From the *pn* junction to the UFSD design

The role of numerical simulation

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Marco Mandurrino, INFN Torino

- I. Overview of semiconductor devices
	- The *pn* junction
	- Low Gain Avalanche Detectors (LGAD)
- II. Electronic device modeling
	- Analytical description
	- Numerical implementation
- III.LGAD design using numerical simulations

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- § **Definition:** the *pn* junction is a semiconductor region where a *p*-type and an *n*-type doped materials are placed side by side.
- § **Example:** the *abrupt junction* of two *uniformly doped* semiconductors.

 $q\chi$ is the electronic affinity (~4.05 eV in Si) *q*Φ is the semiconductor work function

$$
q\Phi_{\mathbf{S}p} = q\chi_{\mathbf{S}} + E_{\mathbf{g}} - (E_{\mathbf{F}} - E_{\mathbf{v}}) = q\chi_{\mathbf{S}} + E_{\mathbf{g}} - k_{\mathbf{B}}T\ln\frac{N_{\mathbf{v}}}{N_{\mathbf{A}}}
$$

$$
q\Phi_{\mathbf{S}n} = q\chi_{\mathbf{S}} + (E_{\mathbf{C}} - E_{\mathbf{F}}) = q\chi_{\mathbf{S}} + k_{\mathbf{B}}T\ln\frac{N_{\mathbf{C}}}{N_{\mathbf{D}}}
$$

§ **Golden-rules to compute the final band-diagram:**

- 1. $E_{\rm g}$ and $q\chi$ are **conserved** by definition;
- 2. E_F must be **constant** across the junction;

3. E_0 and bands must be **continuous** functions (in space *x*).

- § The gradient of carriers concentration produces a **transient**, in which **electrons travel from the** *n***-side to the** *p***-side** (the vice-versa holds for holes). This mechanism behaves as a **diffusion-like dynamics**
- § The diffusion of free charges **depletes a zone** across the junction, called **spacecharge region** (**SCR**), where **fixed charges** (ionized atoms) **are no more compensated by free charges** ($\rho \neq 0$). Far from the junction, we still have compensation (**neutral regions**, $\rho=0$)

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• Within the space-charge region ($\rho \neq 0$) the field is not a constant and **bands are no more straight lines**. In particular, due to the **Poisson equation** of semiconductors

$$
\frac{\mathrm{d}^2 U}{\mathrm{d}x^2} = q\frac{\rho}{\epsilon}
$$

where $U = -q\varphi$ is the *potential energy* felt by free charges, we have

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■ So, finally we have:

What we concluded has several important physical implications:

- 1. $\mathcal{E} \neq 0$ implies the onset of a **drift current** of carriers tending to **compensate the diffusion** of free charges such that $J = 0$;
- 2. A **built-in potential** qV_{bi} , created across the junction, represents an additional **barrier for the diffusion** of electrons towards the *p*-side (and holes in the *n*-side)

$$
qV_{bi} = q\Phi_{Sp} - q\Phi_{Sn} = E_{g} - k_{B}T \ln \frac{N_{v}N_{c}}{N_{A}N_{D}}
$$

= $k_{B}T \ln \frac{N_{v}N_{c}}{n_{i}^{2}} - k_{B}T \ln \frac{N_{v}N_{c}}{N_{A}N_{D}}$
= $k_{B}T \ln \frac{N_{A}N_{D}}{n_{i}^{2}}$

What we concluded has several important physical implications:

3. By integrating the Poisson equation, and thanks to the *neutrality law* $N_A x_p = N_D x_n$, one has

$$
\mathcal{E}(x) = \begin{cases}\n-\frac{qN_A}{\epsilon}(x + x_p) & -x_p \le x < 0 \\
\frac{qN_D}{\epsilon}(x - x_n) & 0 \le x < x_n\n\end{cases}
$$

and

$$
\mathcal{E}_{\max} = \frac{qN_A}{\epsilon} x_p = \frac{qN_D}{\epsilon} x_n
$$

4. In the same way:

$$
\varphi(x) = \begin{cases} \frac{qN_A}{2\epsilon}(x + x_p)^2 & -x_p \le x < 0\\ \frac{qN_D}{2\epsilon}(x - x_n)^2 + \frac{qN_A}{2\epsilon}x_p^2 + \frac{qN_D}{2\epsilon}x_n^2 & 0 \le x < x_n \end{cases}
$$

➤ What happens if the junction is no more at equilibrium?

Direct polarization

- $V > 0, I > 0$
- \blacksquare *J*_{diff} dominates
- electrons from n to p -side
- § holes from *p* to *n*-side
- $qV < qV_{\text{bi}}$

Reverse polarization

- $V < 0, I < 0$
- \blacksquare *J*_{drift} dominates
- electrons from *p* to *n*-side
- \blacksquare holes from *n* to *p*-side
- $qV > qV_{\rm bi}$

➤ What happens if the junction is no more at equilibrium?

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■ *pn* junction at **equilibrium**:

$$
V_{\rm bi}=V_T\log\frac{N_{\rm A}N_{\rm D}}{n_{\rm i}^2}
$$

$$
p_{p0}(-x_p) = N_A
$$
 $p_{n0}(x_n) = n_i^2/N_D$
\n $n_{n0}(x_n) = N_D$ $n_{p0}(-x_p) = n_i^2/N_A$

■ *pn* junction in **reverse polarization**:

$$
n'_p = n_p - n_{p0} \t p'_n = p_n - p_{n0} < 0
$$

- § *V*bias < 0, *I* < 0
- **J**_{drift} dominates
- § electrons from *p* to *n*-side
- holes from *n* to *p*-side
- $qV_{bias} > qV_{bi}$

■ *pn* junction in **forward polarization**:

$$
n'_p = n_p - n_{p0} \t p'_n = p_n - p_{n0} > 0
$$

- $V_{bias} > 0, l > 0$
- **J**_{diff} dominates
- electrons from *n* to *p*-side
- holes from *p* to *n*-side
- \bullet *qV*_{bias} < *qV*_{bi}

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Towards a technological step…

first *n*-*p*-*n* "tip"-transistor

Ultra Fast Silicon Detector

J. Bardeen, W. Brattain, W. Shockley Bell Labs. - NJ (1948)

UFSD Group INFN Torino and FBK Trento (2018)

Extending our application domain to other systems

§ How large the **external biasing voltage** has to be?

➤ What is charge multiplication in LGAD?

- § **Primary charges** (electron/hole pairs) are produced **by ionization**, while the particle is crossing the sensor;
- § Due to the **reverse field**, electrons **drift** towards the *n*-side and holes towards the *p*-side;
- When electrons travel along the p ⁺ **region** (the *gain* or *multiplication*-layer) they experience an **high field**;
- § This field is responsible for the **impact ionization**, which produces an avalanche **multiplication of secondary charges**;
- § Now the **total current** is due to the **additional avalanche contribution**.

➤ Why using LGAD to detect particles at CERN?

I. We need **charge multiplication**:

- 1. LGAD exploit the so-called **avalanche multiplication**, a process which belongs to the class of **generation/recombination (GR) mechanisms**;
- 2. Charge multiplication allows to obtain **large and fast signals**:
	- the **thinner** the sensor, the **faster** the signal;
	- the **higher** the **gain**, the **larger** the signal.

II. We need a good **S/N**:

- 1. Also the **noise** related to the current signal is **proportional to the gain**
- 2. The gain *G* has to be kept as low as required by electronics $(G \sim 10{\text -}20)$

➤ Why using LGAD to detect particles at CERN?

Examples of 50 μ m LGAD performance:

➤ Can we predict the avalanche contribution to the total current?

Let's introduce a bit of physical-mathematics...

- 1. The **avalanche** process is modeled via its **ionization coefficient** α , i.e. the **inverse of the electron/hole mean free path** (cm–1);
- 2. In the literature, several **expressions of** *α* are available. In general, all of them are based on the **Chynoweth's theory** (1958), according to which:

$$
\alpha_{n,p}(\mathcal{E})=\gamma\,A_{n,p}\,\exp\left(-\gamma\frac{B_{n,p}}{\mathcal{E}}\right)
$$

3. Once the coefficient has been obtained, one has to evaluate the **net avalanche generation rate** U_{aval} **, i.e. the number of multiplied** e^{-}/h^{+} **pairs per volume** (cm^{-3}) **per unit time** (s^{-1}) , as:

$$
U_{\text{aval}} = \frac{dn}{dt} = \frac{dp}{dt} = \alpha_n n v_n + \alpha_p p v_p
$$

… Now we need a complete description of the system!

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- We recall the **twofold nature of the current** in a semiconductor device:
	- *a.* **Drift current**, driven by the *electric field*;
	- *b.* **Diffusion current**, due to the density gradient of *free charges*.

§ Then we introduce (all) the **GR mechanisms** through their **net rates** *U*:

$$
U_n = R_n - G_n
$$

\n
$$
\approx \frac{n - n_0}{\tau_n} = \frac{n'}{\tau_n}
$$

\n
$$
U_p = R_p - G_p
$$

\n
$$
\approx \frac{p - p_0}{\tau_p} = \frac{p'}{\tau_p}
$$

- § To derive the **global current density** (field + charge + GR):
	- 1. in a volume $dV = Adx$ the **time variation of the electron density** (similarly for holes) is

field + charge GR
\n
$$
\frac{\partial n}{\partial t} A dx = \frac{J_n(x)}{-q} A - \frac{J_n(x + dx)}{-q} A + G_n A dx - R_n A dx
$$

2. by using the 1st-order Taylor series expansion

$$
J_n(x + dx) \approx J_n(x) + \frac{\partial J_n}{\partial x} dx
$$

and assuming $dx \rightarrow 0$, we obtain the **continuity equations**:

$$
\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} - U_n \qquad \frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} - U_p
$$

§ Since the drift component depends on the **electric field**, we need a third equation to close the system, the **Poisson equation**, which connects the *field* to the *charge densities*.

The final (1D) mathematical framework is:

continuity eqs.
$$
\begin{cases}\n\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} - U_n \\
\frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} - U_p\n\end{cases}
$$
\n**DRIFT-DIFFUSION**\n\n
$$
\frac{\partial \mathcal{E}}{\partial t} = \frac{\rho}{\epsilon}
$$
\nwhere $J_n = q\mu_n n \mathcal{E} + qD_n \frac{\partial n}{\partial x}$, $J_p = q\mu_p p \mathcal{E} - qD_p \frac{\partial p}{\partial x}$ \n**TRANSPORT EQS.**\n\nand $\mathcal{E} = -\frac{\partial \varphi}{\partial x}$, $\rho = q(p - n + N_D^+ - N_A^-)$.

- § Avalanche generation is not the only **GR mechanism** occurring in silicon devices. In general, we have to account for **two different families**:
	- A. **Band-to-band** generation/recombination
		- o *Auger* o *direct tunneling*

- B. **Defect-assisted** generation/recombination
	- o *Shockley-Read-Hall* (*SRH*)
	- o *trap-assisted tunneling*
	-

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		- o *…*

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	-

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		-
		-

- B. **Defect-assisted** generation/recombination
	- o *Shockley-Read-Hall* (*SRH*)
	- o *trap-assisted tunneling*
	- o *…*

■ **SRH** processes are determined by such a net rate statistics

$$
U_{\text{SRH}} = \frac{np - n_i^2}{\tau_p \left(n + n_i e^{\frac{E_{\text{trap}} - E_{\text{F}_i}}{k_{\text{B}}T}}\right) + \tau_n \left(p + n_i e^{\frac{E_{\text{F}_i} - E_{\text{trap}}}{k_{\text{B}}T}}\right)}
$$

where $\tau_{n,p}$ are proper **electron/hole lifetimes**, i.e. the average time interval $(-10^{-7}-10^{-9})$ s) between two consecutive scattering processes originating (or annihilating) e^{-}/h^{+} pairs.

§ Moreover, **band-to-band tunneling** is modeled with the usual Kane expression (1961)

 $U_{\text{tunn}} = A \mathcal{E}^2 \cdot \exp(-B/\mathcal{E})$

with *A* and *B* (V/cm) material-dependent parameters.

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➤ We need a method to compute the DD model

$$
\begin{cases}\n\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} - U_n \\
\frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} - U_p \\
\frac{\partial \mathcal{E}}{\partial x} = \frac{\rho}{\epsilon}\n\end{cases}
$$

where φ **is the input function,** *n***,** *p* **and** ϵ **are the unknowns of the continuity equations and where the Poisson equation closes the system.**

➤ We have to solve a set of *non-linear***,** *secondary-order* **PDEs, in** *space* **and** *time***, for the whole device!**

§ **The strategy**

- Dynamics (bias ramps, transients, …) is treated as a sequence of *small* increments between stationary states at equilibrium: the **quasi-stationary process**;
- At each quasi-stationary step the mathematics has to be simplified through proper approximations and algorithms:

- 1. the **geometry** is **discretized** (e.g.: Delaunay-Voronoï procedure)
- 2. DD system is rewritten and adapted to the mesh grid
- 3. PDEs are linearized and transformed into **ODEs** (**FD schemes**)
- 4. **I.C.** and **B.C.** are defined
- 5. the *new* DD model is solved via **iterative methods** (Newton) in all mesh nodes

1. The **geometry** is **discretized** (e.g.: **Delaunay-Voronoï procedure**)

2. **Drift-Diffusion system** is rewritten and **adapted** to the **mesh grid**

scalar/vector operators and **constants** are transformed: $\frac{\partial}{\partial t}\int\limits_{S}x\,\mathrm{d}s\Rightarrow\frac{\partial x_{i}}{\partial t}\,S_{i}% \,\mathrm{d}s,\quad\mathrm{d}t\int\limits_{S}y_{i}^{2}x_{j}\,\mathrm{d}s\label{eq:2.14}%$ $\oint_{\Gamma} \mathbf{F}_{\perp} d\gamma \Rightarrow \sum_{j} l_{ij} \langle \mathbf{F}_{\perp} \rangle_{ij}$ $\int c ds \Rightarrow c_i S_i$

by **averaging** the **in/out quantities** at each box side, they are computed at **nodes**

3. PDEs are linearized and transformed into **ODEs** (**FD schemes**)

4. **I.C.** and **B.C.** are defined

Boundary Conditions: Initial Conditions: starting polarization at contacts

$$
\frac{\partial n(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} = 0, \quad \frac{\partial p(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} = 0 \quad \text{and} \quad \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} = 0 \quad \text{Neumann homogeneous (insulators, external edges,...)}\n\begin{cases}\nn(\mathbf{r},t) \mu_n \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} = D_n \frac{\partial n(\mathbf{r},t)}{\partial \hat{\mathbf{n}}}\\
p(\mathbf{r},t) \mu_p \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} = -D_p \frac{\partial p(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} \\
\epsilon_s \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} \Big|_{\mathbf{s}} = \epsilon_{\text{diel}} \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} \Big|_{\text{diel}}\n\end{cases} \quad \text{Neumann non-homogeneous (dielectrics)}
$$
\n
$$
\begin{cases}\nn(\mathbf{r},t) = \frac{1}{2} \left(\sqrt{\sum_k C_k^{\pm 2}(\mathbf{r},t) + 4n_i^2} + \sum_k C_k^{\pm}(\mathbf{r},t) \right) \\
p(\mathbf{r},t) = \frac{1}{2} \left(\sqrt{\sum_k C_k^{\pm 2}(\mathbf{r},t) + 4n_i^2} - \sum_k C_k^{\pm}(\mathbf{r},t) \right) \\
\phi(t) = V_{\text{bias}}(t) + \text{const.}\n\end{cases} \quad \text{Dirichlet non-homogeneous (constants)}
$$

- TCAD procedure for each node:
	- a) Choose a **maximum number of iterations** $\#_{\text{max}}$ and a **tolerance** ε
	- b) Impose proper **I.C.** and **B.C.**
	- c) Start from an *initial guess* φ'_0 for the **electrostatic potential**
	- d) The equilibrium solution φ_0 is obtained by solving only the Poisson equation with the **I.C.** and **B.C.**
- § If we have to perform a **voltage ramp** or a **transient**:
	- d) each step *i* of the ramp (with *i* **=1,…,N**) is treated as a **quasi-stationary state**. The potential resulting from the Poisson solution at equilibrium φ_0 is used as initial guess for solving the **DD** equations at steps $i \ge 1$
- **F** If the **solution** is found **within the maximum number of iterations** $\#_{\text{max}}$ and with an **error smaller than the tolerance** ε , then **the system converges** and the scheme go further, otherwise:
	- § The **pitch** of the steps **Δ***i* is **decreased**
	- \blacksquare The **tolerance** ε is **increased**
	- § If the alternatives above fails, then the method is **aborted**

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➤ Why LGAD are so innovative?

- **Example 1** Large signals coupled with low Gain \Rightarrow high S/N
- **•** Fast signals \implies high time resolution
- \blacksquare Simple design \Rightarrow **low production cost**
- Huge ongoing R&D \Rightarrow radiation hardness

➤ How a real LGAD module is made?

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- 2. Analysis about the internal **electric fields**: efficiency issues, …
- 3. **Radiation tolerance**

1. Study of detector static/dynamic characteristics: $I(V)$, $G(V)$, $C(V)$, ...

2. Analysis about the internal **electric fields**: efficiency issues, …

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- § **Two main strategies:**

a. layout scaling

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	- *a. layout scaling*

- 2. Analysis about the internal **electric fields**: efficiency issues, …
- § **Two main strategies:**

b. implement a new readout approach

3. **Radiation tolerance**

empirical **acceptor removal/creation** law

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3. **Radiation tolerance**

empirical **acceptor removal/creation** law

 $N_{A}(\phi, x) = g_{eff} \phi + N_{A}(0, x) e^{-c(N_{A}(0, x))\phi}$

1. Study of detector **static/dynamic characteristics**: *I*(*V*), *G*(*V*), *C*(*V*), …

+ 2. Analysis about the internal **electric fields**: efficiency issues, …

+ 3. **Radiation tolerance**

 $1. + 3.$

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LGAD production: the complete workflow!

Contacts and Info

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- ⇒ To download this presentation and for more info about simulation: <http://personalpages.to.infn.it/~mandurri/teaching.html>
- ⇒ About the RSD experiment: <http://personalpages.to.infn.it/~mandurri/rsdproject.html>
- ⇒ Master Thesis Proposal: http://personalpages.to.infn.it/~mandurri/teaching/Proposta_di_Tesi_LM_RSD.pdf