Challenges in the simulation of hot electrons in radiation detectors

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with thanks to Francesco Bertazzi, Alberto Tibaldi, Marco Mandurrino, Marco Vallone, Giovanni Ghione, Enrico Bellotti

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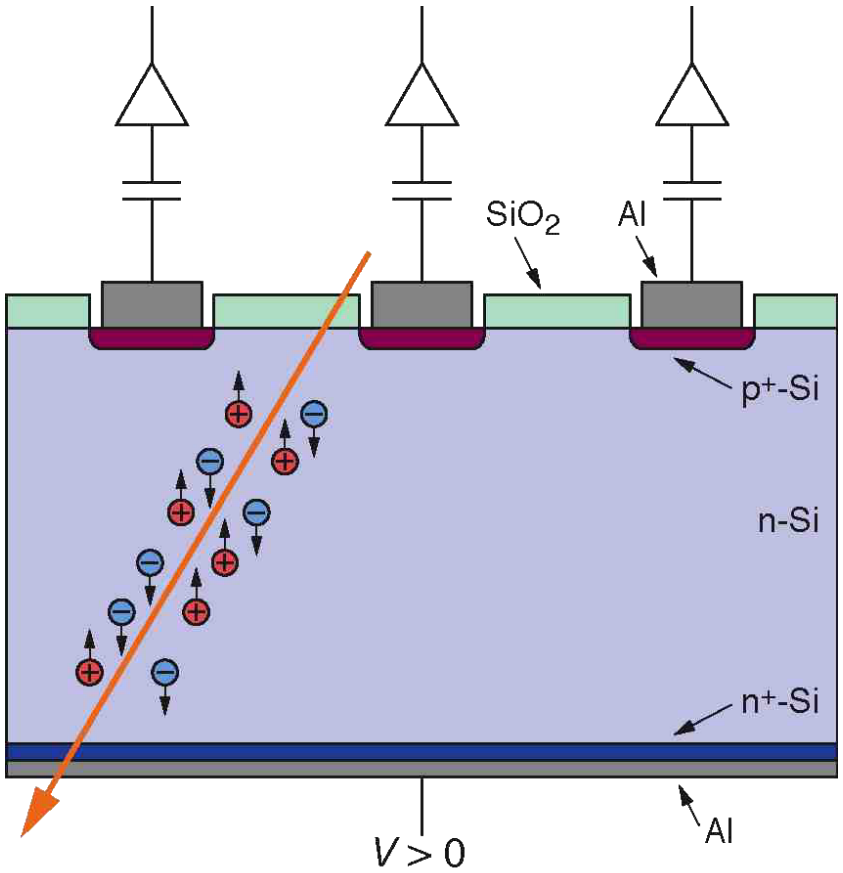
Outline

1. Introduction: disclaimer

This is not a lecture about the design of semiconductor radiation detectors: the target would be too ambitious, since our group has no specific experience on this large and diverse family of devices.

My discussion will be strictly, boringly methodological, and its point of view wil be informed only by the experience of my group on conventional (opto)electronic devices (transistors, LEDs, lasers, photodetectors: e.g., magnetic fields are never mentioned) in several semiconductor materials systems and with different modeling tools.



1. Introduction: hotness is in the eye of the beholder

Depending on the particular experiment or application, high energy physicists have to detect ionizing radiations with energies ranging from TeV to a few keV.

The design of detectors can be based on specialized codes, often implementing Monte Carlo simulation of trajectories in solids, e.g. MCNP (Oak Ridge, LANL; neutrons, photons, electrons), Casino (Université de Sherbrooke; electrons), Geant (CERN; photons, electrons, positrons, etc, with promising «low energy extensions»).

Most of these tools are able to describe the radiation-matter interaction on a very wide energy scale - *down to tens of eV*.

However, the final steps of the thermalization process are usually described through models originally developed for conventional electronic devices – the simulation tools we device engineers use (and sometimes develop) for a living.

1. Introduction: the bottom line

Hence, here is our predicament today:

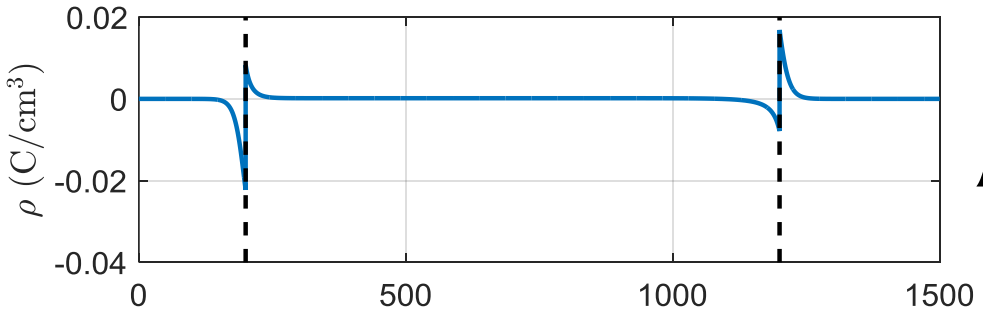
1. to briefly review the conventional model (*drift-diffusion*) available to all practitioners of electronic device simulation
2. to recall that drift-diffusion has <u>not</u> been conceived to deal with *hot* carriers – where a carrier having a (kinetic) energy comparable to the semiconductor energy gap (≈ 1 eV) would be considered definitely hot
3. to derive, from a general reference model (the *BTE*), possibly better approximations (*hydrodynamic* and *energy-balance* models), which are also available (often unbeknownst) to all designers having access to commercial simulation suites
4. to discuss the advantages and limitations of HD and EB
5. to mention the importance and show a few application examples of Monte Carlo transport simulation in semiconductors
6. to provide arguments suggesting that – even if you don't have access to a general, reliable Monte Carlo code for semiconductor device simulation – you definitely should look for a research group with this kind of expertise ;-)

Outline

2. The basics: devices at equilibrium

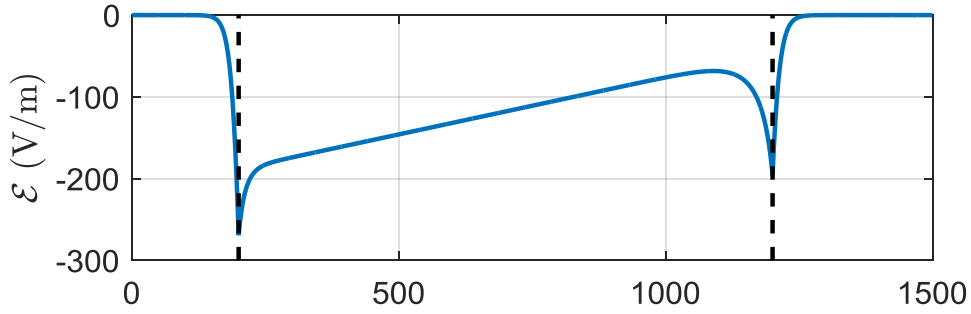
Let's pick a *p-i-n* junction at equilibrium – to recall the interplay between:

- net charge density



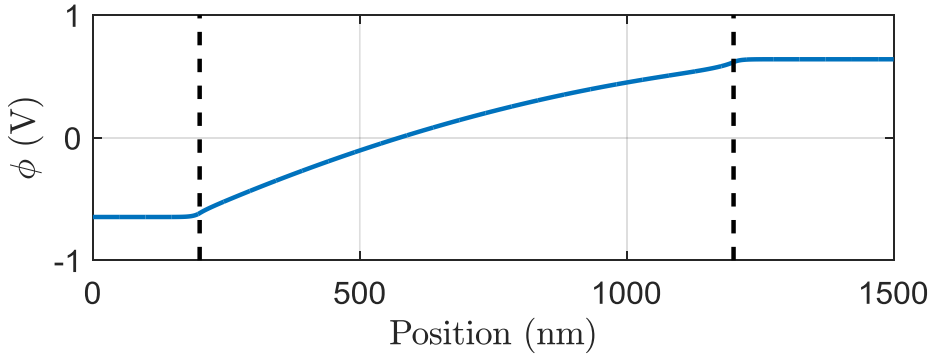
$$\rho = q\left(p - n + N_D^+ - N_A^-\right)$$

- electric field



$$\nabla \cdot \mathcal{E} = \frac{\rho}{\varepsilon}$$ (Gauss law)

- electrostatic potential



$$\nabla^2 \varphi = -\frac{\rho}{\varepsilon}$$ (Poisson equation)

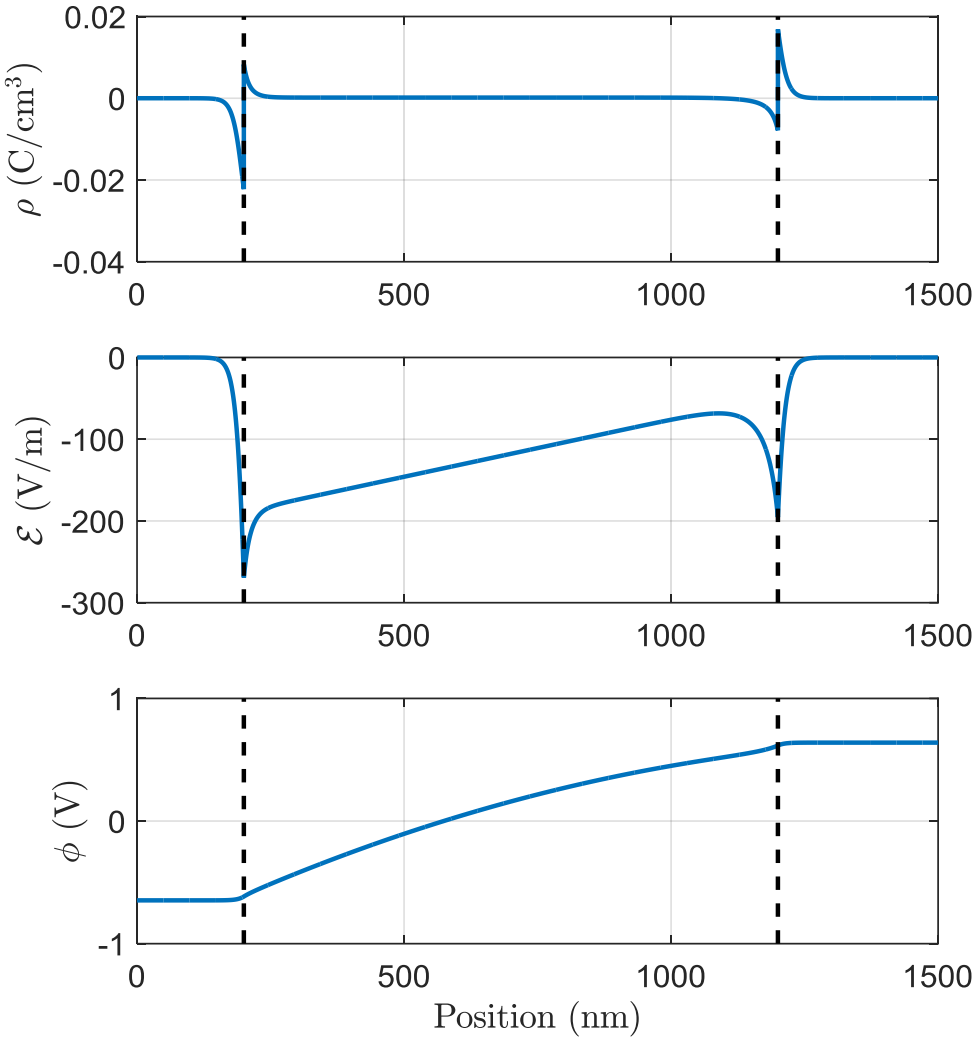
2. The basics: devices at equilibrium

Even at equilibrium, where no current is flowing, we need a *numerical* approach to get correct, consistent profiles, by solving *Poisson equation* (here written for the potential energy):

$$\nabla^2 U_0 = \frac{q^2}{\varepsilon}\left(p - n + N_D^+ - N_A^-\right)$$

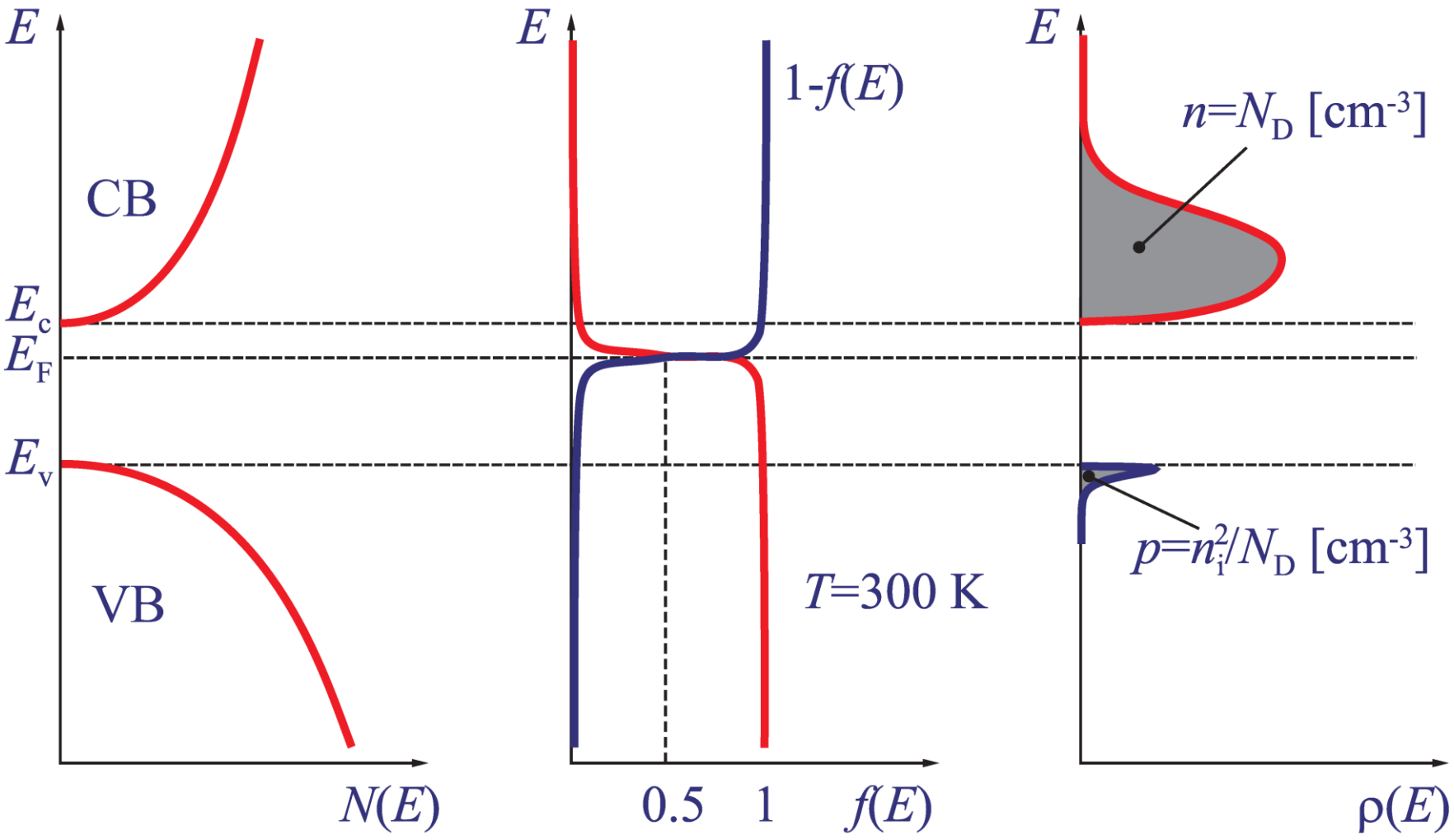
while taking into account also the appropriate *semiconductor statistics*

[simulation results: D1ANA code, developed by Alberto Tibaldi and Francesco Bertazzi]



2. The basics: statistics at equilibrium

In fact, the last ingredient of our Poisson-Fermi (or Poisson-Boltzmann) problem is the *Fermi level* – with the underlying assumption of *Fermi (or Boltzmann) carrier distribution* in energy/momentum space



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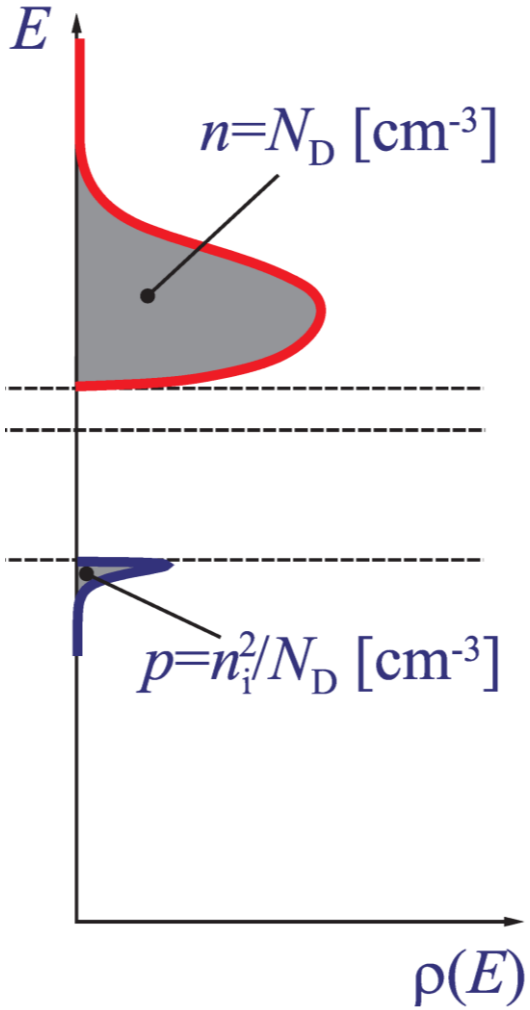
$$n = N_C \mathcal{F}_{1/2}\left[\frac{E_{Fn} - E_C}{k_B T}\right] \approx N_C \exp\left[\frac{E_{Fn} - E_C}{k_B T}\right]$$

$$= N_C \exp\left[\frac{E_{Fn} - (U_0 - \chi)}{k_B T}\right]$$

$$p = N_V \mathcal{F}_{1/2}\left[\frac{E_V - E_{Fp}}{k_B T}\right] \approx N_V \exp\left[\frac{E_V - E_{Fp}}{k_B T}\right]$$

$$= N_V \exp\left[\frac{(U_0 - \chi - E_g) - E_{Fp}}{k_B T}\right]$$



2. The basics: drift-diffusion

If we move out of equilibrium (e.g., we drive the *p-i-n* junction in reverse bias) we'll have to take into account also the *currents* flowing in the device, by including conservation equations for the carrier densities:

- Poisson equation

$$\nabla^2 U_0 = \frac{q^2}{\varepsilon}\left(p - n + N_D^+ - N_A^-\right)$$

- *Continuity* equations

$$\begin{cases} \dfrac{\partial n}{\partial t} = +\dfrac{1}{q}\nabla \cdot \mathbf{J}_n - U_n \\ \dfrac{\partial p}{\partial t} = -\dfrac{1}{q}\nabla \cdot \mathbf{J}_p - U_p \end{cases}$$

This system is the *drift-diffusion model* (DD), implemented in most commercial simulation suites

2. The basics: drift diffusion

The drift-diffusion model takes his name from the *constitutive equations* used to describe the currents in terms of the other unknowns of the system:

(i) carrier densities and

(ii) electric field
(or electrostatic potential)

$$\begin{cases} \mathbf{J}_n = \boxed{qn\mu_n\mathcal{E}} + \boxed{qD_n\nabla n} \\ \mathbf{J}_p = \boxed{qp\mu_p\mathcal{E}} - \boxed{qD_p\nabla p} \end{cases}$$

drift currents

diffusion currents

where the electric field couples the continuity equations to Poisson equation

2. The basics: drift diffusion

These constitutive equations require the definition of *four* additional material parameters:

(i) carrier *mobilities*

(ii) carrier *diffusivities*

$$\begin{cases} \mathbf{J}_n = qn\mu_n\mathcal{E} + qD_n\nabla n \\ \mathbf{J}_p = qp\mu_p\mathcal{E} - qD_p\nabla p \end{cases}$$

which are usually considered to be related through *Einstein relation*:

$$D_{n,p} = \frac{k_B T}{q}\mu_{n,p}$$

2. The basics: quasi-Fermi levels

Under the approximation of Boltzmann statistics and using Einstein relation between diffusivity and mobility, one may rewrite the continuity equations as:

$$\begin{cases} \dfrac{\partial n}{\partial t} = +\dfrac{1}{q}\nabla\cdot(n\mu_n \nabla E_{Fn}) - U_n \\ \dfrac{\partial p}{\partial t} = -\dfrac{1}{q}\nabla\cdot(p\mu_p \nabla E_{Fp}) - U_p \end{cases}$$

In fact:

- however hard you drive a device out of equilibrium, in DD electrons and holes always have *Maxwellian* distributions in energy, albeit with different *quasi-Fermi levels* (intraband relaxation processes are much faster than interband ones)
- nonzero current densities ⇔ nonconstant quasi-Fermi levels

2. The basics: generation-recombination

The last ingredients of the drift-diffusion model are the net recombination rates U_n, U_p, which are used to describe an host of GR processes, e.g.:

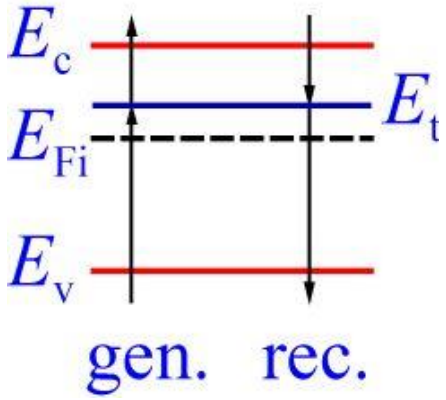
- **Two particle**
  - one step (direct)
    - photogeneration
    - radiative recombination
    - direct thermal generation
    - direct thermal recombination
  - two-step (indirect)
    - Shockley-Read-Hall (SRH) generation-recombination
    - surface generation-recombination
- **Three particle**
  - impact ionization → pure generation process
  - Auger
    - electron emission
    - hole emission

2. The basics: generation-recombination

As an example, the *Shockley-Read-Hall model* is used for indirect processes mediated by *trap levels*:

$$(G-R)_{SRH} = \frac{n_i^2 - np}{\tau_p\left[n + n_i \exp\left(\frac{E_t - E_i}{k_B T}\right)\right] + \tau_n\left[p + n_i \exp\left(\frac{E_i - E_t}{k_B T}\right)\right]}$$

where τ_n and τ_p typically lie in the range between 100 ns and 5 μs.



(A similar description can be used for recombination with surface states)

2. The basics: band diagrams

Now is the time to quote from the Nobel lecture of Herbert Kroemer (2000):

REVIEWS OF MODERN PHYSICS, VOLUME 73, JULY 2001

Nobel Lecture: Quasielectric fields and band offsets: teaching electrons new tricks*

Herbert Kroemer

Electrical and Computer Engineering Department, University of California, Santa Barbara, California 93106-9560

[…] one of the central messages I try to get across early is the importance of energy-band diagrams. I often put this in the form of "Kroemer's Lemma of Proven Ignorance":

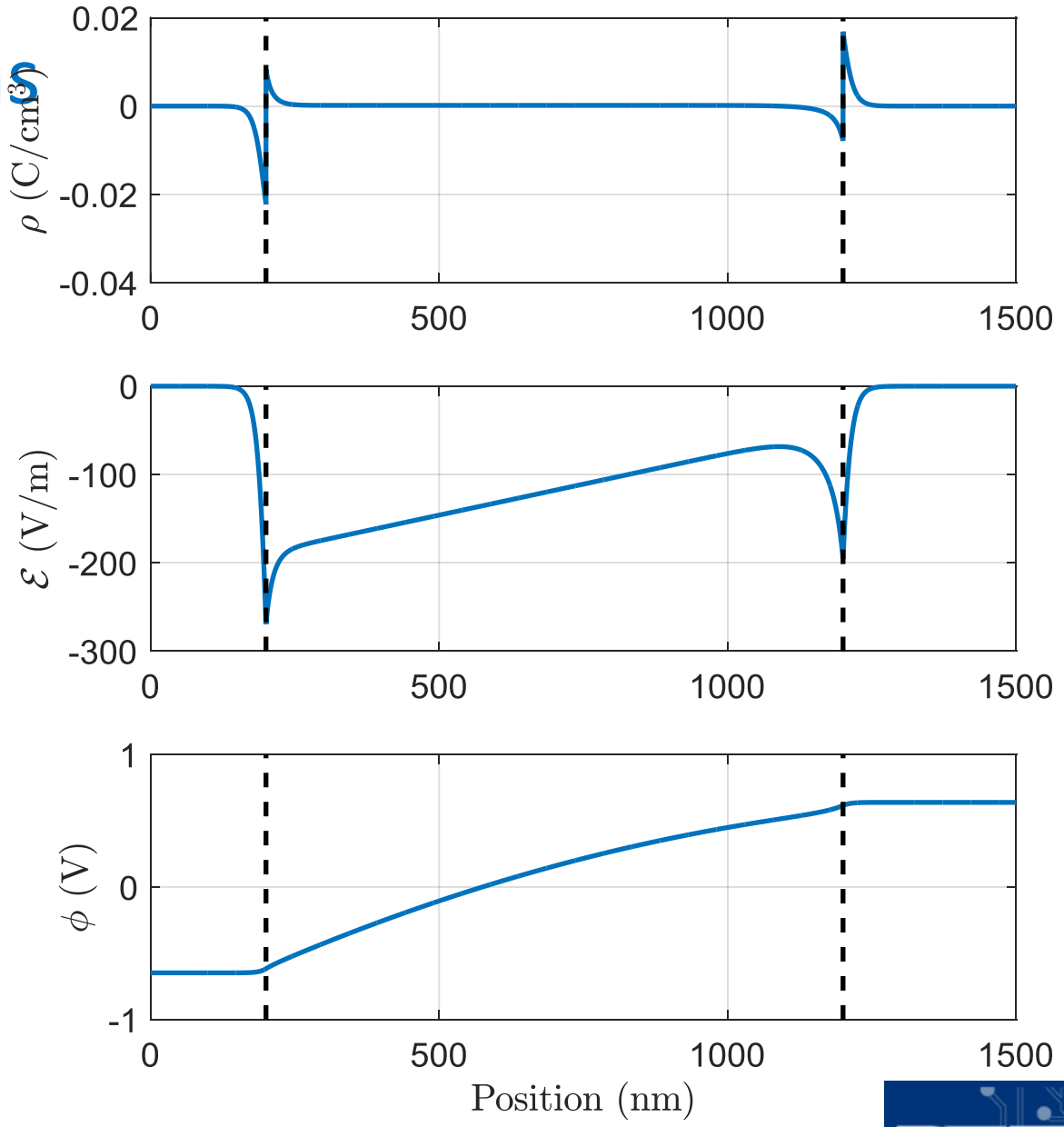
If, in discussing a semiconductor problem, you cannot draw an Energy-Band-Diagram, this shows that you don't know what you are talking about,

with the corollary

If you can draw one, but don't, then your audience won't know what you are talking about.

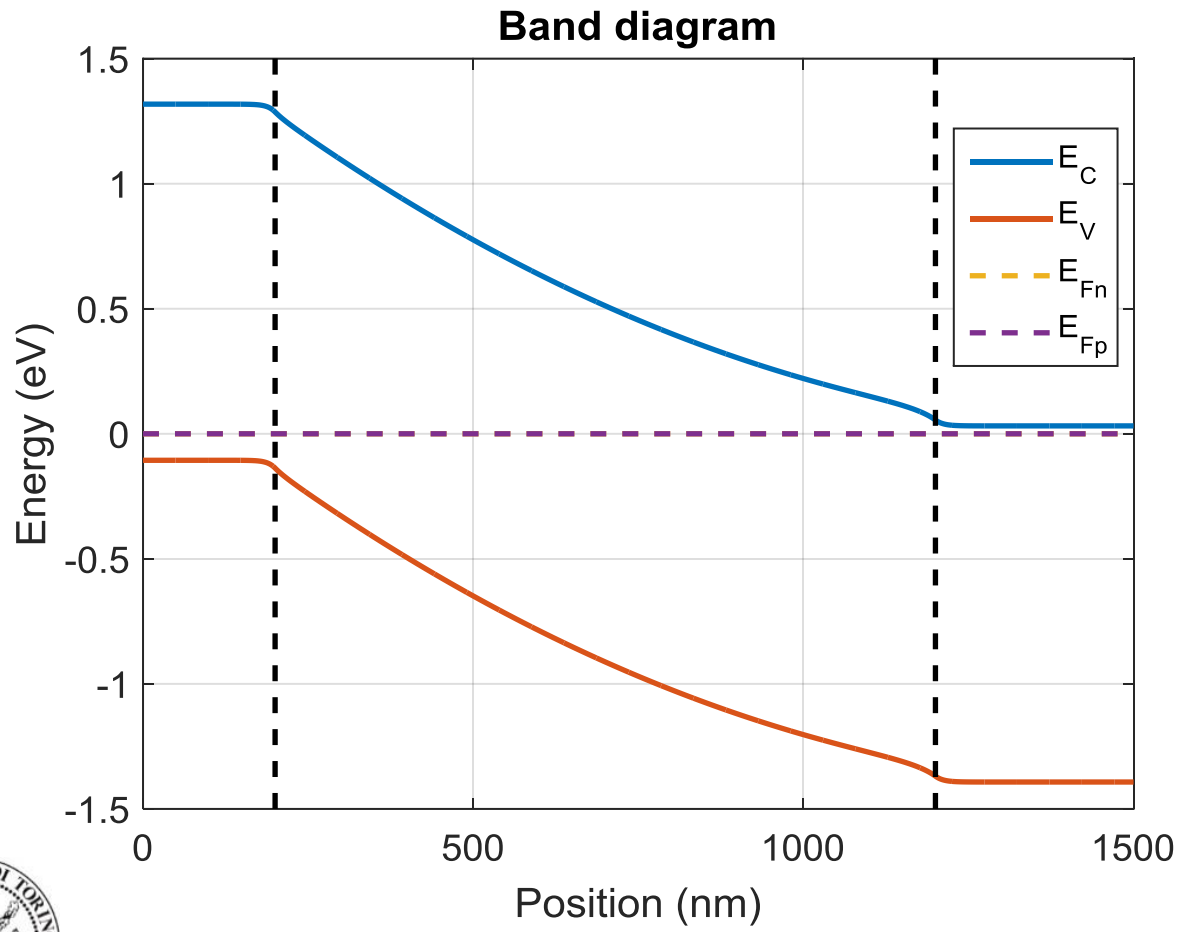
2. The basics: band diagrams

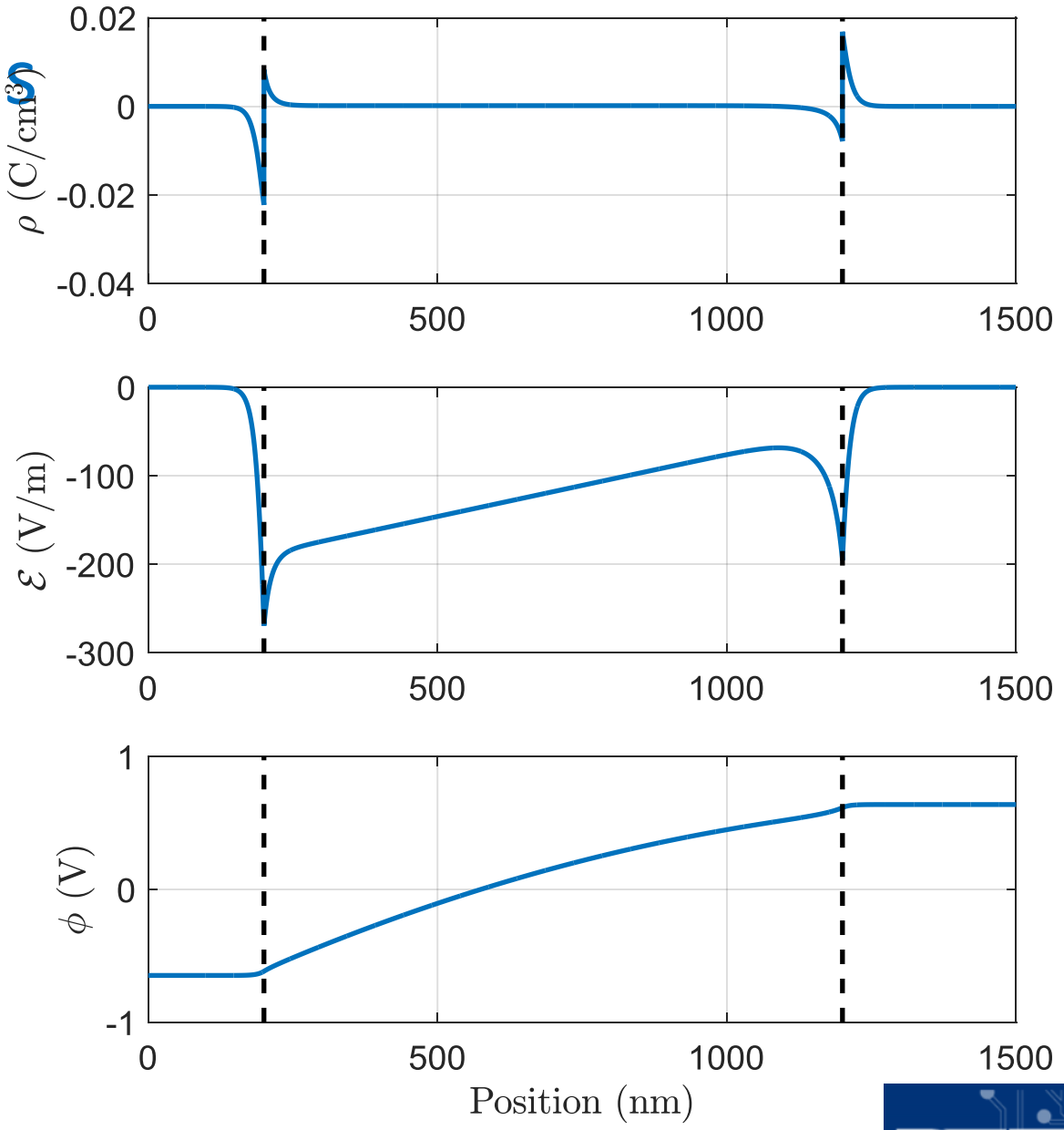
Following Kroemer's injunction, let's pick again our *p-i-n* junction *at equilibrium*, where we have solved the Poisson-Boltzmann problem



2. The basics: band diagrams

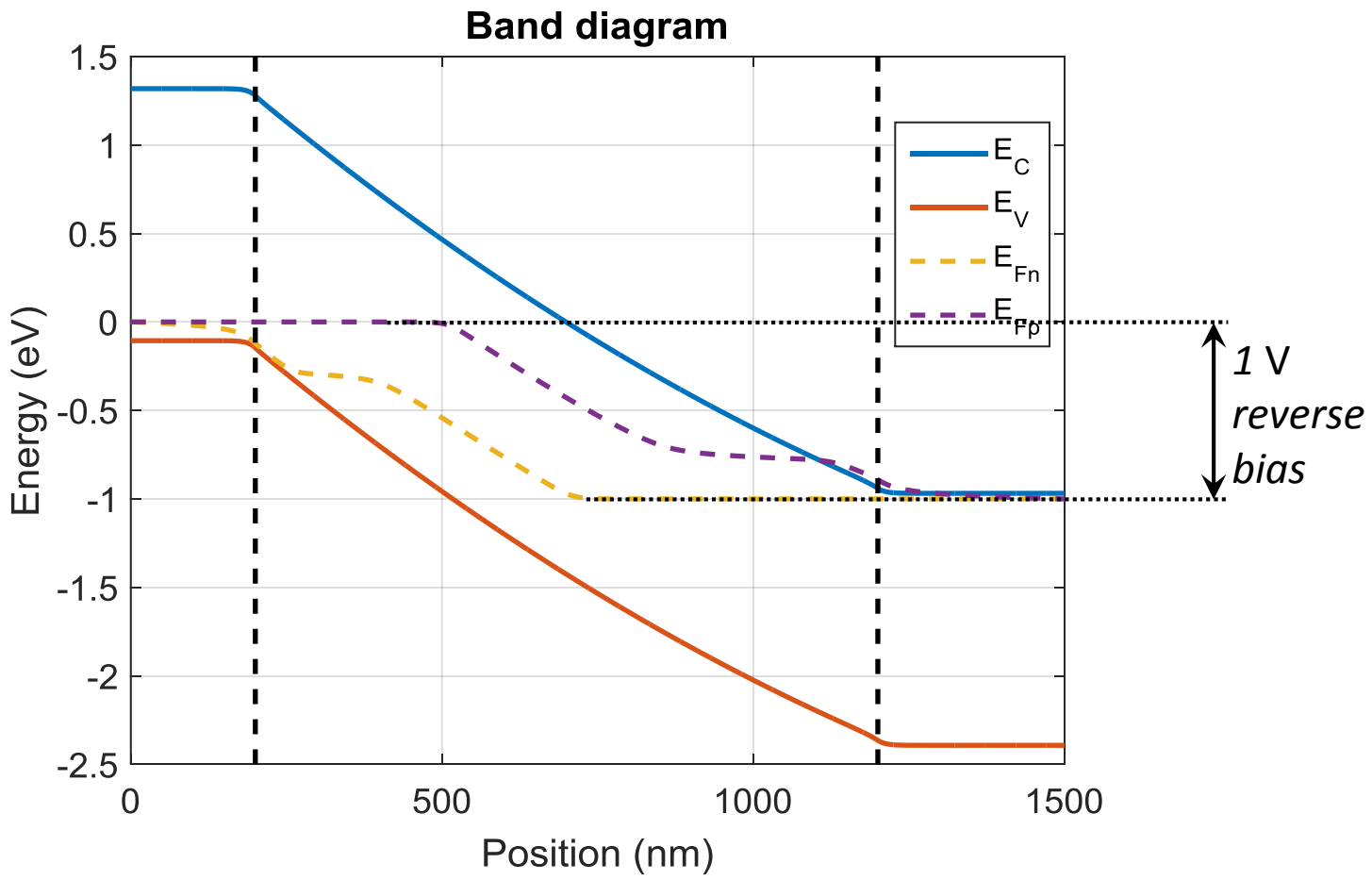
A completely equivalent representation is offered by the corresponding band diagram:





2. The basics: band diagrams

Moving to *reverse bias* (the operating region of most detectors), we can see the quasi-Fermi levels at play



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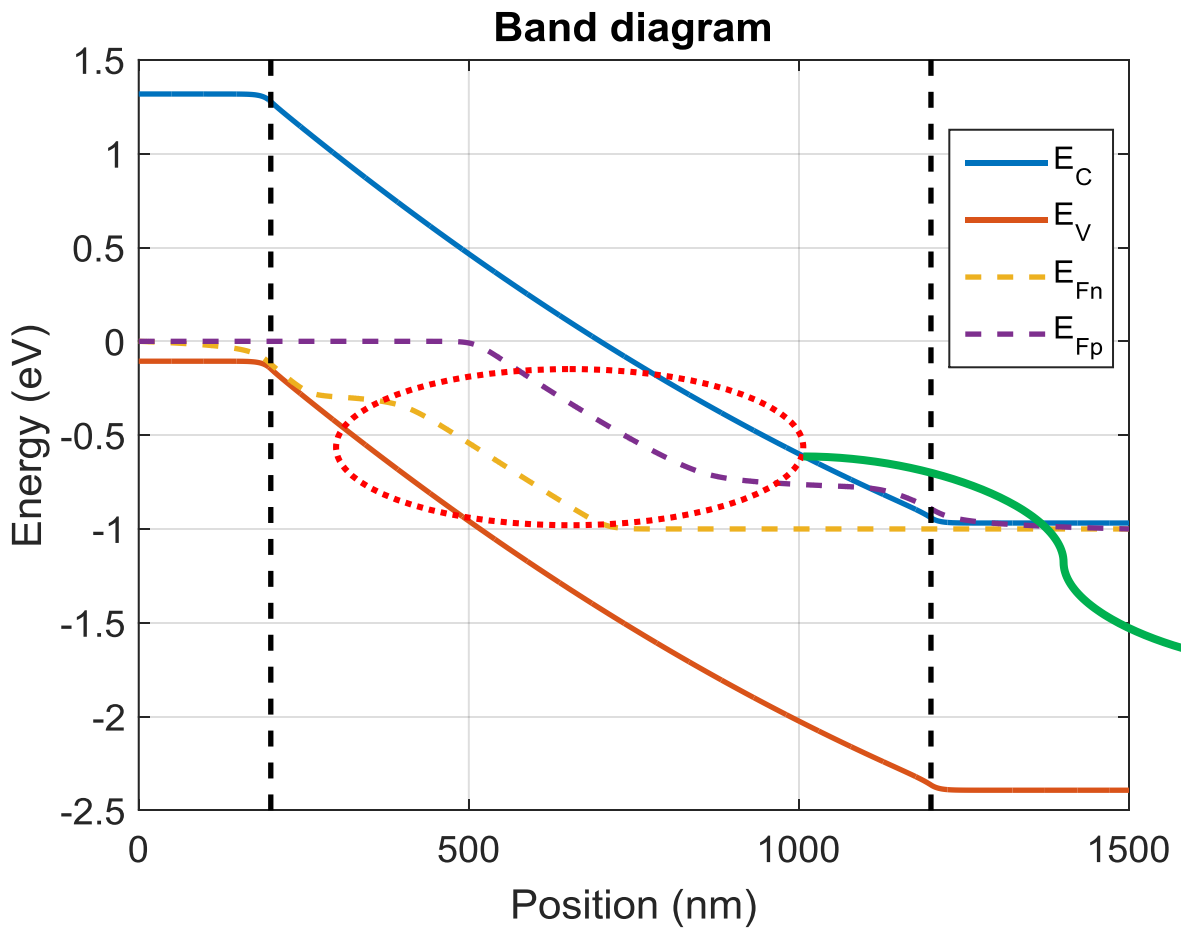
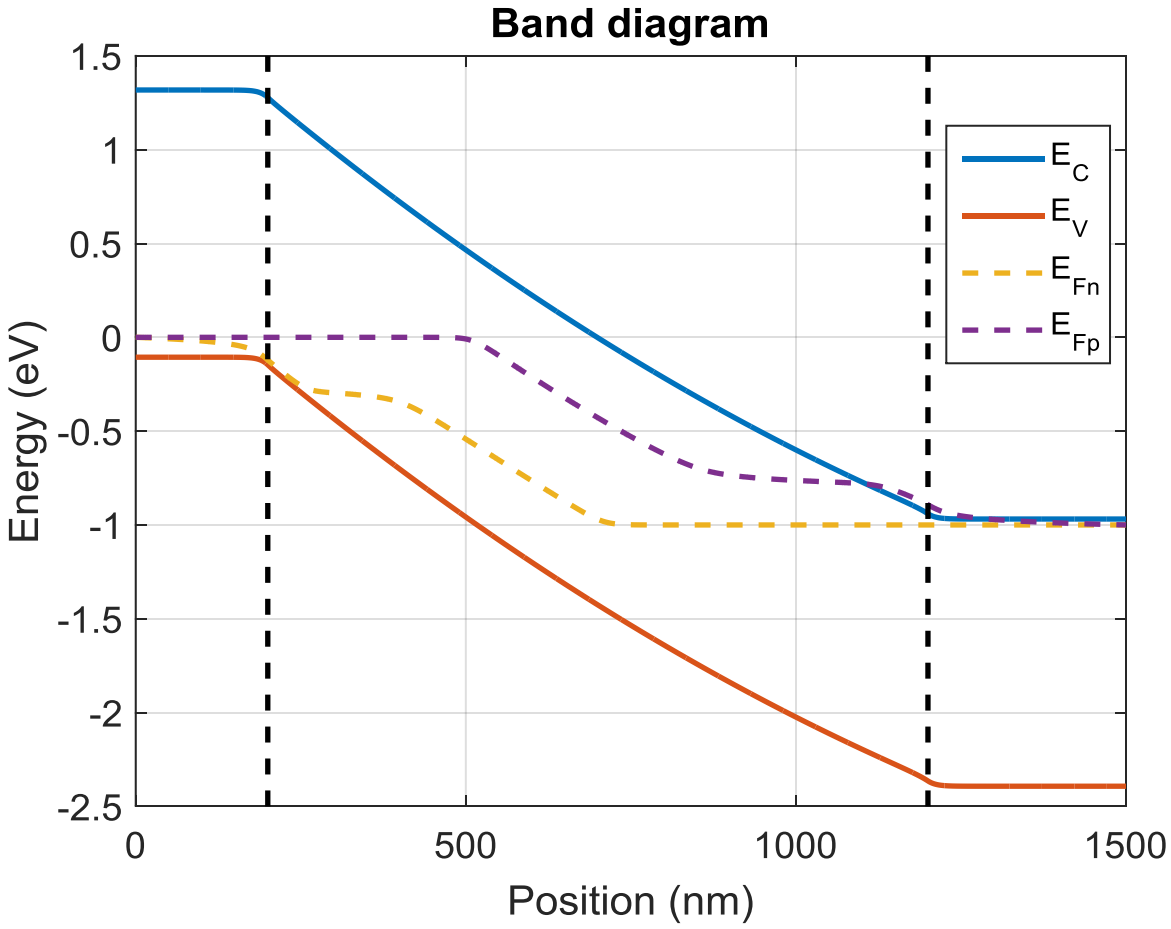
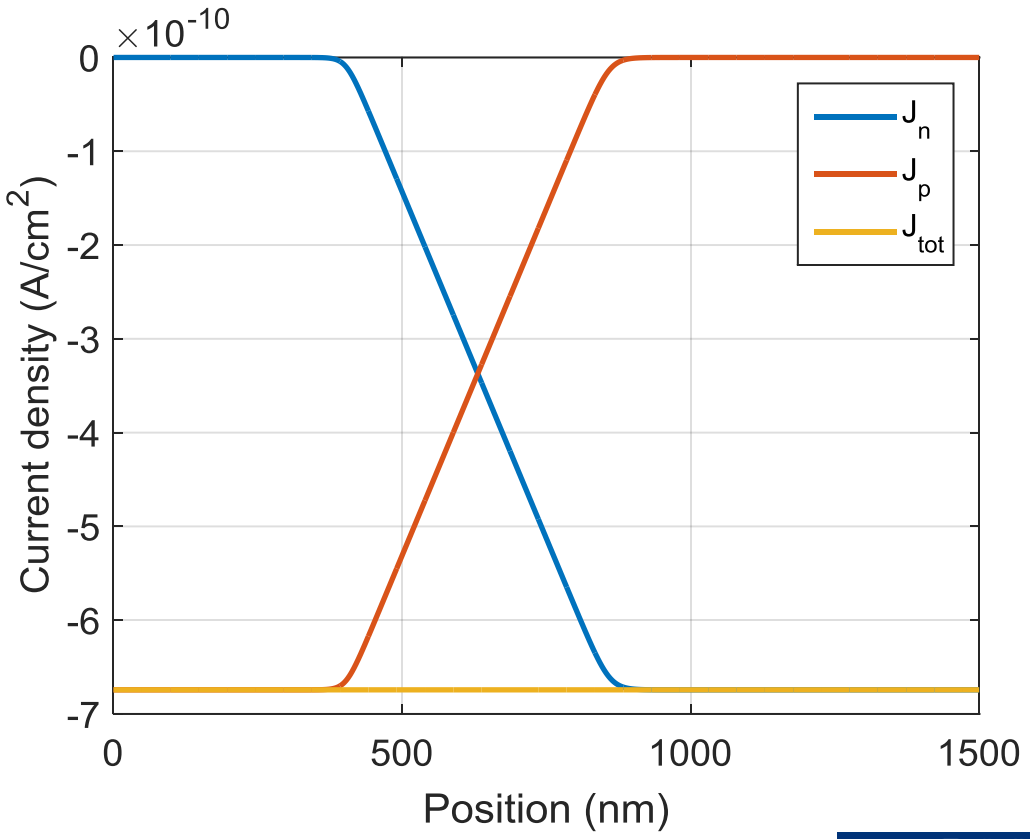


In the depletion region, the quasi-Fermi levels move towards the opposite band edges ⇒ carrier densities are much lower than at equilibrium

2. The basics: band diagrams

Moving to *reverse bias* (the operating region of most detectors), we can see the quasi-Fermi levels at play – whose derivatives also encode information about the corresponding current densities:

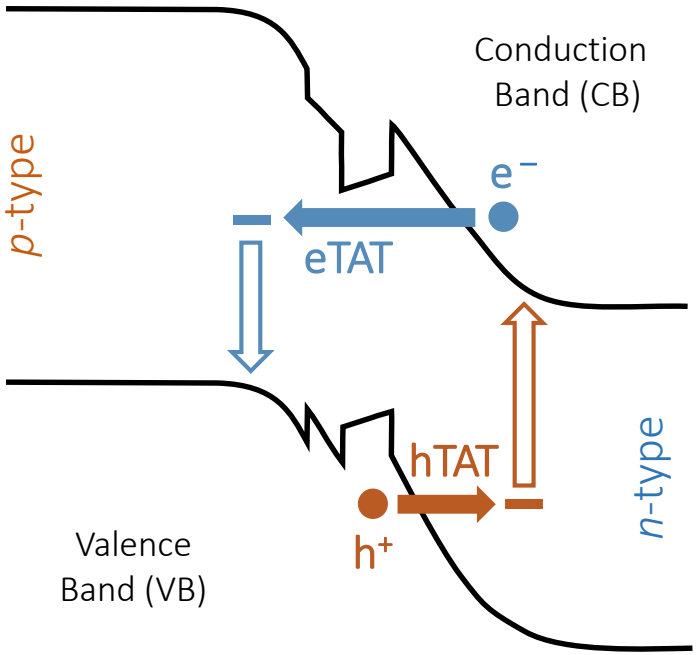


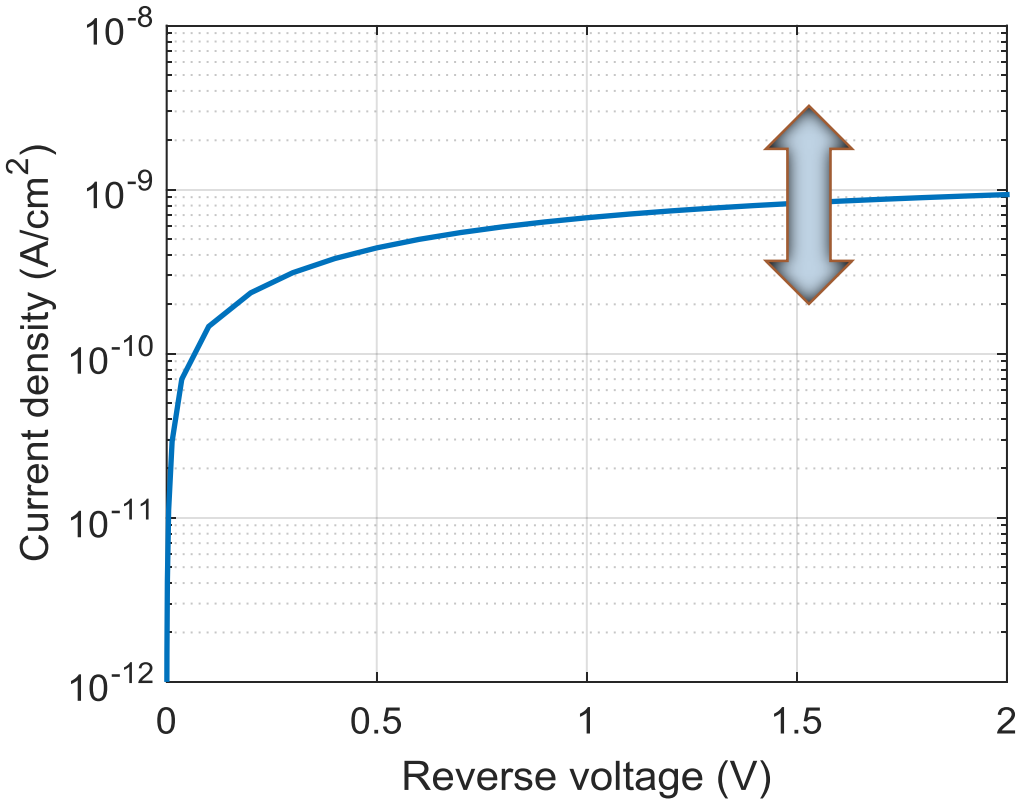


2. The basics: currents and fitting parameters

The drift-diffusion model allows e.g. to predict the current-voltage (*I-V*) characteristics (dark current)

a) The calculated saturation current can be "adjusted" by playing with the GR mechanisms – including quantum effects such as trap-assisted tunneling





2. The basics: currents and fitting parameters

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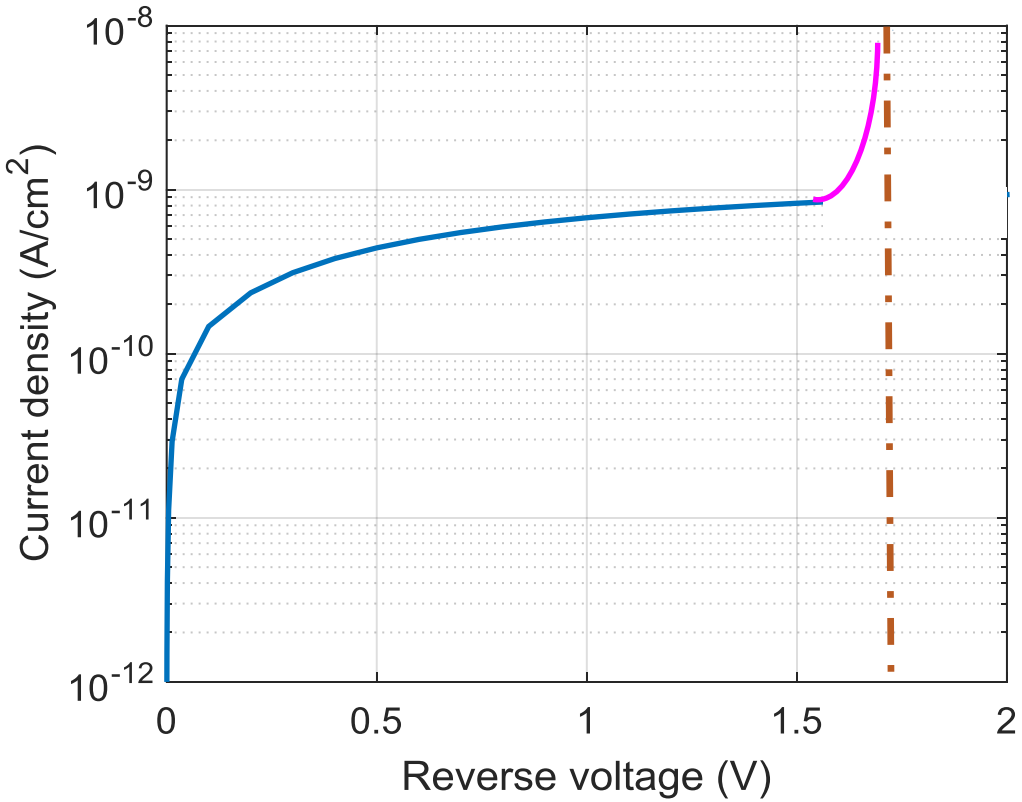
a) The calculated saturation current can be "adjusted" by playing with the GR mechanisms – including quantum effects such as trap-assisted tunneling

b) Even a complex process such as impact ionization can be included semiempirically with yet another (electric-field-dependent) generation mechanism…



Outline

3. Hot electrons and the drift-diffusion model

Here, the cautionary notes begin. Hot electrons affect mainly two sets of ingredients of the DD model:

- The mobility and diffusivity in the constitutive equations for the electron and hole currents

$$\mathbf{J}_n = qn\mu_n\mathcal{E} + qD_n\nabla n$$

$$\mathbf{J}_p = qp\mu_p\mathcal{E} - qD_p\nabla p$$

$$D_{n,p} = V_T\mu_{n,p}$$

$$v_n \approx -\mu_n\mathcal{E}$$

$$v_p \approx +\mu_p\mathcal{E}$$

- The net recombination rates

$$U_n, U_p$$

3. Hot electrons and the drift-diffusion model

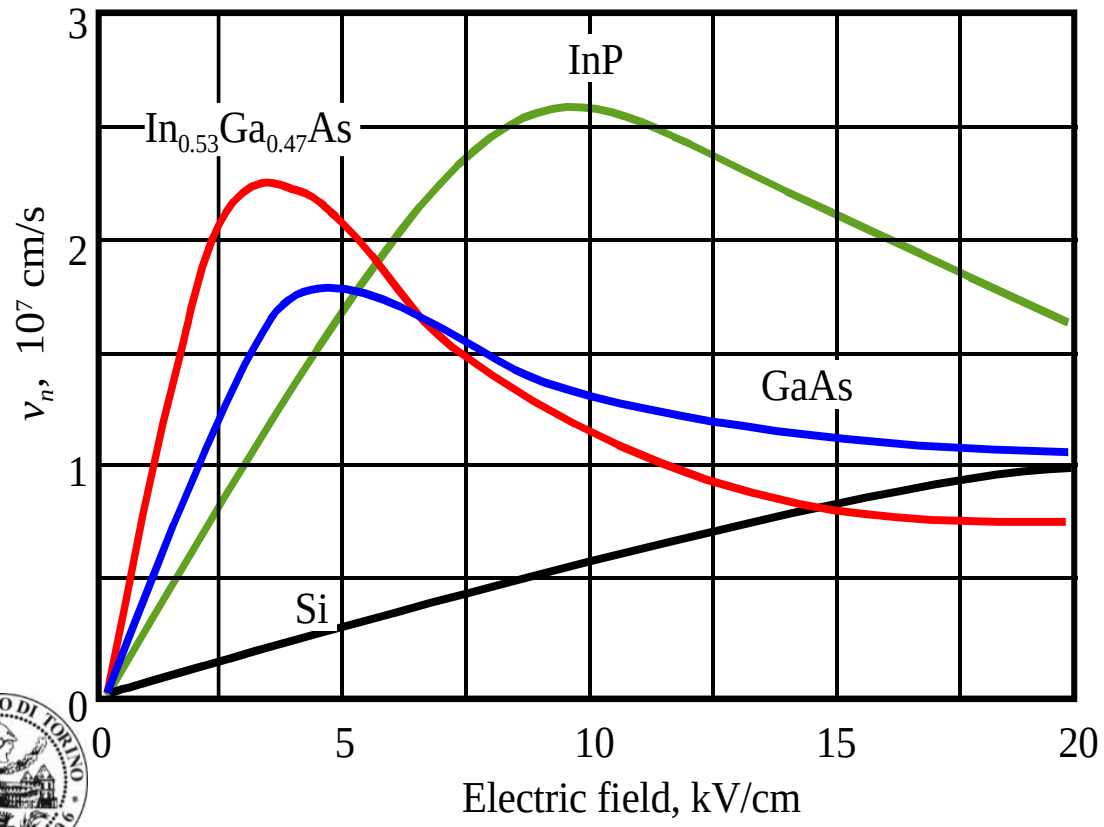
In bulk semiconductors, for low electric fields *at steady state*, the electron and hole average velocities are proportional to the applied field:

$$v_n = -\mu_n \mathcal{E}\,;\, v_p = \mu_p \mathcal{E} \quad \Rightarrow \quad J_{\text{drift},n} = \sigma_n \mathcal{E}\,;\, J_{\text{drift},p} = \sigma_p \mathcal{E}$$

but the picture is more complex for increasing fields

3. Hot electrons and the drift-diffusion model

$$v_n = -\mu_n(\mathcal{E})\mathcal{E}\,;\; v_p = \mu_p(\mathcal{E})\mathcal{E}$$



In order to take into account the carrier *velocity saturation*, empirical *field dependent* mobility models (e.g. the "Canali model") must be introduced and finely tuned:

$$\mu(\mathcal{E}) = \frac{\mu_0}{\left[1+\left(\frac{\mu_0\mathcal{E}}{v_{sat}}\right)^{\beta}\right]^{1/\beta}}$$

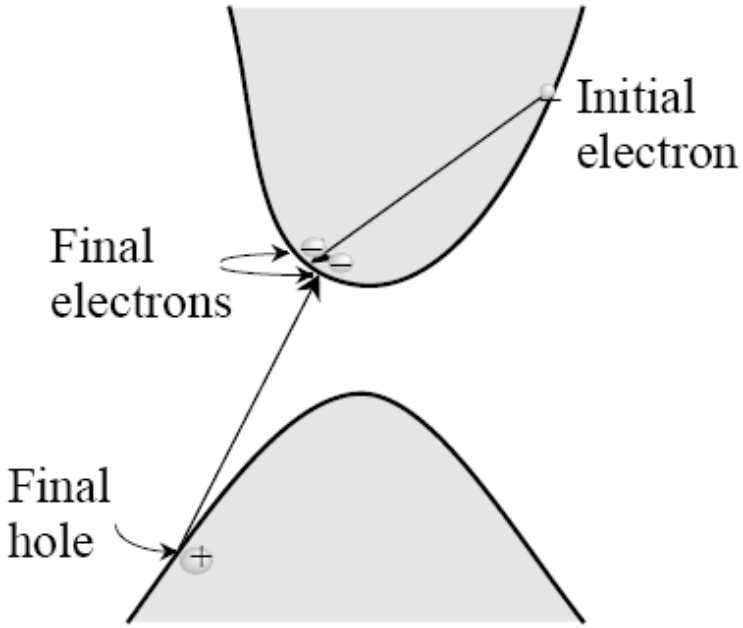
but what about:

- short transients (in time and/or space) where the static $v(\mathcal{E})$ relation is not valid?
- diffusivity and Einstein relation?

3. Hot electrons and the drift-diffusion model

- Under very high fields, carriers may acquire a kinetic energy larger than the energy gap ⇒ a collision with a bound electron in the valence band leads to *impact ionization* (also called *Auger generation*)
- Impact ionization processes may lead to avalanche multiplication (and possibly to device breakdown)

Material	Bandgap (eV)	Breakdown electric field (V/cm)
GaAs	1,43	4×10^5
Ge	0,664	10^5
InP	1,34	5×10^5
Si	1,1	3×10^5
$In_{0,53}Ga_{0,47}As$	0,8	2×10^5
C	5,5	10^7
SiC	2,9	$2\text{-}3 \times 10^6$
SiO_2	9	10^7
Si_3N_4	5	10^7



In the diagram, a hot electron scatters with a valence band electron, producing two conduction band electrons and a hole. Hot holes can undergo a similar process

3. Hot electrons and the drift-diffusion model

- To include impact ionization in drift-diffusion models, *field-dependent carrier generation terms* are inserted in the continuity equations of electrons and holes:

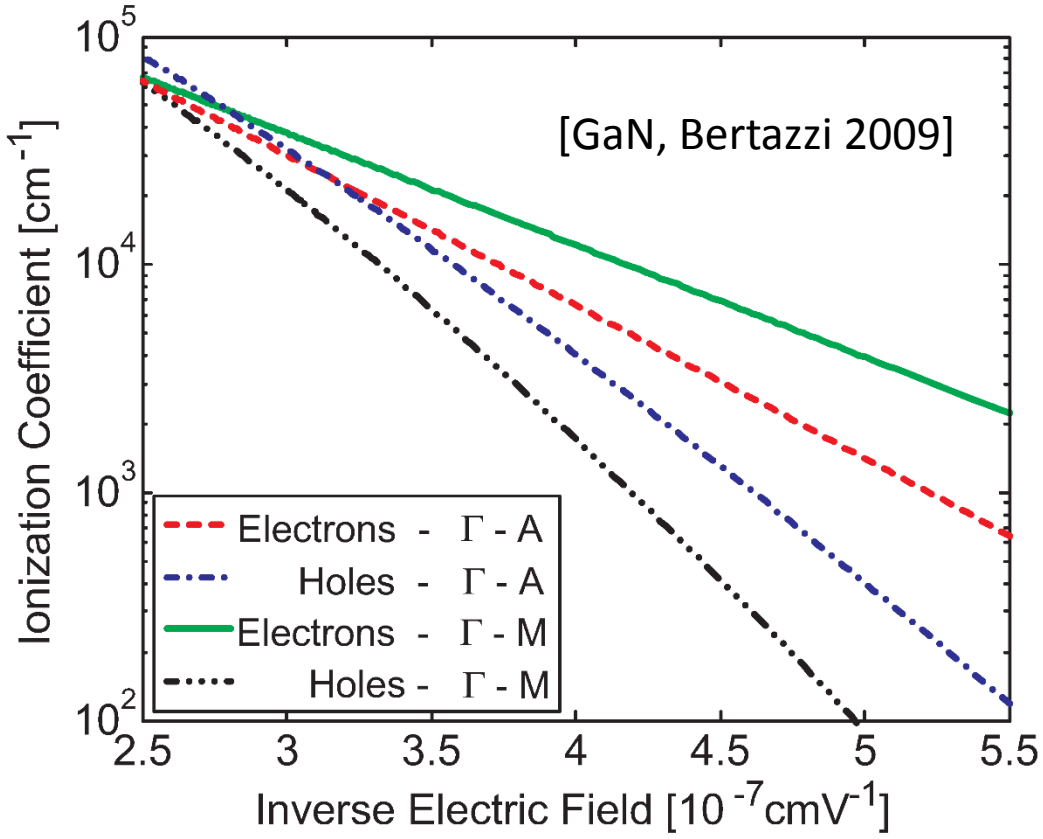
$$-U_n \rightarrow -U_n + G_n(\mathcal{E}) = -U_n + \alpha_n(\mathcal{E})\, J_n / q$$

$$-U_p \rightarrow -U_p + G_p(\mathcal{E}) = -U_p + \alpha_p(\mathcal{E})\, J_p / q$$

- The electron and hole *impact ionization coefficients* α_n, α_h (m^{-1}) increase exponentially with the electric field, and are difficult to estimate via experiments or full-band Monte Carlo simulations (see later)

$$\alpha_n(\mathcal{E}) = A_n \exp\left[-\left(\mathcal{E}_n^{\text{crit}}/\mathcal{E}\right)^{e_n}\right]$$

$$\alpha_p(\mathcal{E}) = A_p \exp\left[-\left(\mathcal{E}_p^{\text{crit}}/\mathcal{E}\right)^{e_p}\right]$$



Because of carrier multiplication, device simulation in the avalanche regime is very challenging within <u>any</u> transport modeling framework

3. Hot electrons and the drift-diffusion model

Most of these hot-carrier corrections to DD

- Have been fine-tuned only for a limited set of materials (Si)
- May lead to convergence issues
- Attempt to describe carriers heated by electric fields - which could be ill-suited to detectors where the high carrier temperature can be due (also) to other reasons

Therefore

- Rather than trying to extend the application of DD well beyond its limits, by including a number of ad hoc semiempirical patches involving scores of fitting parameters, could we move to a more general modeling framework, naturally allowing for hot electrons?
- This has been one of the main goal of *computational electronics* in the last three decades
- The results of these efforts can be arranged in a hierarchy of transport models