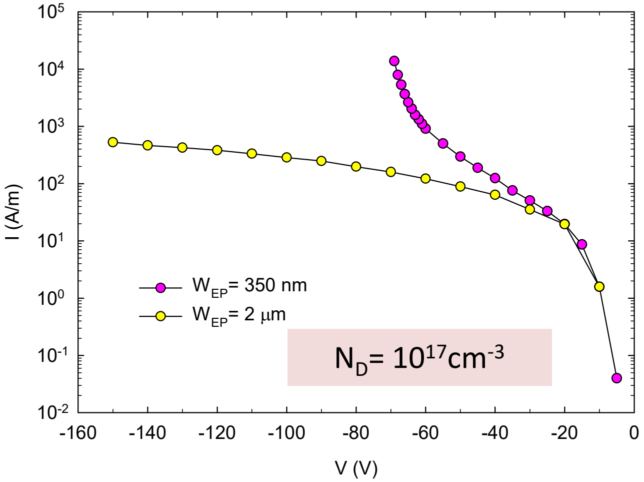


Thicker epilayer

↓

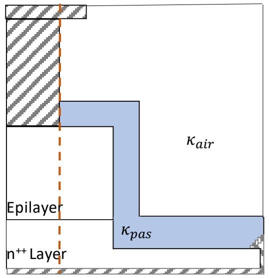
higher breakdown voltage and softer breakdown





N_D= 6x10^{17}cm^{-3}

W_{EP}= 2 µm



Breakdown

↓

impact ionization