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

<table>
<thead>
<tr>
<th>Property</th>
<th>Silicon</th>
<th>Diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bandgap [eV]</td>
<td>1.12</td>
<td>5.47</td>
</tr>
<tr>
<td>Breakdown Field [MV/cm]</td>
<td>0.4</td>
<td>20</td>
</tr>
<tr>
<td>Intrinsic Resistivity @ R. T. [Ω cm]</td>
<td>2.3x10^5</td>
<td>&gt; 10^{11}</td>
</tr>
<tr>
<td>Intrinsic Carrier Density [cm^{-3}]</td>
<td>1.5x10^{10}</td>
<td>10^{-27}</td>
</tr>
<tr>
<td>Dielectric Constant</td>
<td>11.9</td>
<td>5.7</td>
</tr>
<tr>
<td>Electron Mobility</td>
<td>1350</td>
<td>1900-3800</td>
</tr>
<tr>
<td>Hole Mobility</td>
<td>480</td>
<td>2300-4500</td>
</tr>
<tr>
<td>Saturation Velocity</td>
<td>1x10^7</td>
<td>2.7x10^7</td>
</tr>
<tr>
<td>Displacement Energy [eV/atom]</td>
<td>13-20</td>
<td>43</td>
</tr>
<tr>
<td>Thermal Conductivity [W cm^{-1} K^{-1}]</td>
<td>1.5</td>
<td>20</td>
</tr>
<tr>
<td>Energy to create e-h pair [eV]</td>
<td>3.62</td>
<td>11.6 - 16</td>
</tr>
<tr>
<td>Radiation Length [cm]</td>
<td>9.36</td>
<td>12.2</td>
</tr>
<tr>
<td>Energy Loss for MIPs [MeV/cm]</td>
<td>3.21</td>
<td>4.69</td>
</tr>
<tr>
<td>Aver. Signal Created / 100 μm</td>
<td>8892</td>
<td>3602</td>
</tr>
</tbody>
</table>

- high field operation
- low leakage current
- fast signal
- radiation hardness
- heat dissipation

Also problems......
→ small dimensions; high cost;
low signal
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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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)

\[
\nabla \cdot \left( -\varepsilon_s \nabla \varphi \right) = q \left( N_D^+ - N_A^- + p - n \right)
\]

\[
\frac{\partial n}{\partial t} - \frac{1}{q} \nabla \cdot \vec{J}_n = G - R
\]

\[
\frac{\partial p}{\partial t} + \frac{1}{q} \nabla \cdot \vec{J}_p = G - R
\]

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

\[
\vec{J}_p = -q\mu_p p \nabla \varphi - qD_p \nabla p
\]
Physical Characterization of Diamond

Material = "Diamond"

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

* Bandgap
  \[ \chi_0 = 1.3 \] # [eV]
  \[ E_g = 5.47 \] # [eV]

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

* Incomplete Ionization
  \[ N_d = 1.0 \times 10^{20} \] # [cm\(^{-3}\)]
  \[ N_a = 3.1 \times 10^{19} \] # [cm\(^{-3}\)]

\[ \mu_{\text{const}} = \mu_{\text{max}} \left( \frac{T}{T_0} \right)^\text{Exponent} \]
  \[ \mu_{\text{max}} = 4.5 \times 10^3, 3.8 \times 10^3 \] # [cm\(^2\)/(Vs)]
  \[ \text{Exponent} = 1.55, 1.55 \] # [1]

* \[ N_v(T) = N_{v300} \times \left( \frac{T}{300} \right)^{3/2} \]
  \[ N_{v300} = 1.8000 \times 10^{19} \] # [cm\(^{-3}\)]

* \[ N_c(T) = N_{c300} \times \left( \frac{T}{300} \right)^{3/2} \]
  \[ N_{c300} = 5.0000 \times 10^{18} \] # [cm\(^{-3}\)]
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Setting the simulation domain: 2D vs 3D approach

The 2D section of the actual device has been considered for simulation purposes. → save up simulation time

Actual device

Simulated Structure

Area Factor

Contacts

Top view

5 mm

500 µm

5 mm

5 mm

500 µm

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

Numerical Model of MIP in the TCAD environment:

Physics {

...  
AreaFactor=AF
HeavyIon(

...  
\[ Let_f = \frac{57.67 \text{ pC/\mu m}}{AF \text{ \mu m}} \]

...  

MIP

Area Factor

MIP

\[ t = 0 \text{ ps} \]  \[ t = 5 \text{ ps} \]  \[ t = 10 \text{ ps} \]  \[ t = 20 \text{ ps} \]
Setting the simulation domain: 2D vs 3D approach (1)

Numerical Model of MIP in the TCAD environment:

Physics {
  ...
  AreaFactor=AF
  HeavyIon(
    ...
    Let \( f = \frac{57.67\, pC/\mu m}{AF \cdot \mu m} \)
  }

→ save-up simulation time and computing resources

\[ t = 0 \, ps \quad t = 5 \, ps \quad t = 10 \, ps \quad t = 20 \, ps \]
Charge Generation Shape

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

Gaussian

Gaussian, effect of the standard deviation

Beta particle

Alpha Particle

\[ \text{Current (\mu A)} \]

\[ \text{Time (ns)} \]
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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

Intrinsic Concentration Issue

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

This concentration is too low for the numerical analyses with TCAD

Possible strategies to fit the experimental data:
- \( n_i = \text{? cm}^{-3} \) [1][2][3]
- Constant Carrier Generation (bulk)
- Trap Levels

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 × 10^{-44} A
1.97 × 10^{-16} A
1.99 × 10^{-11} A
1.99 × 10^{-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).

[Image of a diagram showing energy levels and transitions between them.]

“de-pumping” processes “pumping” processes

DC: Single Trap vs Position

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

Intrinsic Diamond

Conduction Band

Valence Band

$E_C$ 

$E_V$

$V = 600$

$V = 600$

$0.55 \text{ eV}$

$2.75 \text{ eV}$

$5.5 \text{ eV}$

$10^18 \text{ cm}^{-3}$

$10^{12} \text{ cm}^{-3}$

$10^{15} \text{ cm}^{-3}$

Current (A)

Energy from BC (eV)
Band Gap Model

A=Acceptor
B=Donor

Conduction Band

Valence Band

$\sigma_e=1\times10^{-13}\text{cm}^2$
$\sigma_h=1\times10^{-18}\text{cm}^2$

$\sigma_e=5\times10^{-16}\text{cm}^2$
$\sigma_h=1\times10^{-13}\text{cm}^2$
TV Analyses Results

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

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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

Si ~ 55 e/h pairs/µm
Dia ~ 36 e/h pairs/µm

MIP

t = 0

t = 5 ps
SoD: Effect of the Interface

Electric Field distribution

Aluminum Interface

No Interface

Si

Diamond

E Field (V/cm)

Depth (um)
SoD: Effect of the Interface

Electrostatic Potential

- Aluminum Interface
- No Interface
- Si ++ Interface
- SiO$_2$ Interface
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
  ▪ ...

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

Thank you for your kind attention!!!