RADFAC Day - 26 March 2015

Modelling of Diamond Devices with TCAD Tools

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Outline

- ✓ Introduction: Motivation and Aim.
- ✓ Device-level Numerical Simulation with TCAD: Settings.
- ✓ Physical Characterization of Diamond
- ✓ Design and development of the proper simulation methods and methodologies
  - ✓ 2D vs 3D approach
  - ✓ Charge Generation Shape
  - ✓ Time discretization
- ✓ Simulation Results (Steady-State and Transient Results)
  - ✓ Doping dependence
  - ✓ Constant Carrier Generation
  - ✓ Traps
- ✓ Silicon on Diamond Device
  - ✓ Effect of the interface
- ✓ Conclusions and Future works

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Motivation and Aim

	Silicon	Diamond
Bandgap [eV]	1,12	5,47
Breakdown Field [MV/cm]	0,4	20
Intrinsic Resistivity @ R. T. [Ω cm]	$2{,}3 \times 10^{5}$	$> 10^{11}$
Intrinsic Carrier Density [cm^{-3}]	$1{,}5 \times 10^{10}$	10^{-27}
Dielectric Constant	11,9	5,7
Electron Mobility	1350	1900-3800
Hole Mobility	480	2300-4500
Saturation Velocity	1×10^{7}	$2{,}7 \times 10^{7}$
Displacement Energy [eV/atom]	13-20	43
Thermal Condutivity [W cm^{-1} K^{-1}]	1,5	20
Energy to create e-h pair [eV]	3,62	11,6 - 16
Radiation Length [cm]	9,36	12,2
Energy Loss for MIPs [MeV/cm]	3,21	4,69
Aver. Signal Created / 100 µm	8892	3602

high field operation

low leakage current

fast signal

radiation hardness

heat dissipation

Also problems……
→ small dimensions;
high cost;

low signal

Motivation and Aim (1)

- ✓ Goal: development of numerical methods and methodologies in order to simulate, at device-level, the steady-state and time-variant analysis of a Diamond and Silicon on Diamond device.

- ✓ The design of the set-up is a critical issue in a TCAD simulation
  - ✓ Robust and reusable simulation set-up.
  - ✓ Wrong choices on spatial and time domain discretization or methodologies, lead to wrong results.

- ✓ Diamond is a novel material in electronic applications

  → is not included in the material library of the state-of-the-art TCAD software.

  → diamond added by-hand in the TCAD material's library

  → No fitting parameters of existing insulator/semiconductor materials.

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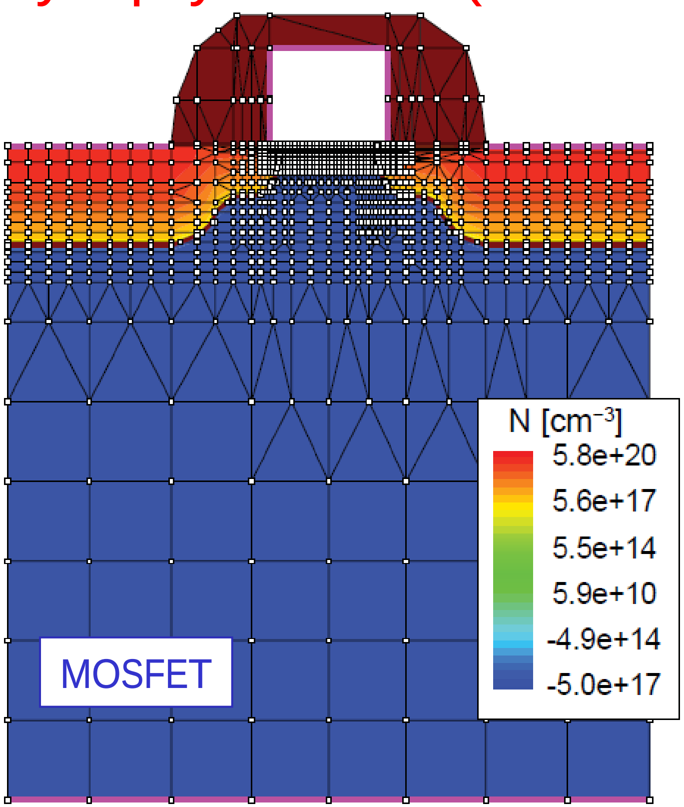
Technology Computer-Aided Design (TCAD)

- ✓ Device simulation tools simulate the electrical characteristics of semiconductor devices, as a response to external electrical, thermal or optical boundary conditions imposed on the structure.

- ✓ Synopsys© TCAD (Sentaurus)



$$\begin{cases} \nabla\cdot\left(-\varepsilon_s\nabla\varphi\right)=q\left(N_D^+-N_A^-+p-n\right) \\ \dfrac{\partial n}{\partial t}-\dfrac{1}{q}\nabla\cdot\vec{J}_n=G-R \\ \dfrac{\partial p}{\partial t}+\dfrac{1}{q}\nabla\cdot\vec{J}_p=G-R \end{cases}$$

$$\vec{J}_n=-q\mu_n n\nabla\varphi+qD_n\nabla n$$

$$\vec{J}_p=-q\mu_p p\nabla\varphi-qD_p\nabla p$$

Physical Characterization of Diamond

```
Material = "Diamond"

* Ratio of the permittivities of material and vacuum
        epsilon          = 5.7      # [1]

* Bandgap
        Chi0      = 1.3      # [eV]
        Eg0       = 5.47     # [eV]

* Lattice thermal conductivity
        kappa     = 20             # [W/(K cm)]

* Incomplete Ionization
NdCrit              = 1.0e+20            # [cm - 3]
NaCrit              = 3.1e+19            # [cm - 3]

* mu_const    = mumax (T/T0)^(   - Exponent )
        mumax             = 4.5e+03 ,  3.8e+03        # [cm^2/(Vs)]
        Exponent          = 1.55    ,  1.55           # [1]

* Nv(T) = Nv300 * (T/300)^3/2
        Nv300    = 1.8000e+19       # [cm - 3]

* Nc(T) = Nc300 * (T/300)^3/2
        Nc300    = 5.0000e+18       # [cm - 3]
```

New material added by-hand in the TCAD material library

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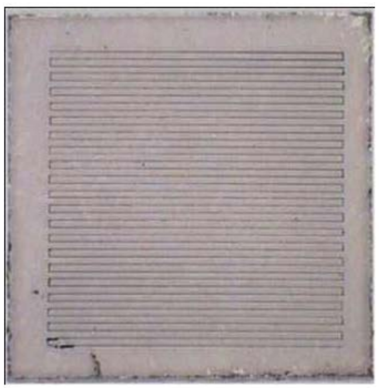
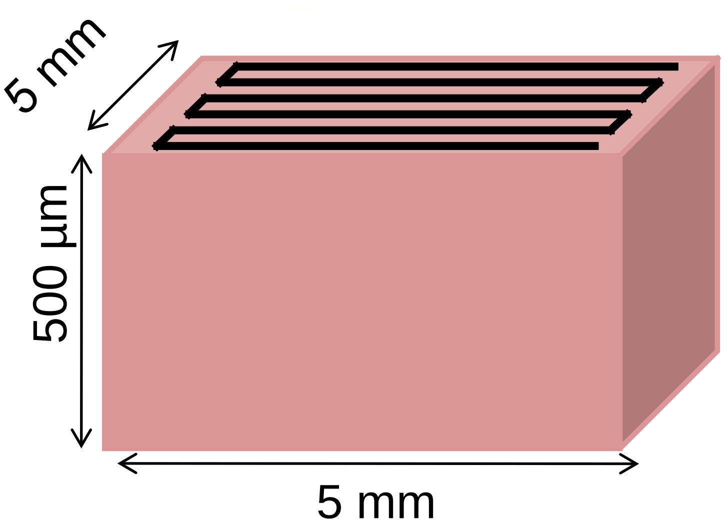
Setting the simulation domain: 2D vs 3D approach

Actual device

Top view

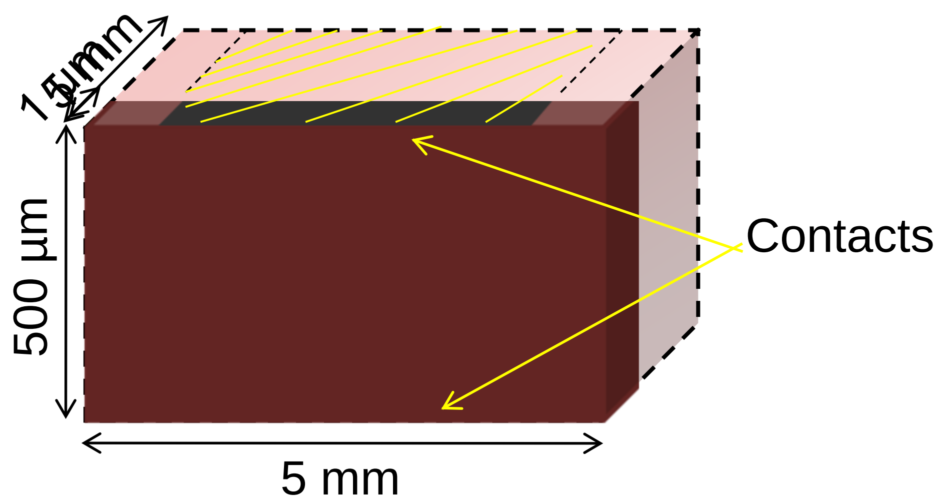




Simulated Structure

The 2D section of the actual device has been considered for simulation purposes.

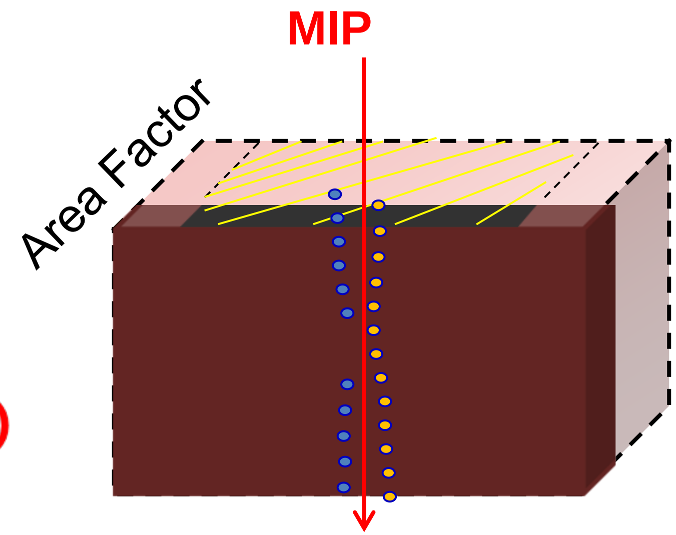
→ save up simulation time

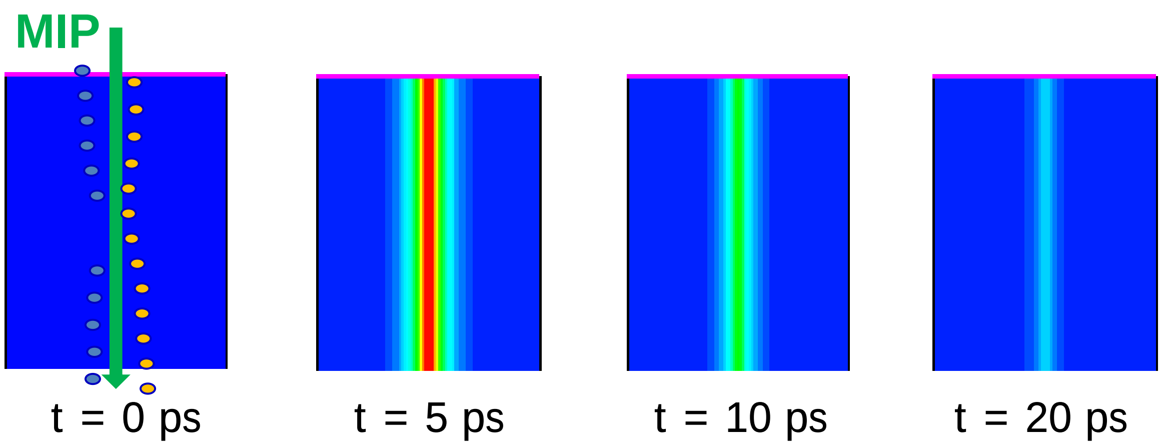


Setting the simulation domain: 2D vs 3D approach (1)

Numerical Model of MIP in the TCAD environment:

Physics {
  ...
  AreaFactor=AF
  HeavyIon(
    ...
    $$Let_f = \frac{57{,}67}{AF}\frac{pC/\mu m}{\mu m})$$
    }





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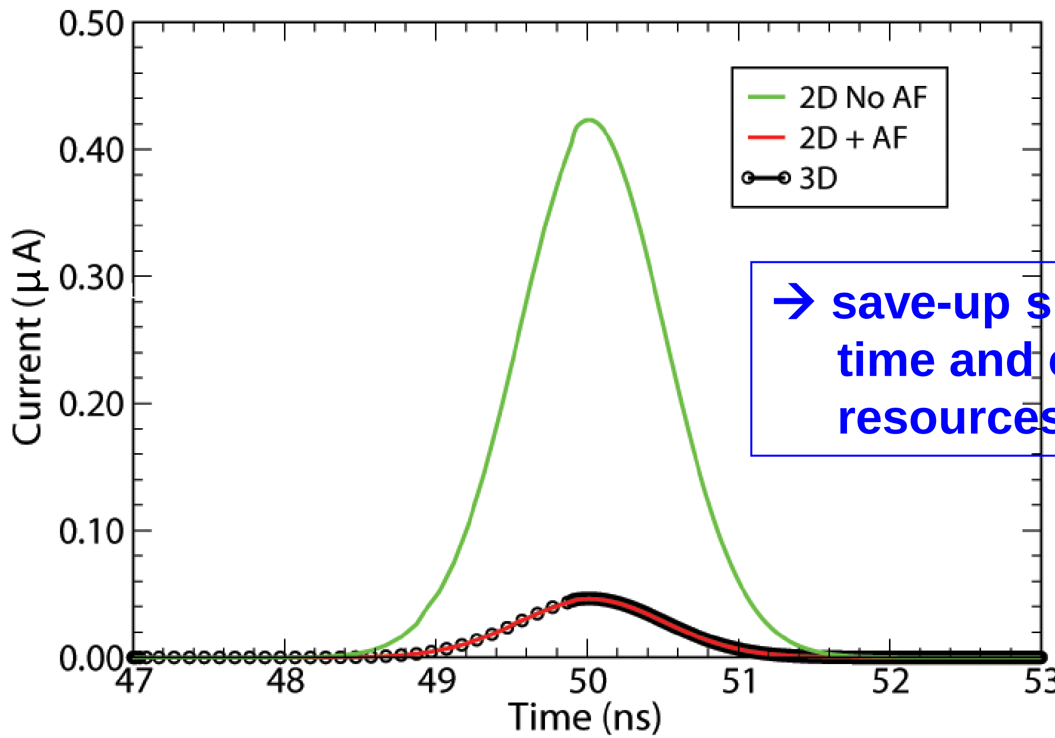
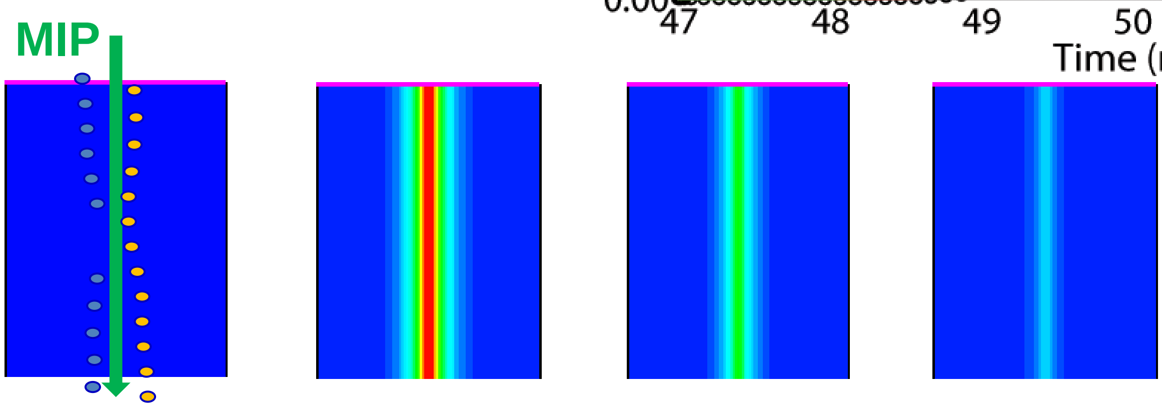
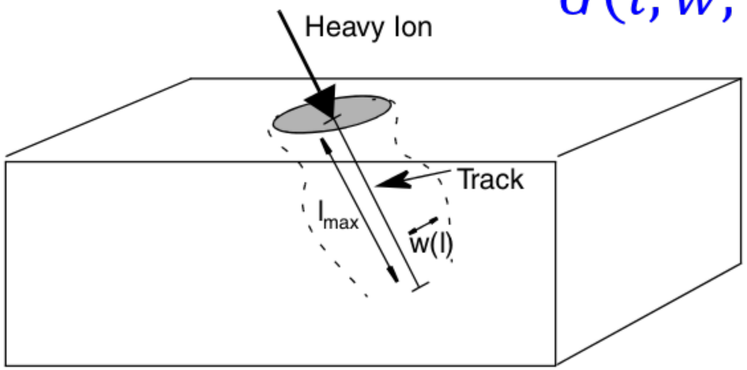


→ save-up simulation time and computing resources



t = 0 ps t = 5 ps t = 10 ps t = 20 ps

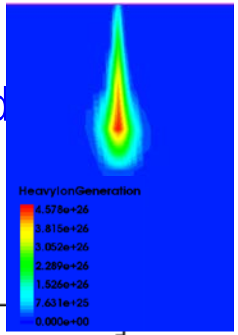
Charge Generation Shape



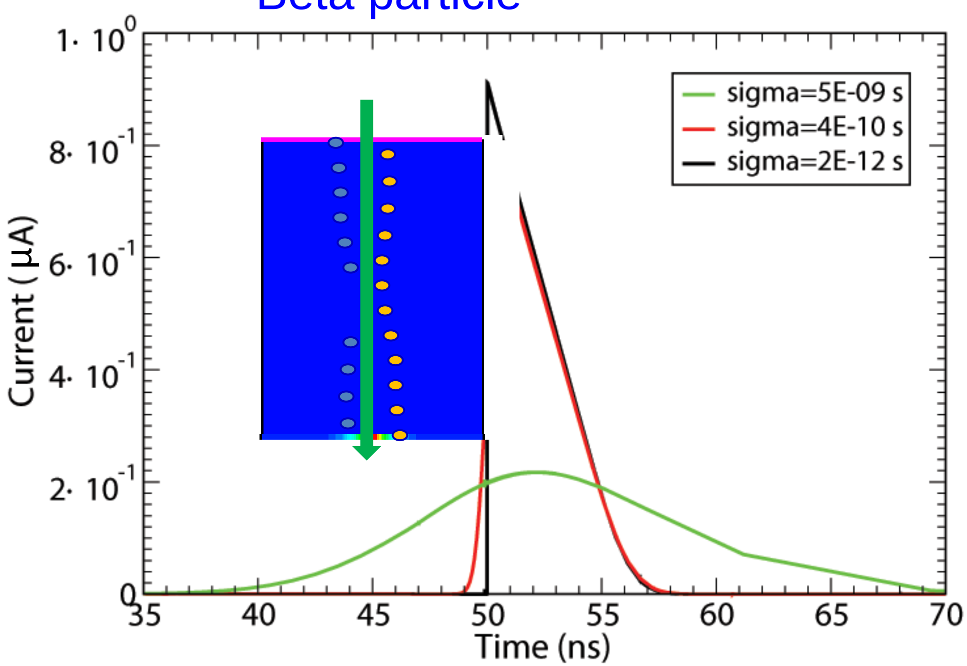
$$G(l,w,t) = G_{LET}(l)\, R(w,l)\, T(t)$$

Gaussian

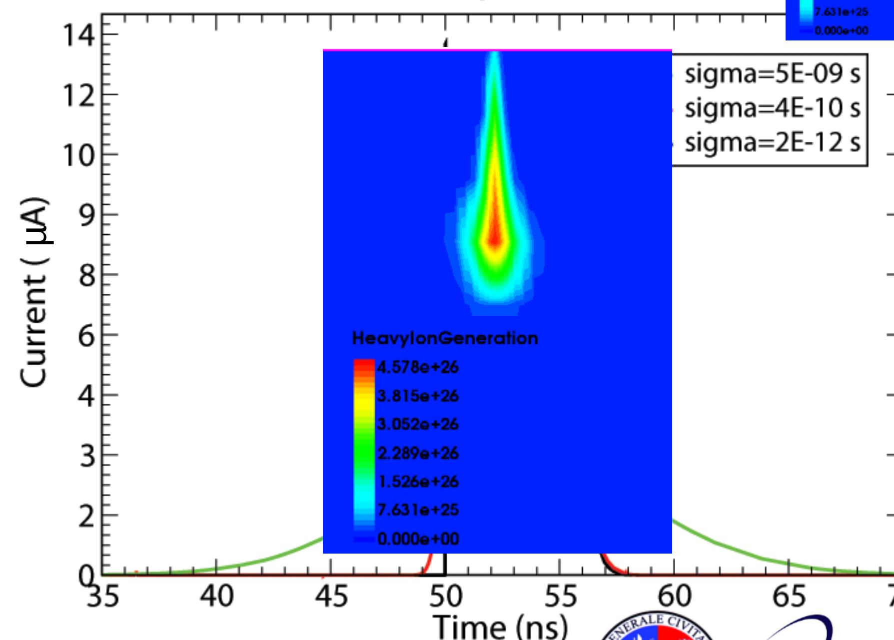
Gaussian,
→effect of the standard



Beta particle



Alpha Particle



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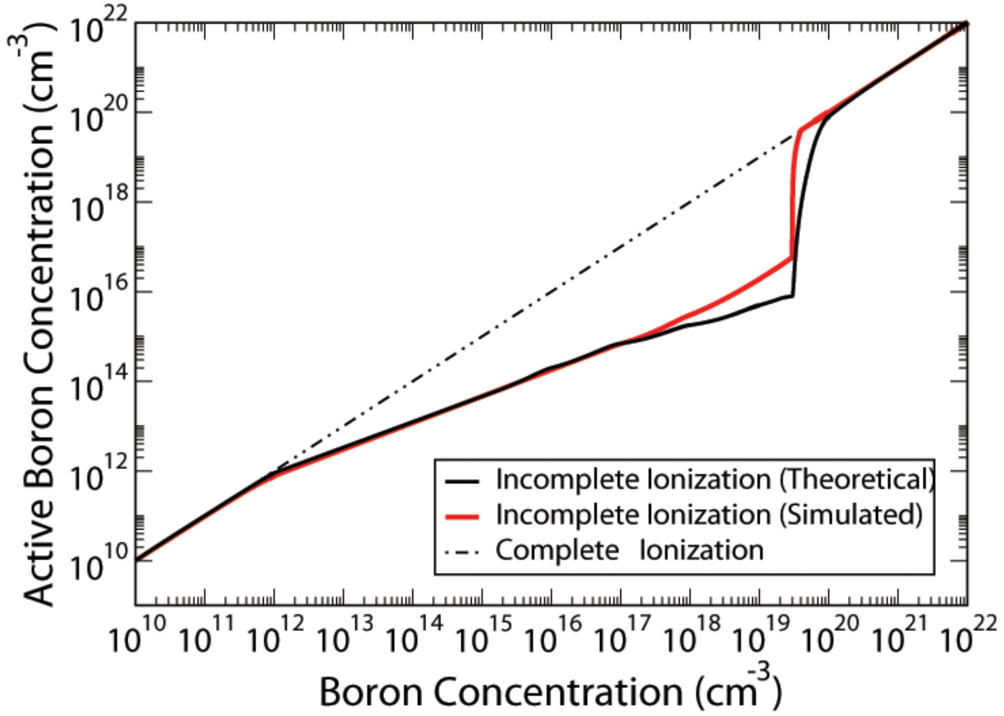
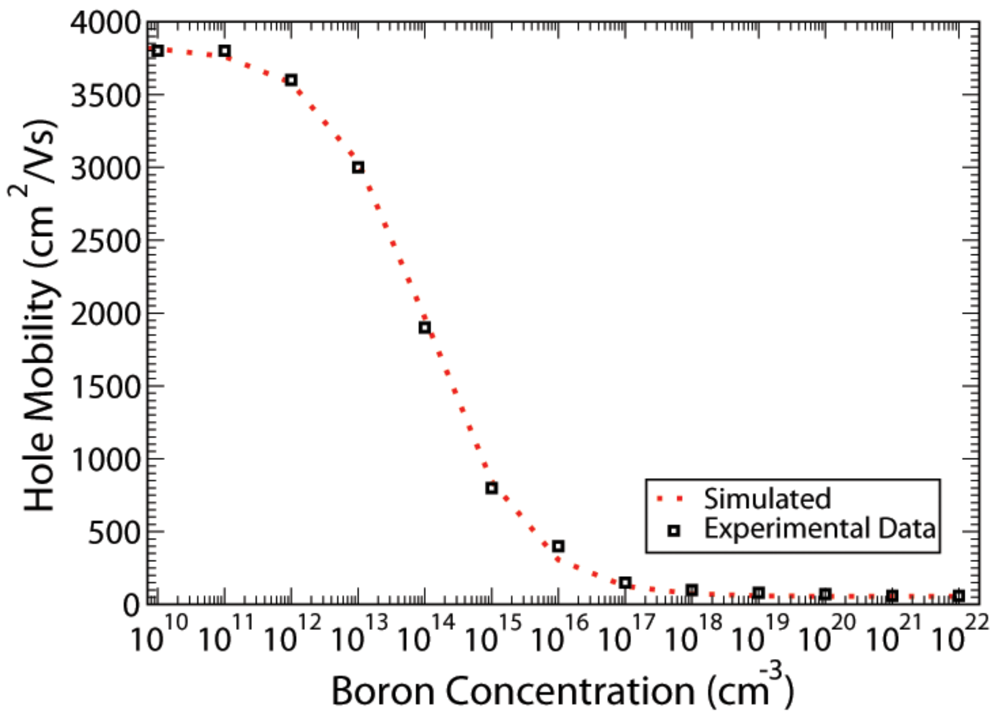
Single-Crystal CVD diamond

Intrinsic Diamond



Ionized acceptor concentration versus dopant concentration in boron doped sCVD diamond at 300K



Hole mobility versus dopant concentration in boron doped sCVD diamond at 300K

[Rashid et al., Numerical Parametrization of Chemical-Vapor-Deposited (CVD) Single-Crystal Diamond for Device Simulation and Analysis, IEEE Trans Electr. Dev., vol 55, October 2008]

Intrinsic Concentration Issue

Diamond has a large Bandgap (5.47 eV) → $n_i = 10^{-27}$ cm^{-3} at 300K

This concentration is too low for the numerical analyses with TCAD

↓

Possible strategies to fit the experimental data:

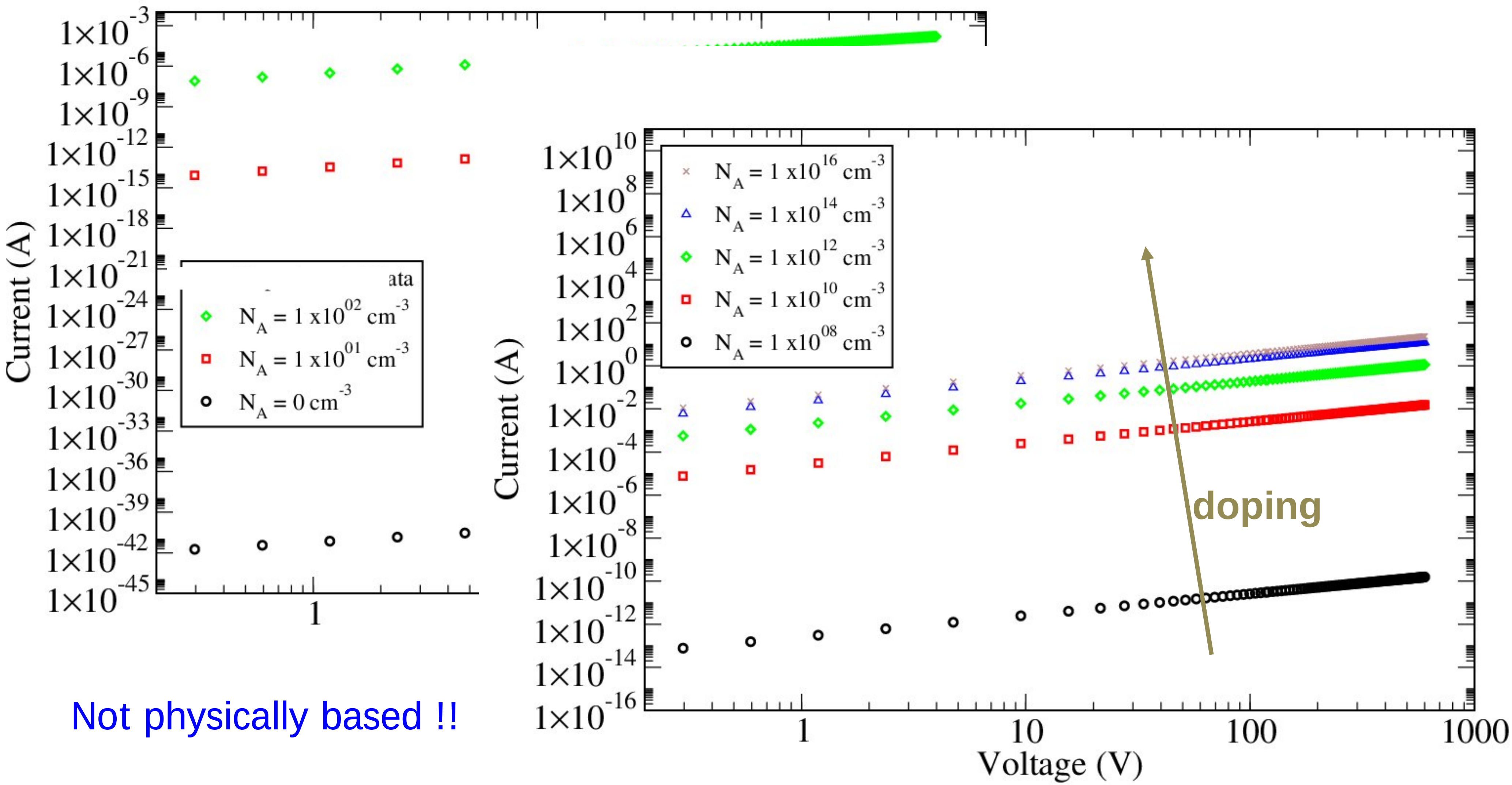
- n_i = ? cm^{-3} [1][2][3]
- Constant Carrier Generation (bulk)
- Trap Levels

[1] Rashid et al., Numerical Parametrization of Chemical-Vapor-Deposited (CVD) Single-Crystal Diamond for Device Simulation and Analysis, IEEE Trans Electr. Dev., vol 55, October 2008

[2] Rahid et al, Modelling of single-crystal diamond Schottky diodes for high-voltage applications, Diamond and Rel. Materials, 15 (2006) 317-323

[3] M. Brezeanu et al., Single crystal diamond M-i-P diodes power electronics, Iet Circuits Devices Syst., 2007, 1, (5), pp. 380-386

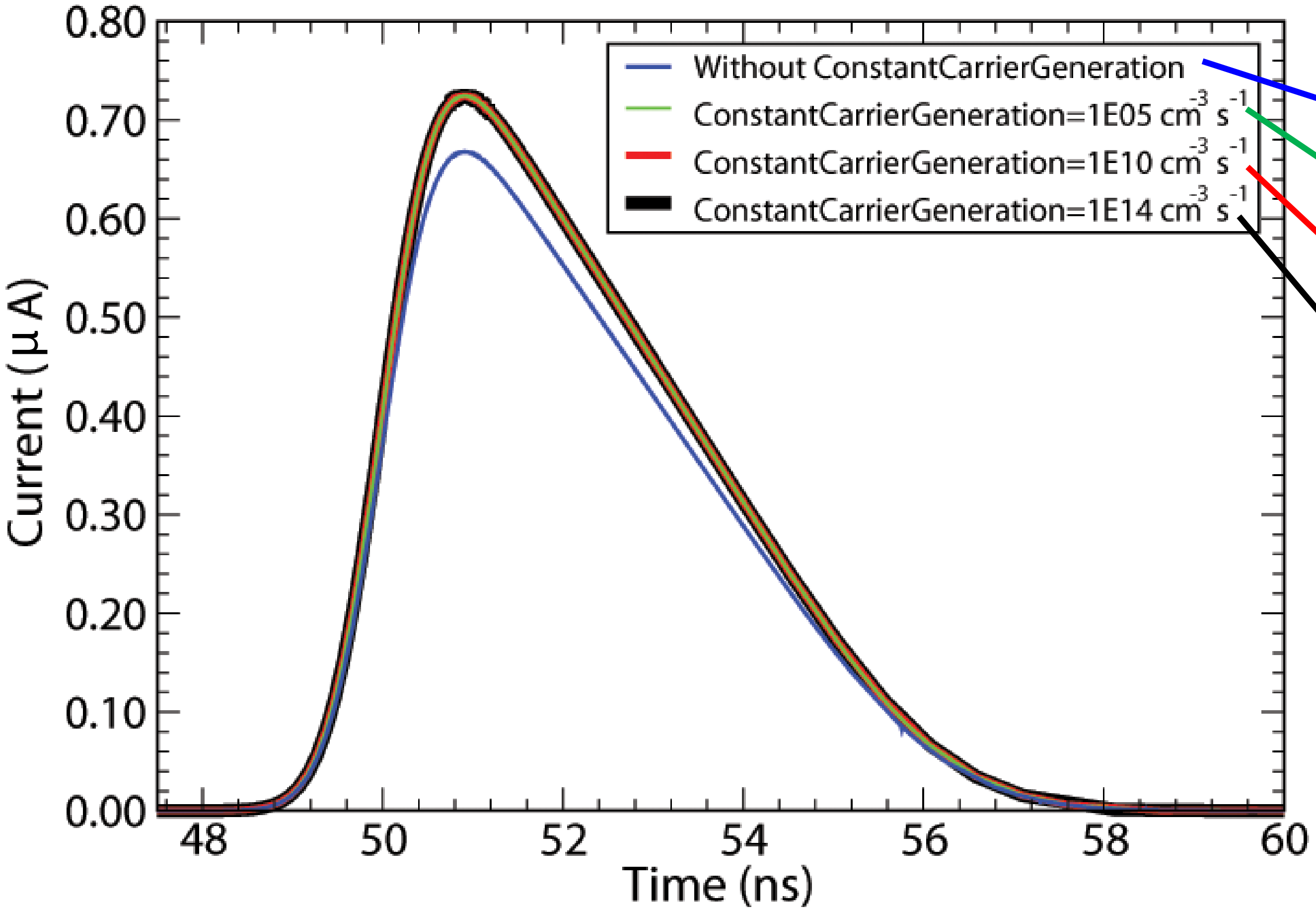
DC Analyses: Effect of Doping



Not physically based !!

The diamond is intrinsic and not doped

DC and TV Analyses: Constant Carrier Generation Effect



More realistic DC currents

$1{,}14\times10^{-44}$ A

$1{,}97\times10^{-16}$ A

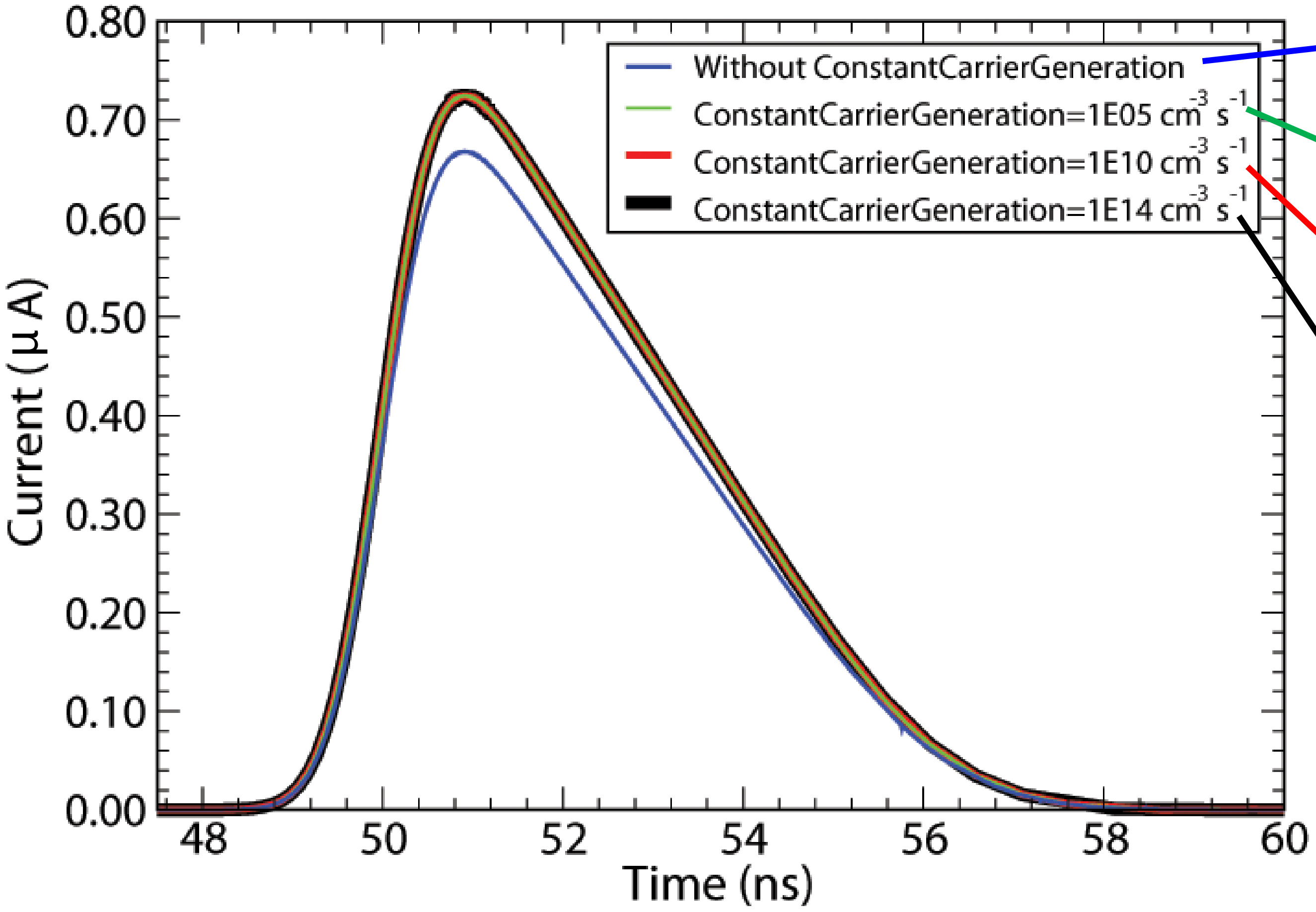
$1{,}99\times10^{-11}$ A

$1{,}99\times10^{-07}$ A

DC and TV Analyses: Constant Carrier Generation Effect

Nominal Generated Charge 2,88 fC

Collected Charge:



2,5689 fC

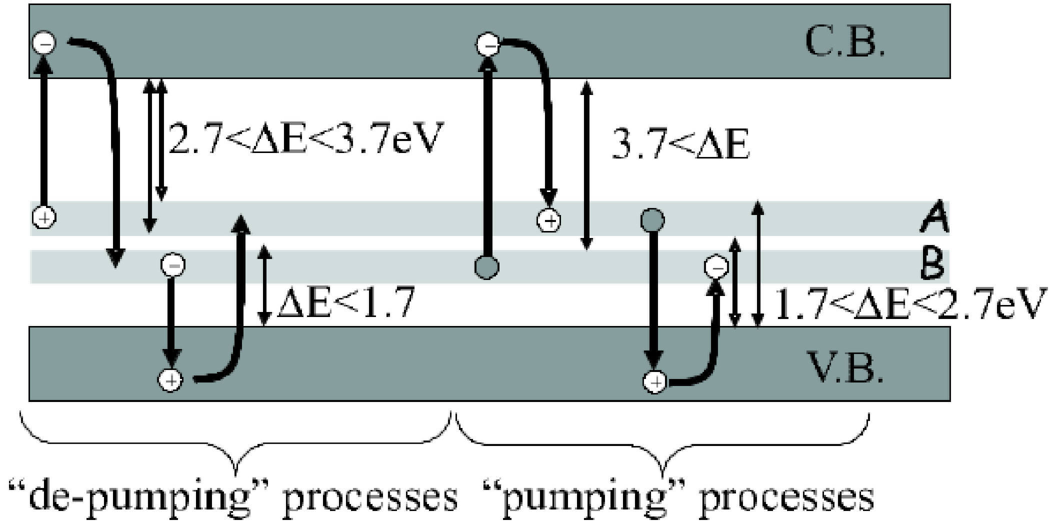
2,7875 fC

2,7877 fC

2,7876 fC

Trapping and Recombination Centers in pCVD

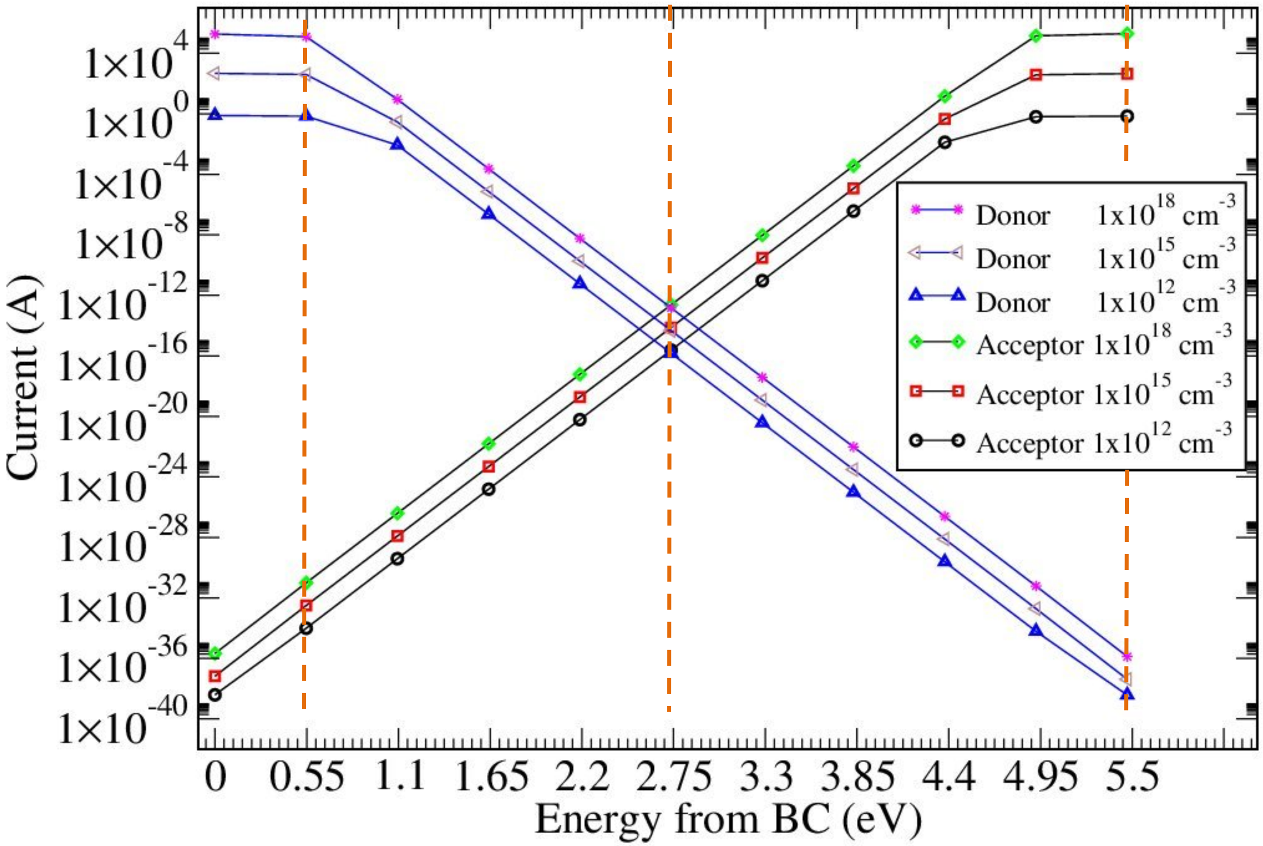
A model of electronic transport in polycrystalline (pCVD) has been included in the simulation, accounting for two distributions of defect levels: a mid-gap group of recombination centers (Band A) and a distribution of traps closer to one of the band edges (Band B).



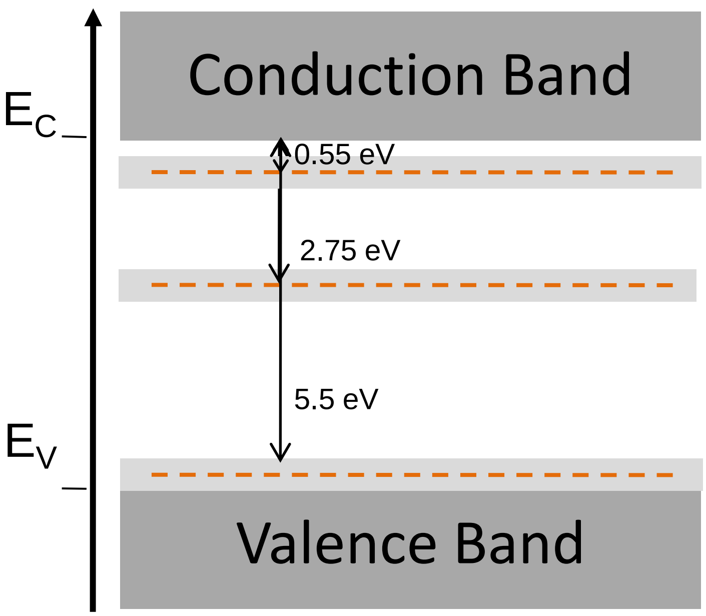
[S. Lagomarsino and S. Sciortino Modeling of the Transport Properties of Diamond Radiation Sensors Carbon - Topics in Applied Physics Volume 100, 2006, pp 303-327]

DC: Single Trap vs Position

Strong effect of the position of Trapping and Recombination Centers within the Bandgap



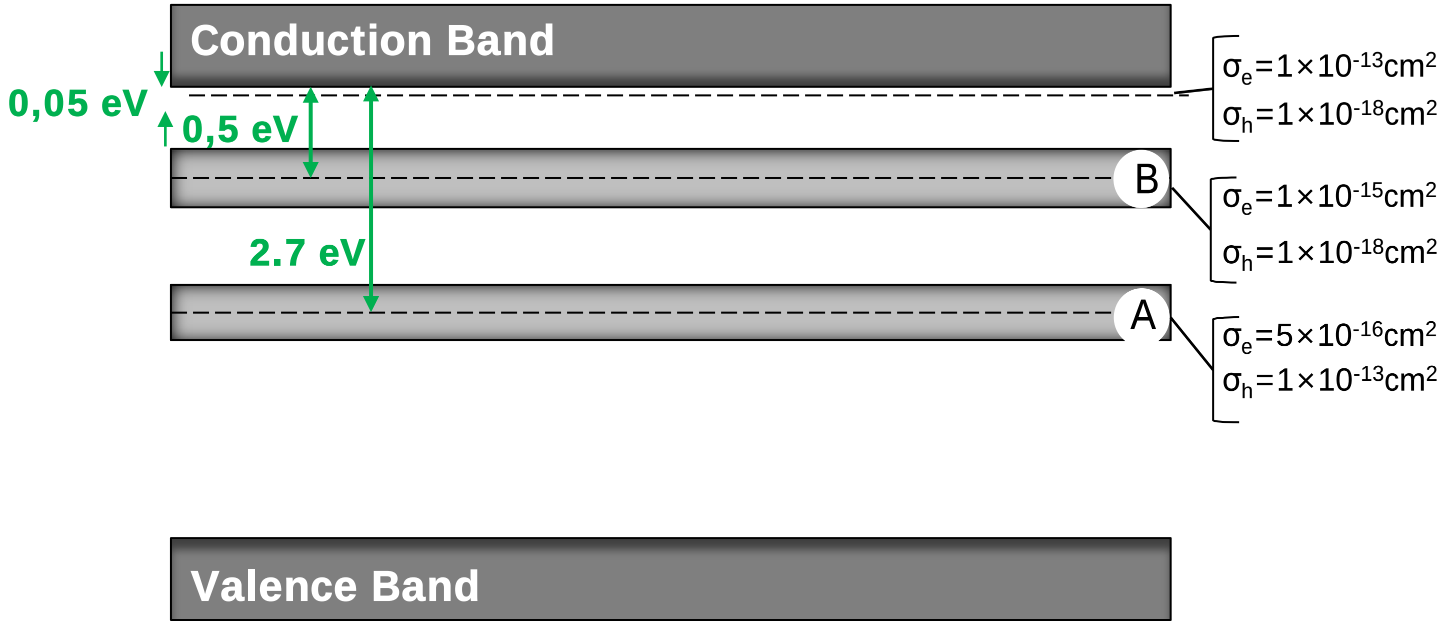
Intrinsic Diamond



V = 600

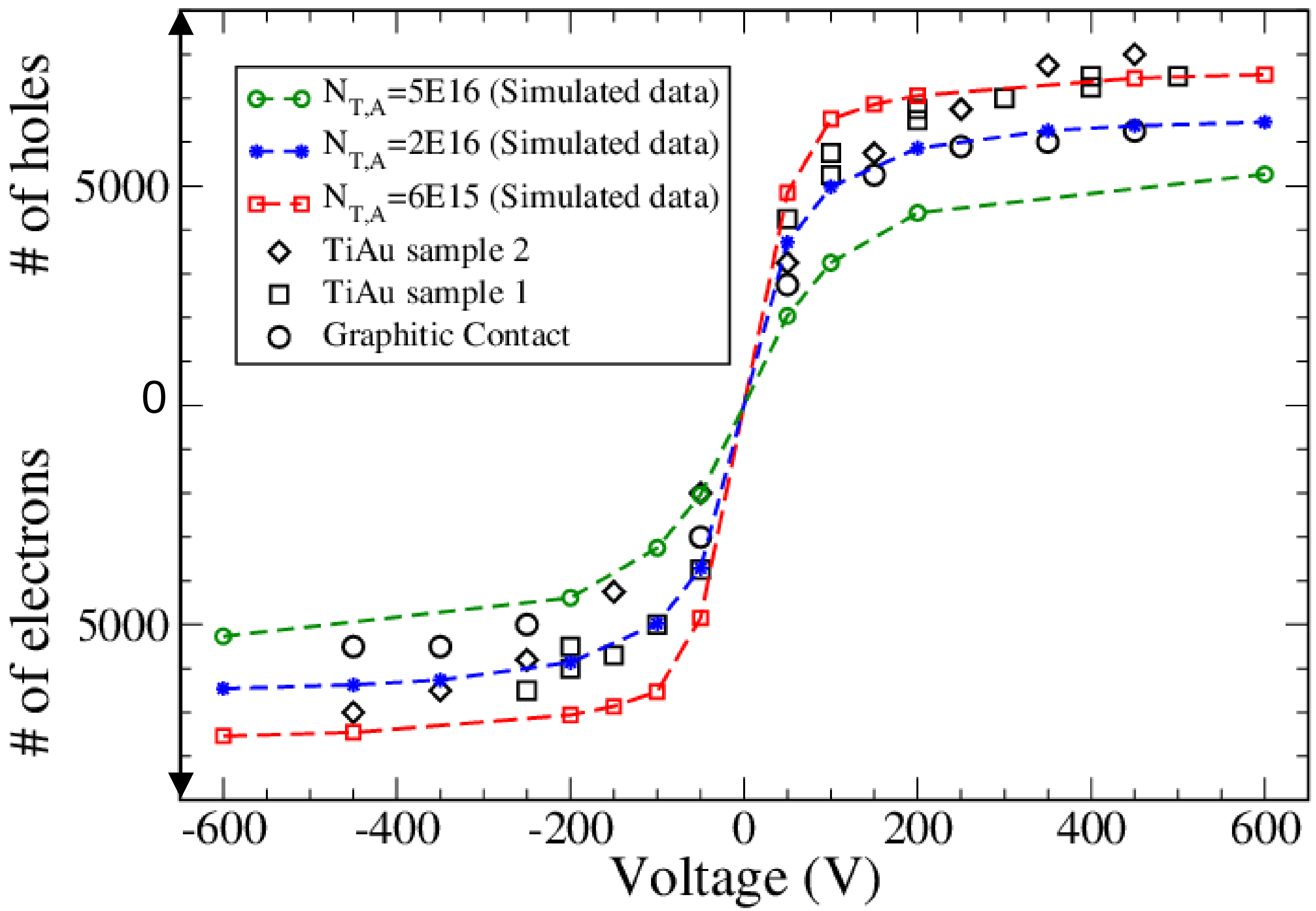
Band Gap Model

A=Acceptor
B=Donor



TV Analyses Results

Charge Collection of the simplified model compared with experimental results of a diamond with planar TiAu contacts



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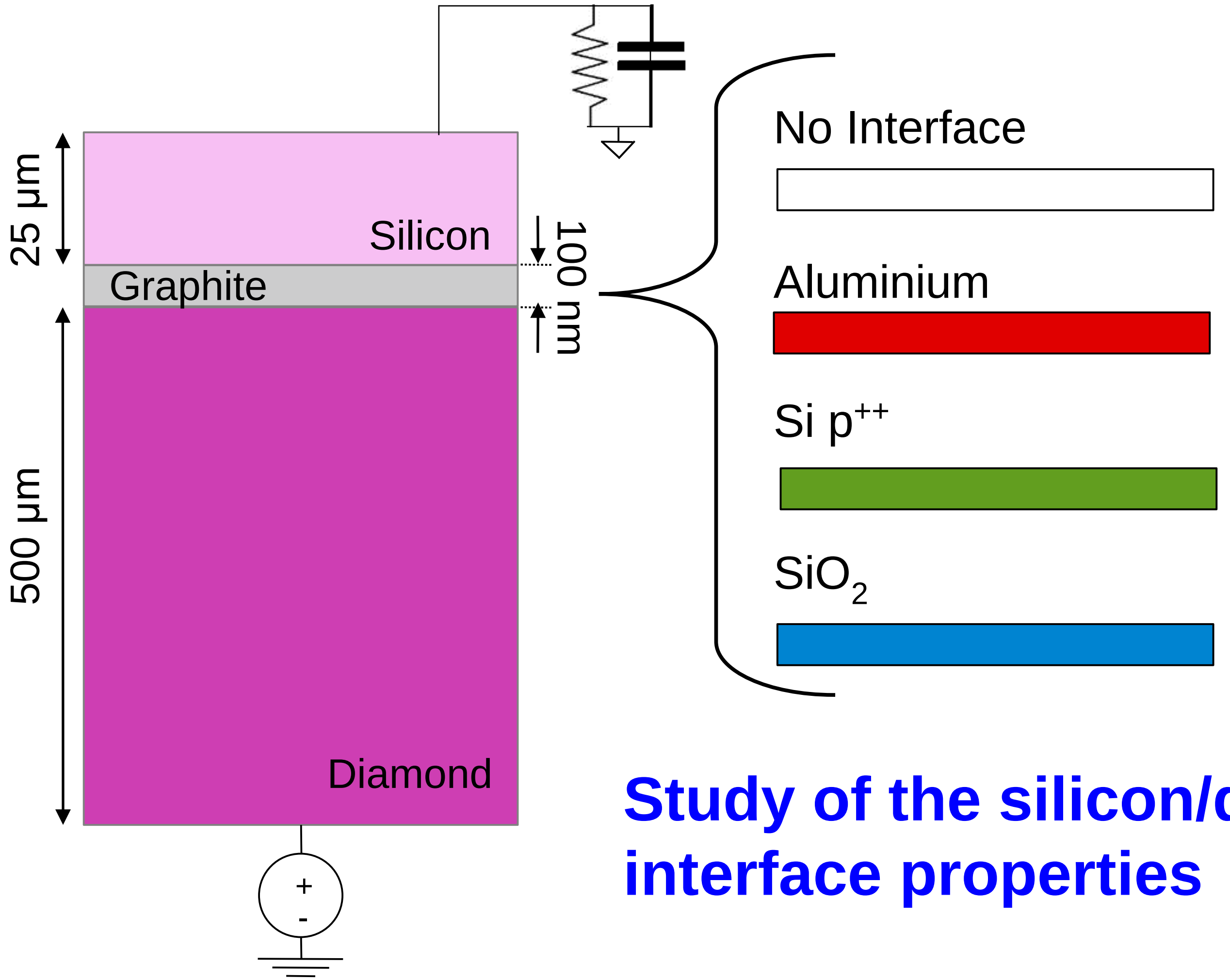
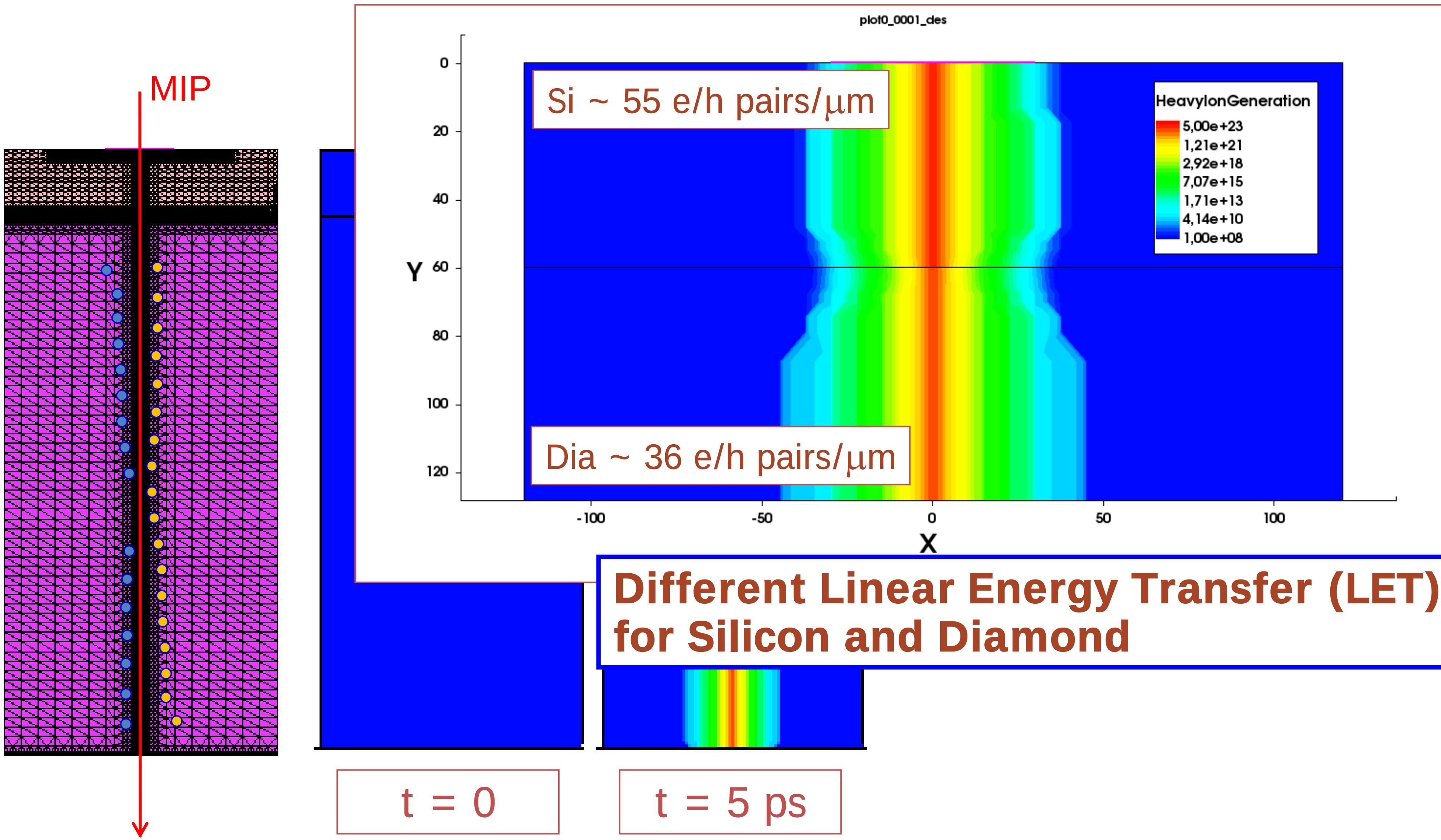
Silicon on Diamond (SoD)

Goal: connect a full CMOS readout chip to a diamond substrate to obtain a device for charged particle detection.



Study of the silicon/diamond interface properties

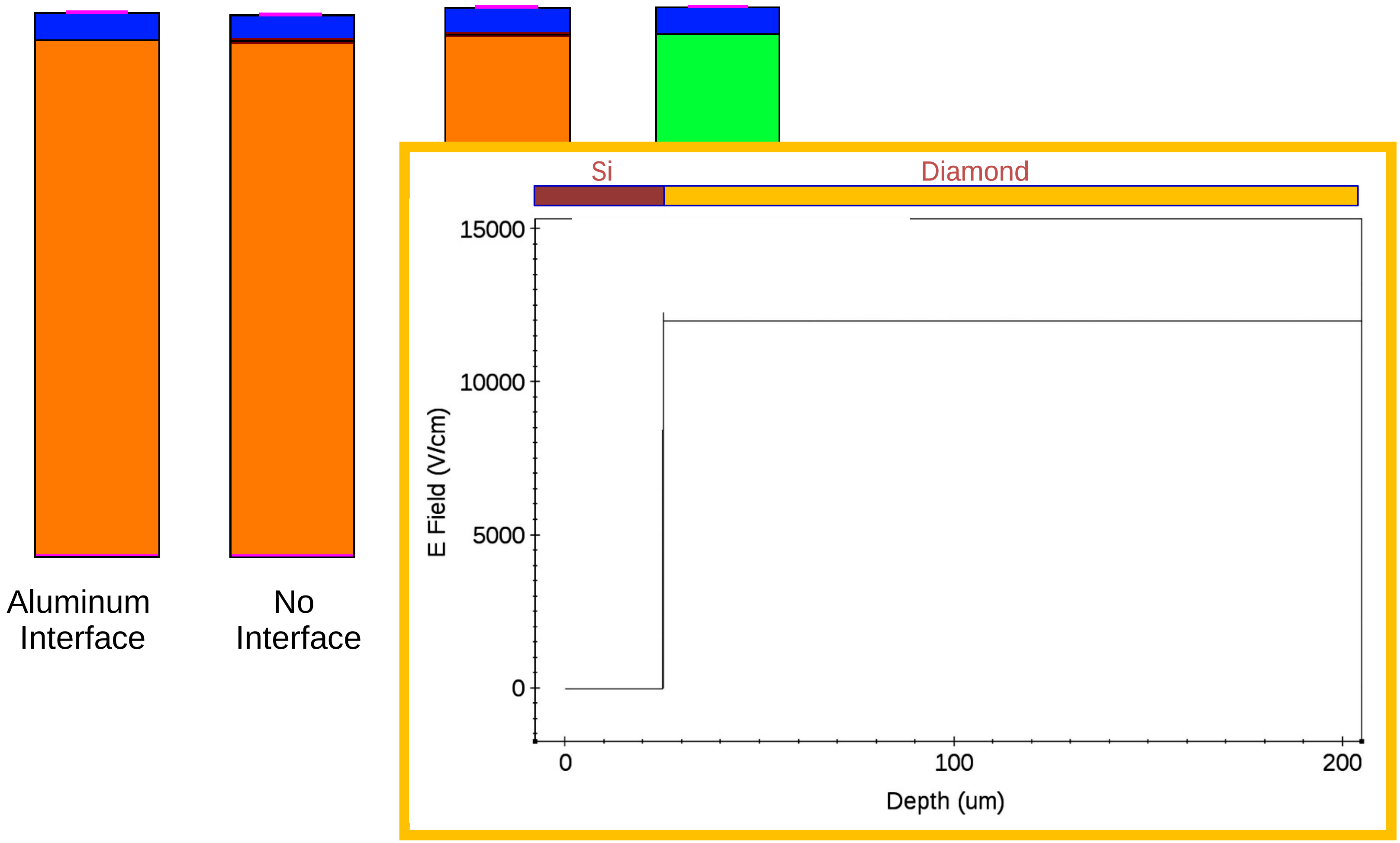
SoD: Heavy Ion Generation



Different Linear Energy Transfer (LET) for Silicon and Diamond

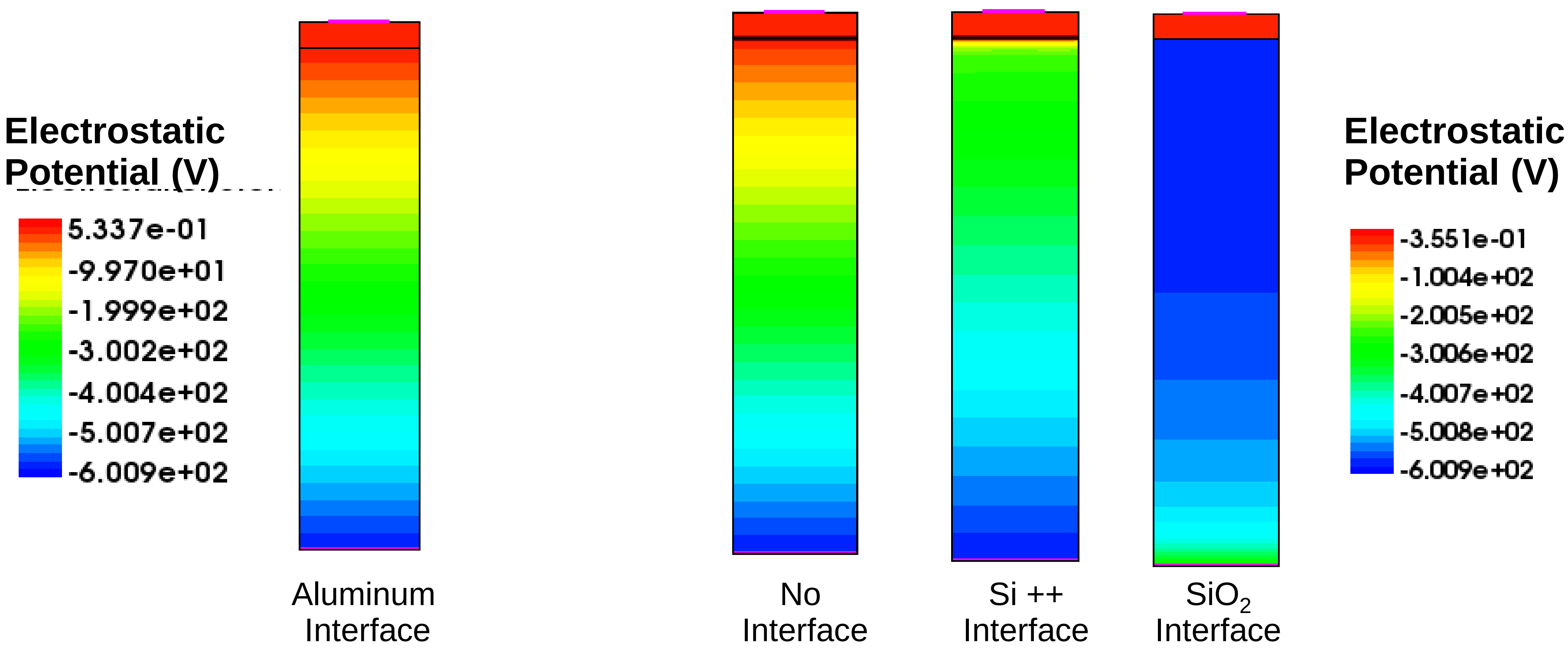
SoD: Effect of the Interface

Electric Field distribution



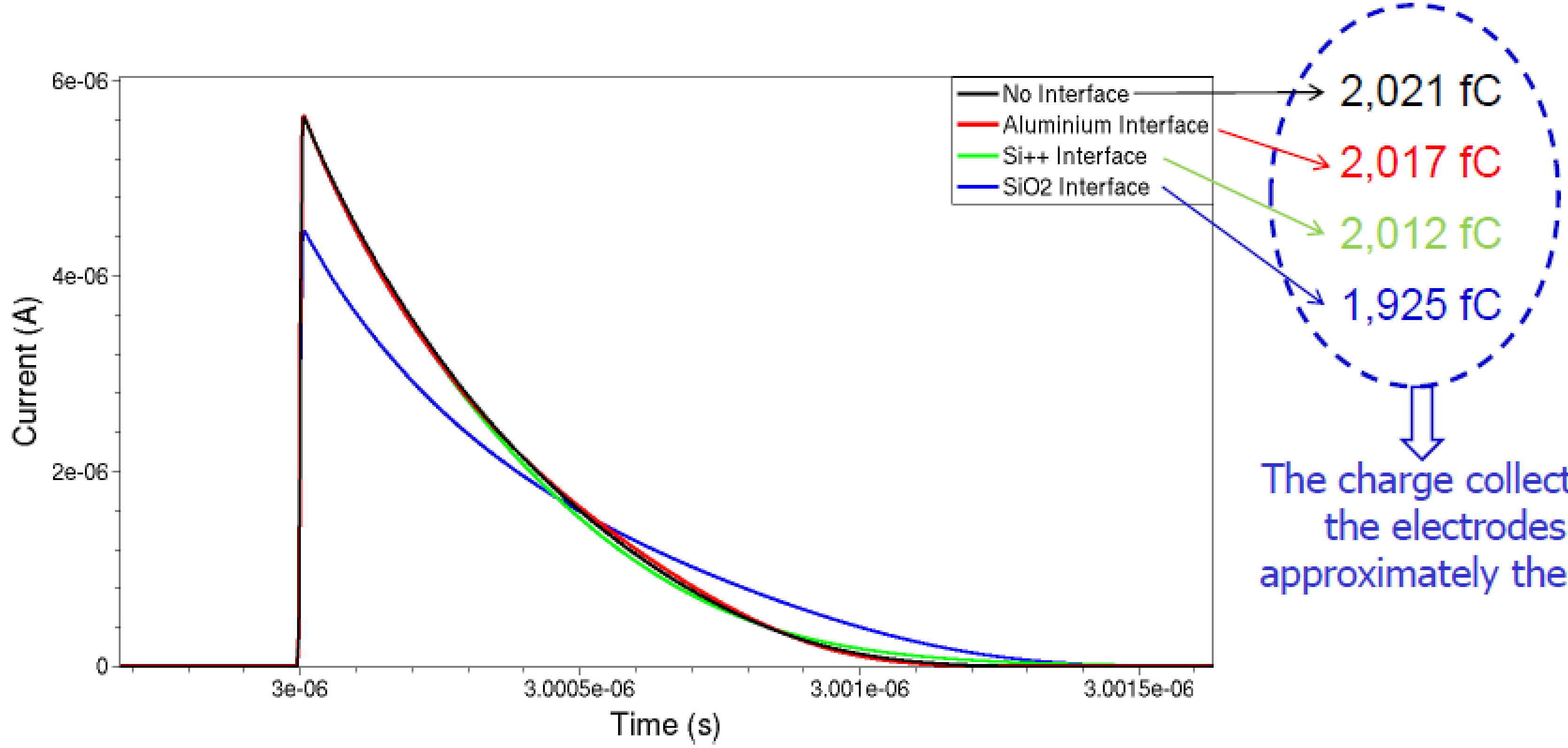
SoD: Effect of the Interface

Electrostatic Potential



SoD: Transient Analyses

Charge Collected through the different interfaces



The charge collected by the electrodes is approximately the same

Conclusions

- ✓ Technology CAD (TCAD) tools customization for the study of diamond and silicon on diamond structures (models and methodologies).
- ✓ Development of an accurate and physically based model of diamond to predict the DC and TV behavior
  - ✓ Intrinsic + ConstantCarrierGeneration for scCVD
  - ✓ Intrinsic + ConstantCarrierGeneration + Traps for pcCVD
- ✓ The proposed TCAD modeling scheme is a suitable way to reproduce the behavior of real devices and can be used as predictive tool for the optimization of:
  - SoD devices
  - 3D detectors
  - …

Thank you for your kind attention!!!

- ✓ The SoD interface has to be deeply studied, in order to comprehend the method to reproduce a realistic interface efficiency.

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