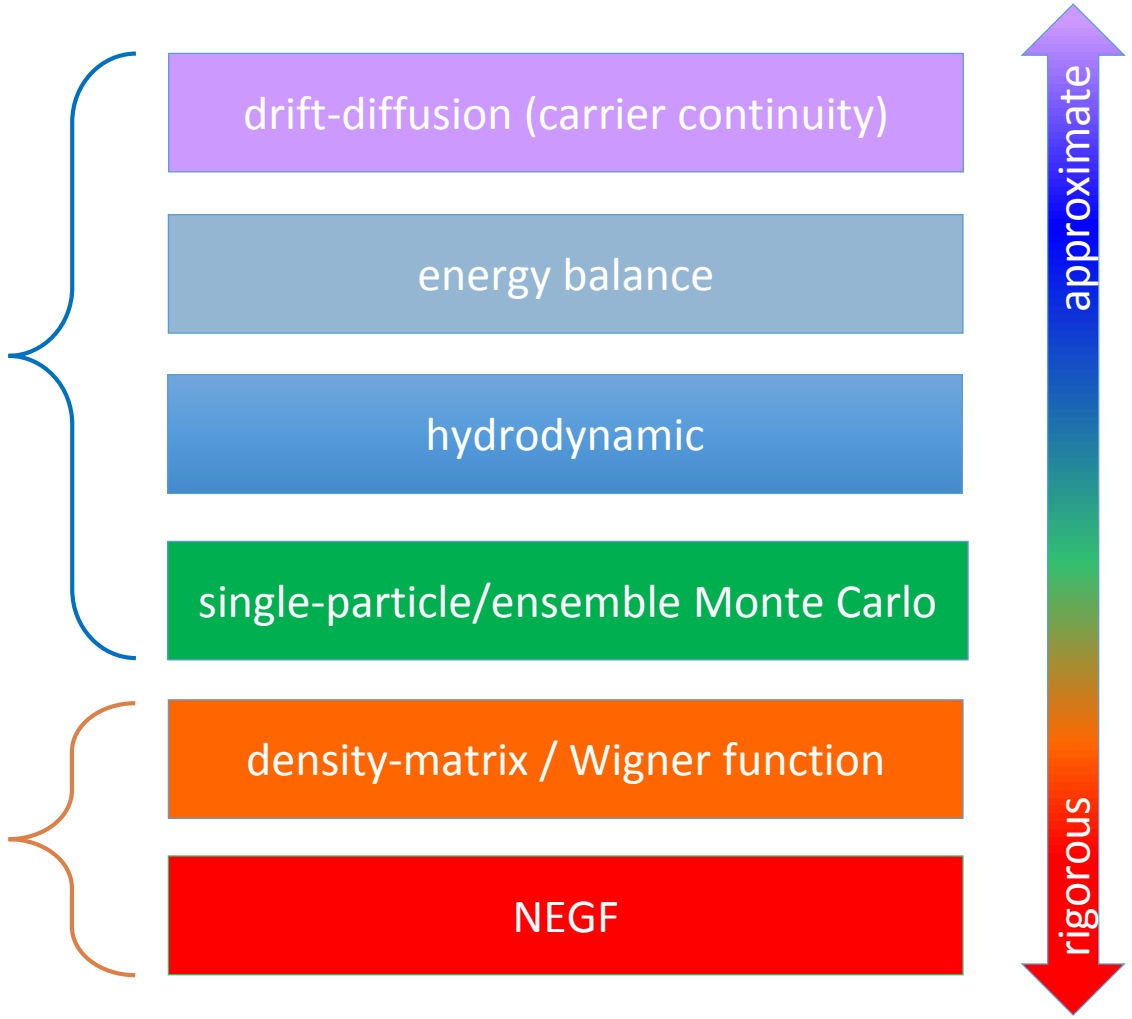
Outline

1. Introduction
2. The basics
3. Hot electrons and the drift-diffusion model
4. Beyond drift-diffusion
5. Limits of the drifted Gaussian
6. Monte Carlo transport simulation
7. Conclusions

4. Beyond drift-diffusion: a hierarchy of transport models

semiclassical models based on Boltzmann transport equation

quantum transport models



4. Beyond drift-diffusion: a hierarchy of transport models

- No general solver of the BTE is available to the general public for device simulation…
- …but almost all commercial simulation suites include hydrodynamic and/or energy balance solvers
- HD and EB are PDE models, just like drift-diffusion: what's the difference? Is it worth moving from DD to HD/EB?
- Let's take a top-down approach, briefly recalling the BTE and then deriving from it the HD/EB description

4. Beyond drift-diffusion: the BTE

- The Boltzmann transport Equation (BTE) is the reference model for semiclassical transport. It is a conservation equation for the particle distribution function $f(\mathbf{v},\mathbf{r},t)$, which gives the probability of finding a particle (in our case, electron or hole) having velocity between $\mathbf{v}$ and $\mathbf{v}+d\mathbf{v}$ and in the region $\mathbf{r}$ to $\mathbf{r}+d\mathbf{r}$
- We assume that $\mathbf{v}$ and $\mathbf{r}$ are given simultaneously → classical particles
- $f(\mathbf{v},\mathbf{r},t)$ allows us to calculate *ensemble averages* over *velocity and space*:

$$\langle A(t)\rangle = \int d\mathbf{r}\int d\mathbf{v} A(\mathbf{v},\mathbf{r},t) f(\mathbf{v},\mathbf{r},t)$$

- For this to give the proper averages, f is normalized:

$$\int d\mathbf{r}\int d\mathbf{v} f(\mathbf{v},\mathbf{r},t) = 1$$

- The distribution function should satisfy a *continuity equation* in a 6D phase space defined by the independent variables:

$$x, y, z, v_x, v_y, v_z$$

4. Beyond drift-diffusion: the BTE

- The classical form of this continuity equation is:

$$\frac{\partial f(\mathbf{r},\mathbf{v},t)}{\partial t} = \boxed{-\mathbf{v}\cdot\nabla_r f - \frac{\mathbf{F}}{m}\cdot\nabla_v f} + \left.\frac{\partial f}{\partial t}\right|_{Coll} + \left.\frac{\partial f}{\partial t}\right|_{G-R}$$

  where the first two terms on rhs are *streaming terms*

- For Bloch electrons in a semiconductor, we may consider a 6D space *x, y, z,* k_x, k_y, k_z, where **k** is the wavevector and $\mathbf{v} = \nabla_k E(\mathbf{k})/\hbar$.

- This implies in principle to know the *electronic structure* of the material in the *entire Brillouin zone*

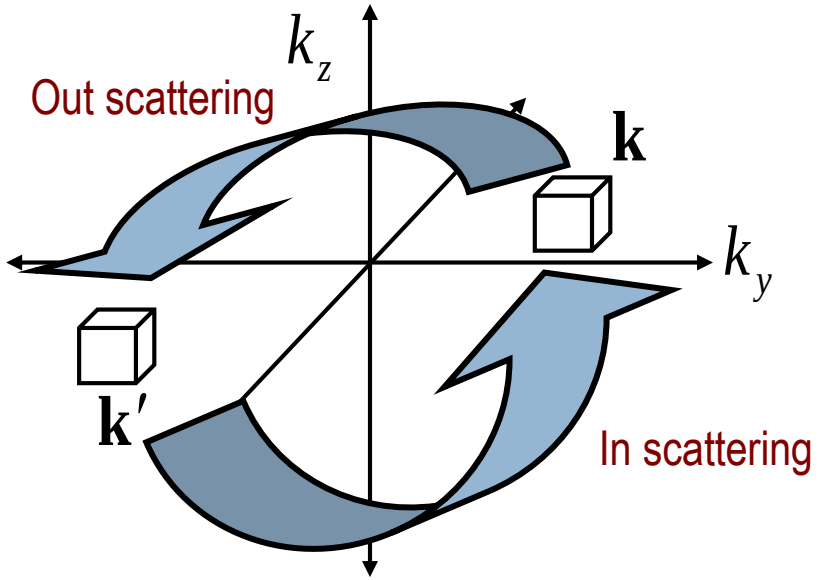
- The semiclassical BTE for transport of Bloch electrons is therefore:

$$\frac{\partial f(\mathbf{r},\mathbf{k},t)}{\partial t} = -\frac{1}{\hbar}\nabla_k E(\mathbf{k})\cdot\nabla_r f - \frac{\mathbf{F}}{\hbar}\cdot\nabla_k f + \left.\frac{\partial f}{\partial t}\right|_{Coll} + \left.\frac{\partial f}{\partial t}\right|_{G-R}$$

4. Beyond drift-diffusion: the BTE

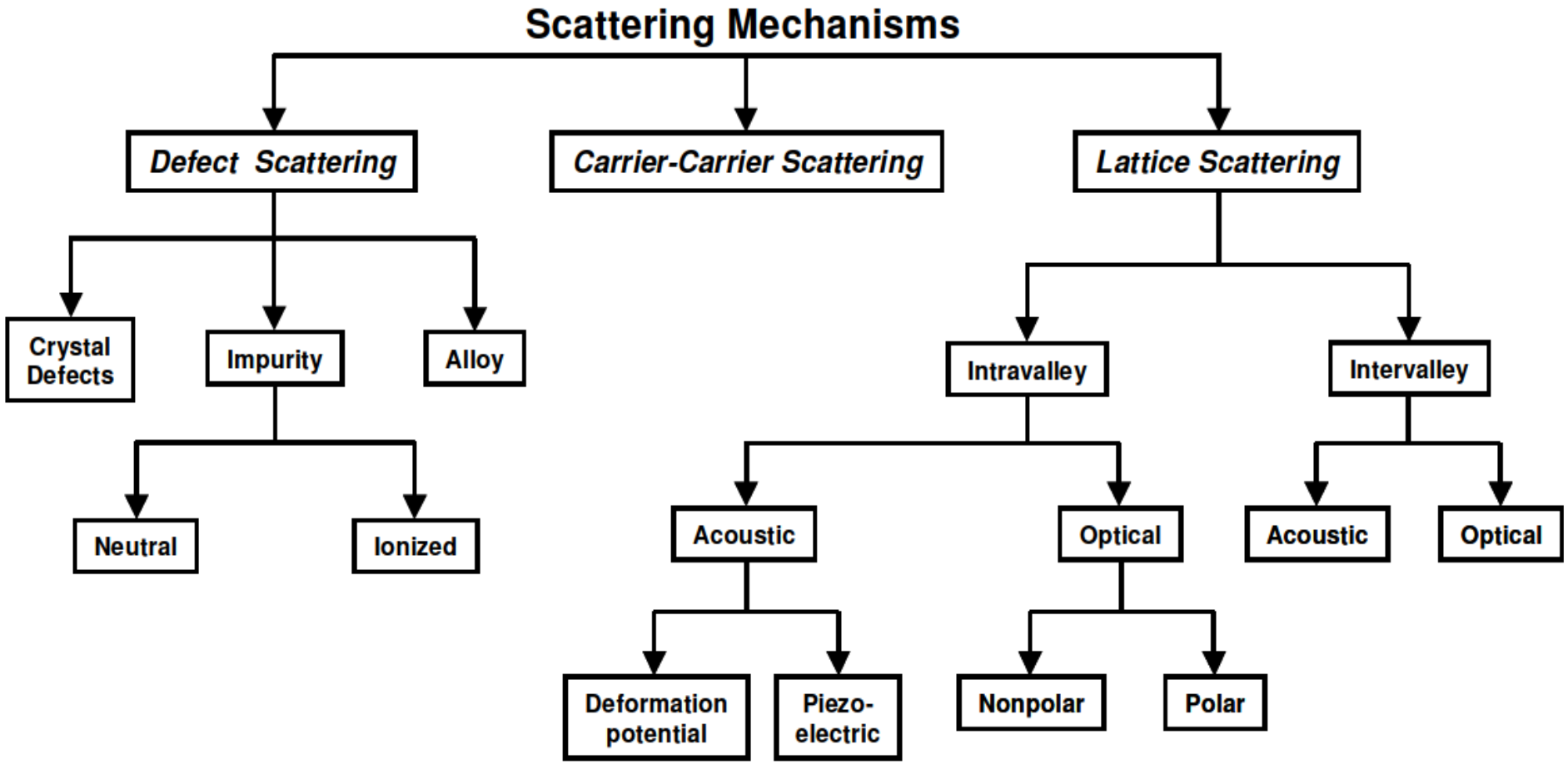
- Assuming instantaneous collisions (*scattering events*) which take particles from **k** to **k′** (*out scattering*) or from **k′** to **k** (*in scattering*), the BTE becomes:

$$\frac{\partial f_k}{\partial t} + \frac{1}{\hbar}\nabla_k E \cdot \nabla_r f_k + \frac{\mathbf{F}}{\hbar}\nabla_k f_k = \frac{V}{8\pi^3}\int d\vec{k}' \left\{ \underbrace{f_{k'}\left[1 - f_k\right]\Gamma_{k'k}}_{\text{in scattering}} - \underbrace{f_k\left[1 - f_{k'}\right]\Gamma_{kk'}}_{\text{out scattering}} \right\}$$



- The quantity $\Gamma_{kk'}$ is the transition rate (scattering rate, dimension 1/s) per particle from **k** to **k′**
- The square brackets take into account Pauli's exclusion principle

4. Beyond drift-diffusion: the BTE



4. Beyond drift-diffusion: from BTE to HD

Moments of the distribution function $f(\mathbf{r},\mathbf{k},t)$ give us information about particle concentration, current density, average energy…

$$M_0 = \int_k f\left(\vec{k},\vec{r},t\right)\mathrm{d}\vec{k} = n\left(\vec{r},t\right)$$

$$M_1 = \int_k \vec{k}\, f\left(\vec{k},\vec{r},t\right)\mathrm{d}\vec{k} \propto n\left\langle \vec{p}_n \right\rangle \propto J_n\left(\vec{r},t\right)$$

$$M_2 = \int_k k^2 f\left(\vec{k},\vec{r},t\right)\mathrm{d}\vec{k} \propto n\left\langle E_n \right\rangle$$

$$M_3, M_4 \ldots M_\infty$$

(for parabolic valleys, $\vec{p} = \hbar\vec{k} = m^*\vec{v}$ and $E = \hbar^2 k^2 / 2m^*$)

4. Beyond drift-diffusion: from BTE to HD

Generalized moments of *i*-th order over *k* space of the BTE give us equations involving moments of the distribution function up to order *i*+1. For orders 0 through 2 we get:

$$\int_k (\mathrm{BTE})\mathrm{d}\vec{k} \rightarrow M_0, M_1 : n, \vec{p}_n$$

$$\int_k \vec{k}(\mathrm{BTE})\mathrm{d}\vec{k} \rightarrow M_0, M_1, M_2 : n, \vec{p}_n, E_n$$

$$\int_k k^2(\mathrm{BTE})\mathrm{d}\vec{k} \rightarrow M_0, M_1, M_2, M_3 : n, \vec{p}_n, E_n, Q_n$$

i.e.,

- a continuity (conservation) equation for the charge density n
- a transport equation for the momentum p_n
- a conservation equation for the kinetic energy E_n

(M_3 is related to the heat flow due to electrons Q_n.)

4. Beyond drift-diffusion: from BTE to HD

As an example, we may evaluate the components of the 0th order moment over *k* space of the BTE:

$$\frac{\partial f_k}{\partial t} + \vec{v}_g \cdot \nabla_r f_k + \frac{\vec{F}}{\hbar} \cdot \nabla_k f_k = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}} + \left.\frac{\partial f}{\partial t}\right|_{\text{G-R}}$$

$$\int_k \frac{\partial f\left(\vec{k},\vec{r},t\right)}{\partial t} \mathrm{d}\vec{k} = \frac{\partial}{\partial t}\int_k f\left(\vec{k},\vec{r},t\right)\mathrm{d}\vec{k} = \frac{\partial}{\partial t} n\left(\vec{r},t\right)$$

4. Beyond drift-diffusion: from BTE to HD

As an example, we may evaluate the components of the 0th order moment over *k* space of the BTE:

$$\frac{\partial f_k}{\partial t} + \vec{v}_g \cdot \nabla_r f_k + \frac{\vec{F}}{\hbar} \cdot \nabla_k f_k = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}} + \left.\frac{\partial f}{\partial t}\right|_{\text{G-R}}$$

$$\int_k \vec{v}_g(k) \cdot \nabla_r f\left(\vec{k}, \vec{r}, t\right) \mathrm{d}\vec{k} =$$

$$= \nabla_r \cdot \int_k \vec{v}_g(k) f\left(\vec{k}, \vec{r}, t\right) \mathrm{d}\vec{k} = \nabla_r \cdot \left(n\left(\vec{r}, t\right)\vec{v}\right)$$

4. Beyond drift-diffusion: from BTE to HD

As an example, we may evaluate the components of the 0th order moment over *k* space of the BTE:

$$\frac{\partial f_k}{\partial t} + \vec{v}_g \cdot \nabla_r f_k + \frac{\vec{F}}{\hbar} \cdot \nabla_k f_k = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}} + \left.\frac{\partial f}{\partial t}\right|_{\text{G-R}}$$

$$\int_k \frac{\mathbf{F}}{\hbar} \cdot \nabla_k f\left(\vec{k},\vec{r},t\right) \mathrm{d}\vec{k} = -\frac{\mathbf{F}}{\hbar} \cdot \int_k \left(\nabla_k 1\right) f\left(\vec{k},\vec{r},t\right) \mathrm{d}\vec{k} = 0$$

4. Beyond drift-diffusion: from BTE to HD

As an example, we may evaluate the components of the 0th order moment over *k* space of the BTE:

$$\frac{\partial f_k}{\partial t} + \vec{v}_g \cdot \nabla_r f_k + \frac{\vec{F}}{\hbar} \cdot \nabla_k f_k = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}} + \left.\frac{\partial f}{\partial t}\right|_{\text{G-R}}$$

The integral of the collision term is the variation of the (spatial) density of carriers in *k* space, i.e. the net recombination rate:

$$U_n = -\left.\frac{\partial f}{\partial t}\right|_{G-R}$$

4. Beyond drift-diffusion: from BTE to HD

Hence, the 0th order moment over *k* space of the BTE gives us the continuity (conservation) equation for the electron (or hole) density:

$$\int_k \left(\mathrm{BTE}\right)\mathrm{d}\vec{k} \;\rightarrow\; \frac{\partial n}{\partial t} + \nabla\cdot\left(n\vec{v}_n\right) = -U_n$$

which involves both carrier density and average velocity. Hence, we need *an additional closure relation*. The standard choice is a constitutive equation for the velocity as a function of the other quantities, leading to the drift-diffusion description:

$$n\vec{v}_n \propto \mathbf{J}_n\left(\vec{r},t\right) \;\Rightarrow\; \mathbf{J}_n/q = \underbrace{n\mu_n\mathcal{E}}_{\textit{drift}} + \underbrace{D_n\nabla n}_{\textit{diffusion}}$$

where the electric field is determined through Poisson's equation, and two critical parameters (*mobility* and *diffusivity*) are introduced. As an alternative, one may take into account higher-order moments of the BTE.

4. Beyond drift-diffusion: from BTE to HD

The moments of the 1st and 2nd order yield 2 more transport equations, one for the momentum and one for the energy:

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot \left(n\vec{v}_n \right) = -U_n \\ \dfrac{\partial \vec{p}_n}{\partial t} + \dfrac{1}{n}\nabla\left(nk_B T_e \right) + \left(\vec{v}_n \cdot \nabla \right)\vec{p}_n + q\vec{\mathcal{E}} = -\dfrac{\vec{p}_n}{\tau_{\vec{p}n}\left(E \right)} \\ \dfrac{\partial E_n}{\partial t} + \vec{v}_n \cdot \nabla E_n + \dfrac{1}{n}\nabla \cdot \left(n\vec{v}_n k_B T_e \right) + \dfrac{1}{n}\nabla \cdot \vec{Q}_n = -q\vec{v}_n \cdot \vec{\mathcal{E}} - \dfrac{E_n - E_0}{\tau_{En}\left(E \right)} \end{cases}$$

Assume an electric field as the only external force

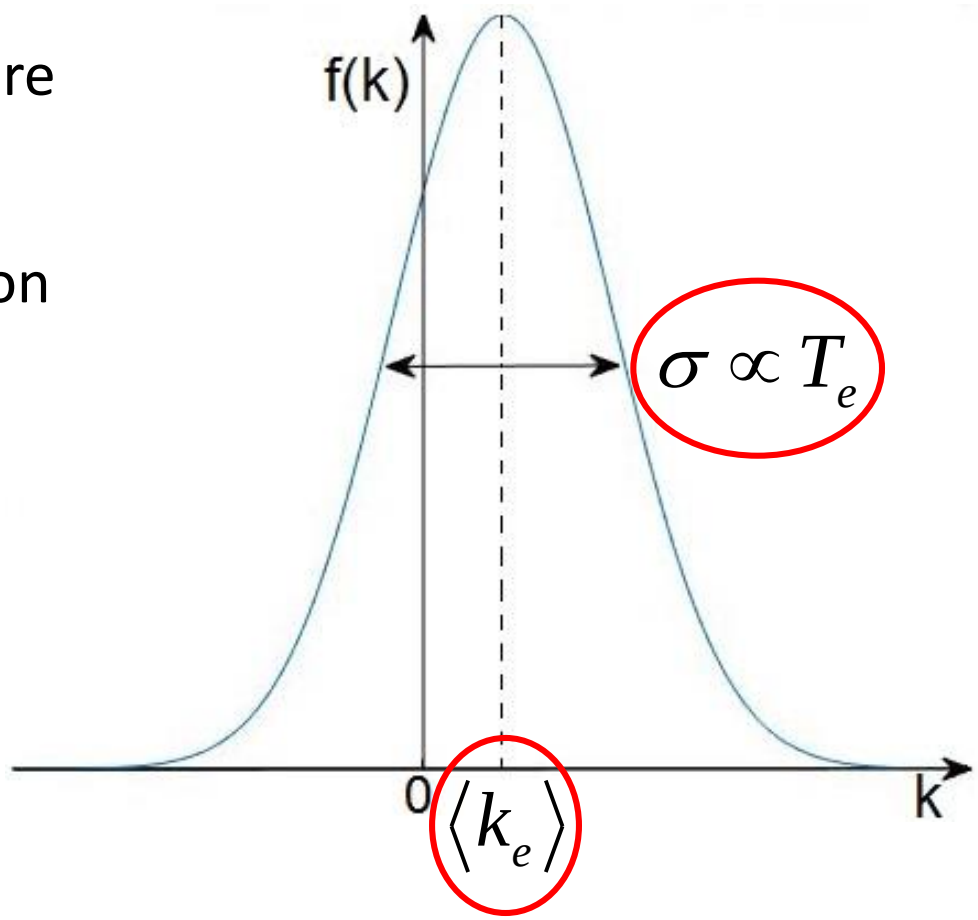
Joule effect

where a relaxation time approximation has been introduced for both energy and momentum. This *hydrodynamic* (HD) model is completed by the three corresponding equations for holes + Poisson equation (quasi static approximation for the electromagnetic field) + another *closure* relation.

4. Beyond drift-diffusion: the drifted Gaussian

The term T_e refers to the temperature of a gas of electrons; if, out of equilibrium, we assume a *«drifted» Gaussian distribution* for the electron gas, then the mean energy of the carriers is given by

$$E_e = \frac{h^2 k_e^{\ 2}}{2m_e^{\ *}} + \frac{3}{2} k_B T_e$$



where the first term is the kinetic energy due to external forces (electric fields) causing the electrons to drift, while the second is the disordered thermal energy.

4. Beyond drift-diffusion: energy balance

To make things more manageable, since the relaxation time of momentum τ_{pn} is shorter than τ_{En}, the transport equation for p_n may be assumed to be at equilibrium ($\partial p_n/\partial t \approx 0$):

$$\frac{\partial n}{\partial t} + \nabla \cdot \left(n\vec{v}_n \right) = -U_n$$

$$\frac{\partial \vec{p}_n}{\partial t} + \frac{1}{n}\nabla\left(nk_B T_e \right) + \left(\vec{v}_n \cdot \nabla \right)\vec{p}_n + q\vec{\mathcal{E}} = -\frac{\vec{p}_n}{\tau_{\vec{p}n}\left(E \right)}$$

$$\frac{\partial E_n}{\partial t} + \vec{v}_n \cdot \nabla E_n + \frac{1}{n}\nabla \cdot \left(n\vec{v}_n k_B T_e \right) + \frac{1}{n}\nabla \cdot \vec{Q}_n = -q\vec{v}_n \cdot \vec{\mathcal{E}} - \frac{E_n - E_0}{\tau_{En}\left(E \right)}$$

becoming an algebraic equation:

$$\left(1 + \tau_{\vec{p}n}\vec{v}_n \cdot \nabla \right)\vec{v}_n \approx -\frac{q\tau_{\vec{p}n}}{m^*}\vec{\mathcal{E}} - \frac{\tau_{\vec{p}n}}{m^* n}\nabla\left(nk_B T_e \right)$$

4. Beyond drift-diffusion: energy balance

The resulting *energy balance* (EB) model is:

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot (n\vec{v}_n) = -U_n \\ \dfrac{\partial E_n}{\partial t} + \vec{v}_n \cdot \nabla E_n + \dfrac{1}{n}\nabla \cdot (n\vec{v}_n k_B T_e) + \dfrac{1}{n}\nabla \cdot \vec{Q}_n = -q\vec{v}_n \cdot \vec{\mathcal{E}} - \dfrac{E_n - E_0}{\tau_{En}} \end{cases}$$

where the velocity includes a drift and a diffusion term (dependent on the carrier density gradient)

$$\vec{v}_n \approx \overbrace{-\mu_n(E_n) \times (\vec{\mathcal{E}} + \frac{k_B}{q}\nabla T_e)}^{\text{drift term}} \overbrace{- \frac{\mu_n(E_n)}{n} D_n(E_n)\nabla n}^{\text{diffusion term}}$$

4. Beyond drift-diffusion: closure

In both HD and EB, a closure equation must be introduced due to the presence of the *heat flow* Q (related to the 3rd order moment of the BTE) in the transport equation for the energy (2nd order moment). The relation usually adopted for approximating the heat flow is:

$$\vec{Q}_n \approx -\kappa_n \nabla T_e$$

where the thermal conductivity of the electron gas κ is often assumed to be proportional to the electrical conductivity σ through the Wiedemann-Franz law:

$$\kappa_n = \frac{\pi^2}{3}\left(\frac{k_B}{q}\right)^2 T_e \sigma_n$$

4. Beyond drift-diffusion: velocity overshoot

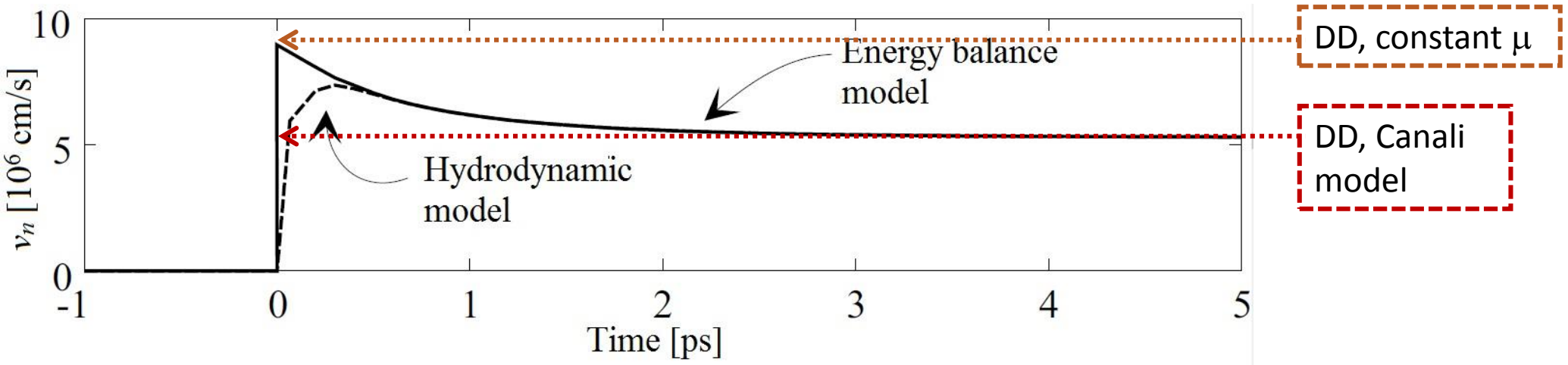
Advantages of the HD/EB models:

- Mobility and diffusivity are not constant (or, at best, instantaneous local functions of the electric field) anymore, but become functions of the spatial distribution of the carrier energy

- Very short transients, as well as abrupt changes of potential and electric field, may be accurately described, but care must be taken in dealing with possibly spurious *velocity overshoot* effects

4. Beyond drift-diffusion: velocity overshoot

If, at t=0, the electric field is abruptly increased, the EB model assumes carrier velocity to be at its steady-state value, hence v_n is computed by using the initial (low field) carrier mobility.

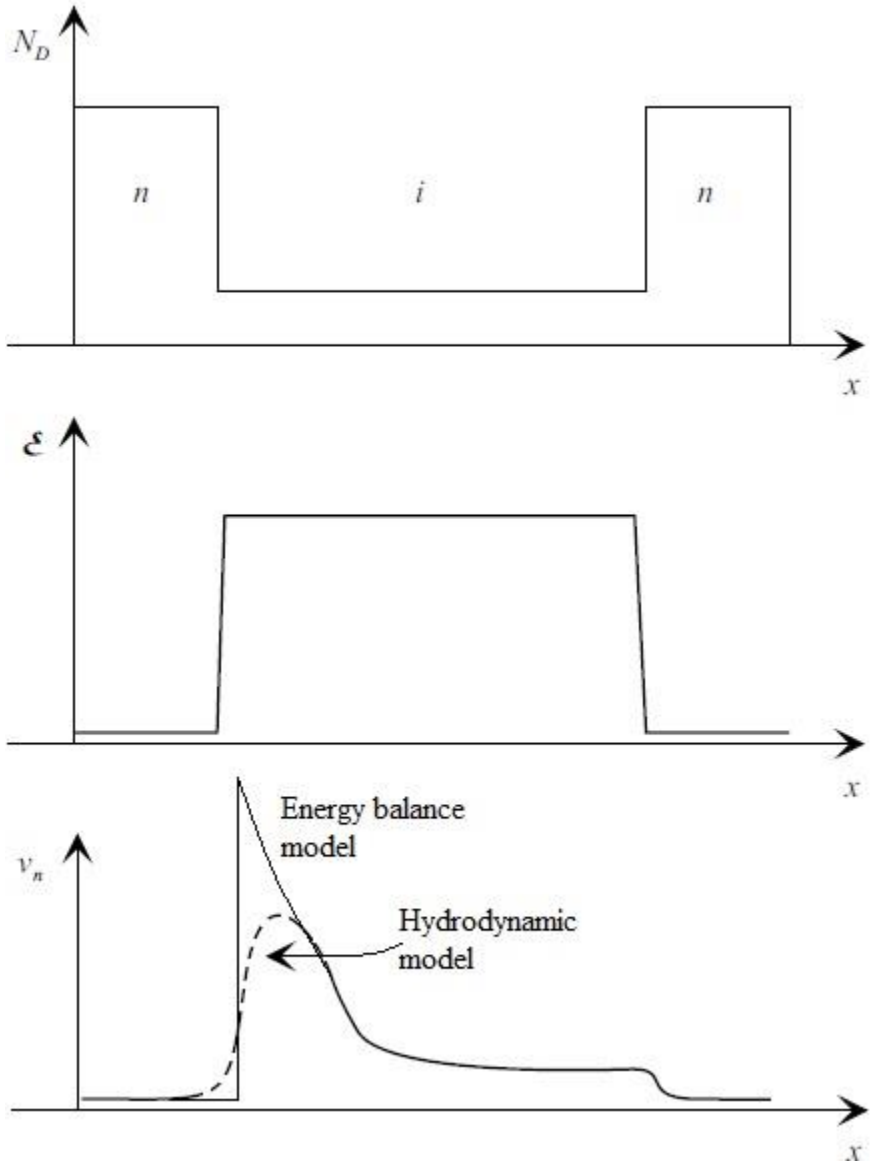


As the energy increases (energy transport equation), though, the mobility (and thus v_n) decreases. The result is a *velocity overshoot*, not present when considering also the dynamics of carrier momentum (HD model).

4. Beyond drift-diffusion: velocity overshoot

Another case that emphasizes such EB limitation appears in abrupt *nin* (and *pin*) junctions; the electric field is rather low in the doped regions and raises quickly at the intrinsic region boundaries, with an almost step-like spatial profile.

Here again the EB model predicts an abrupt velocity profile and a significant overshoot, while the HD model yields a more realistic, gradual behaviour.



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5. Limits of the drifted Gaussian

Disadvantages of the HD/EB models:

i. The solution of the HD system is intrinsically more difficult (the PDEs are not elliptic)

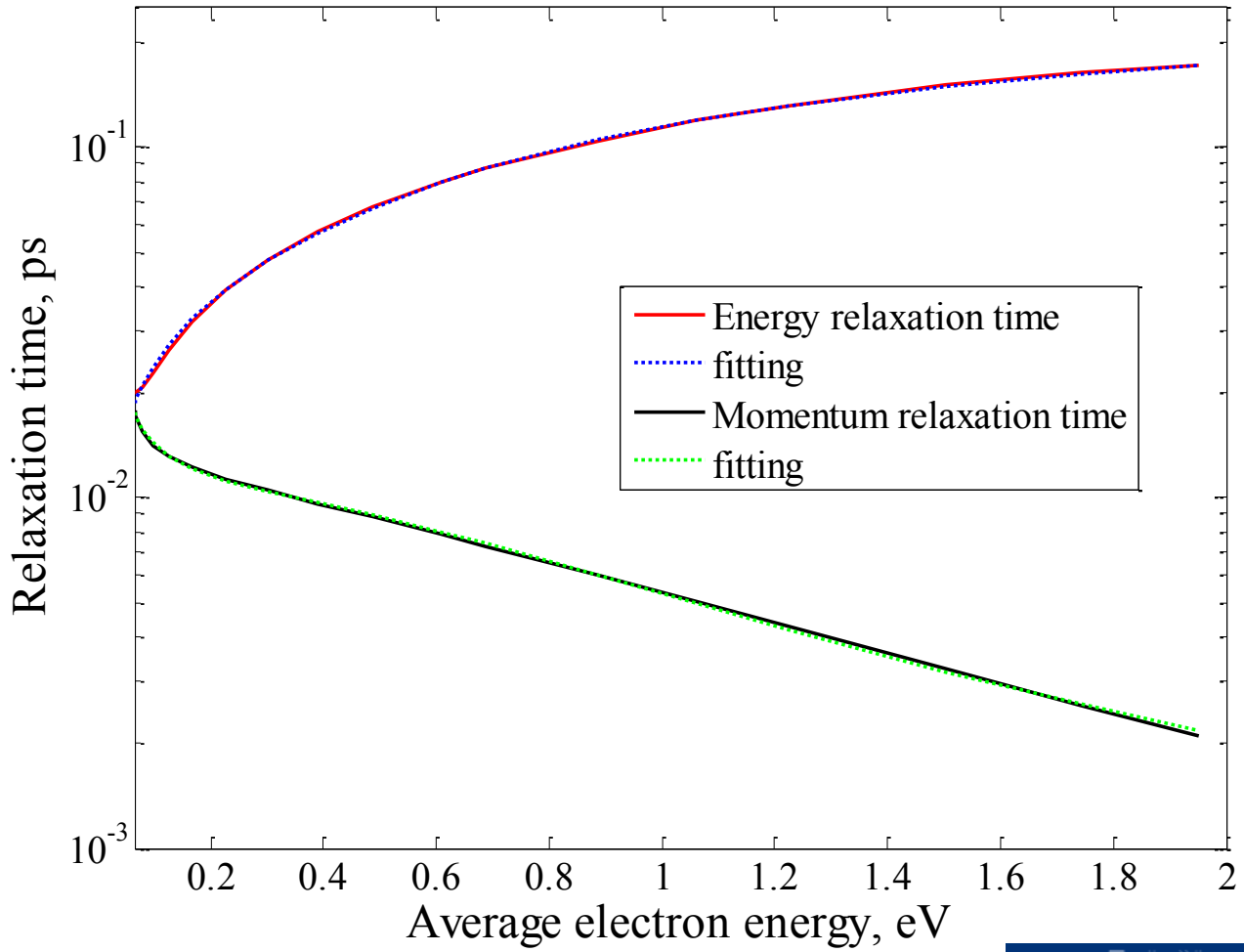
5. Limits of the drifted Gaussian

Disadvantages of the HD/EB models:

ii. Several additional parameters have to be defined; the most critical are probably the energy and momentum relaxation times, which are functions of the carrier energy, and whose determination usually relies on Monte Carlo simulations

$$\tau_E(\bar{E}) = \frac{\bar{E} - \bar{E}_0}{q\mathcal{E}v_n(\bar{E})}$$

$$\tau_m(\bar{E}) = \frac{m(\bar{E})v_n(\bar{E})}{q\mathcal{E}}$$

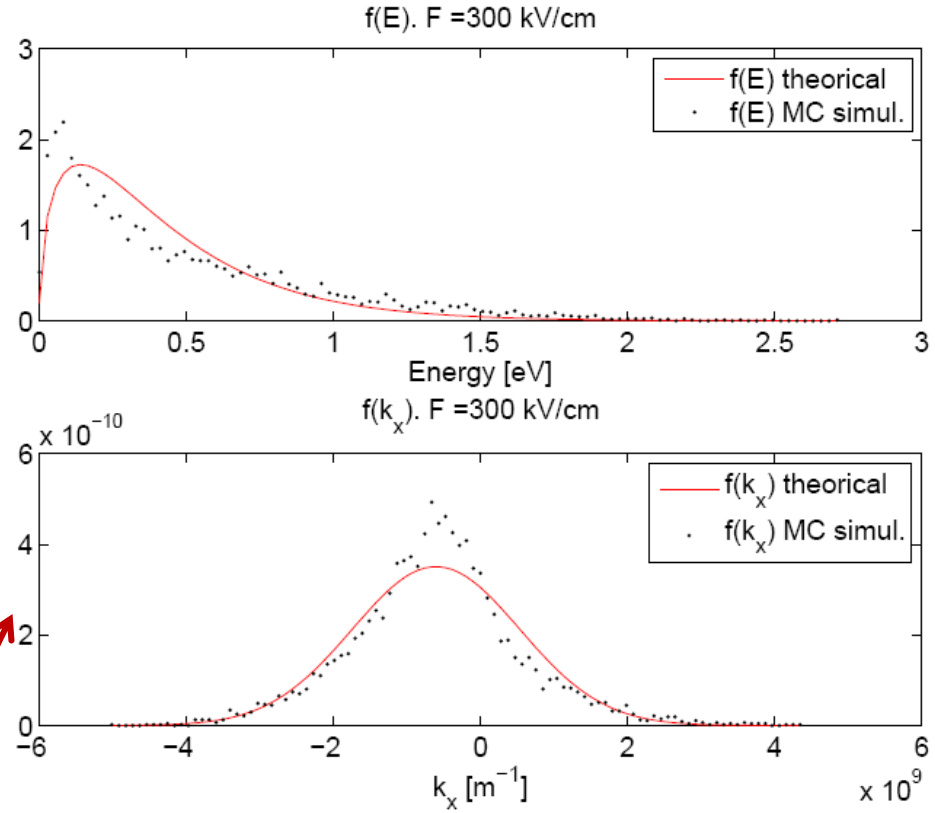


[ZnO, Solid-State Electron. **52**, 1796, 2008]

5. Limits of the drifted Gaussian

Disadvantages of the HD/EB models:

iii. The definition of a carrier temperature is unequivocal only for classical particles with a perfectly parabolic dispersion relation: for realistic electrons/holes, one gets different T_e values from the Maxwellian-like *f(E)* and from the Gaussian-like *f(k)*



$$f(E) = \frac{2}{\sqrt{\pi}}\left(\frac{1}{k_B T}\right)^{\frac{3}{2}} \sqrt{E}\,\exp\left(-\frac{E}{k_B T}\right)$$

$$\overline{E} = \int_0^{+\infty} E f(E) dE = \frac{3}{2} k_B T_e + \frac{\hbar^2 k_i^2}{2 m_n^*}$$

$$T_e = \frac{2}{3 k_B}\left(\overline{E} - \frac{\hbar^2 k_i^2}{2 m_n^*}\right)$$

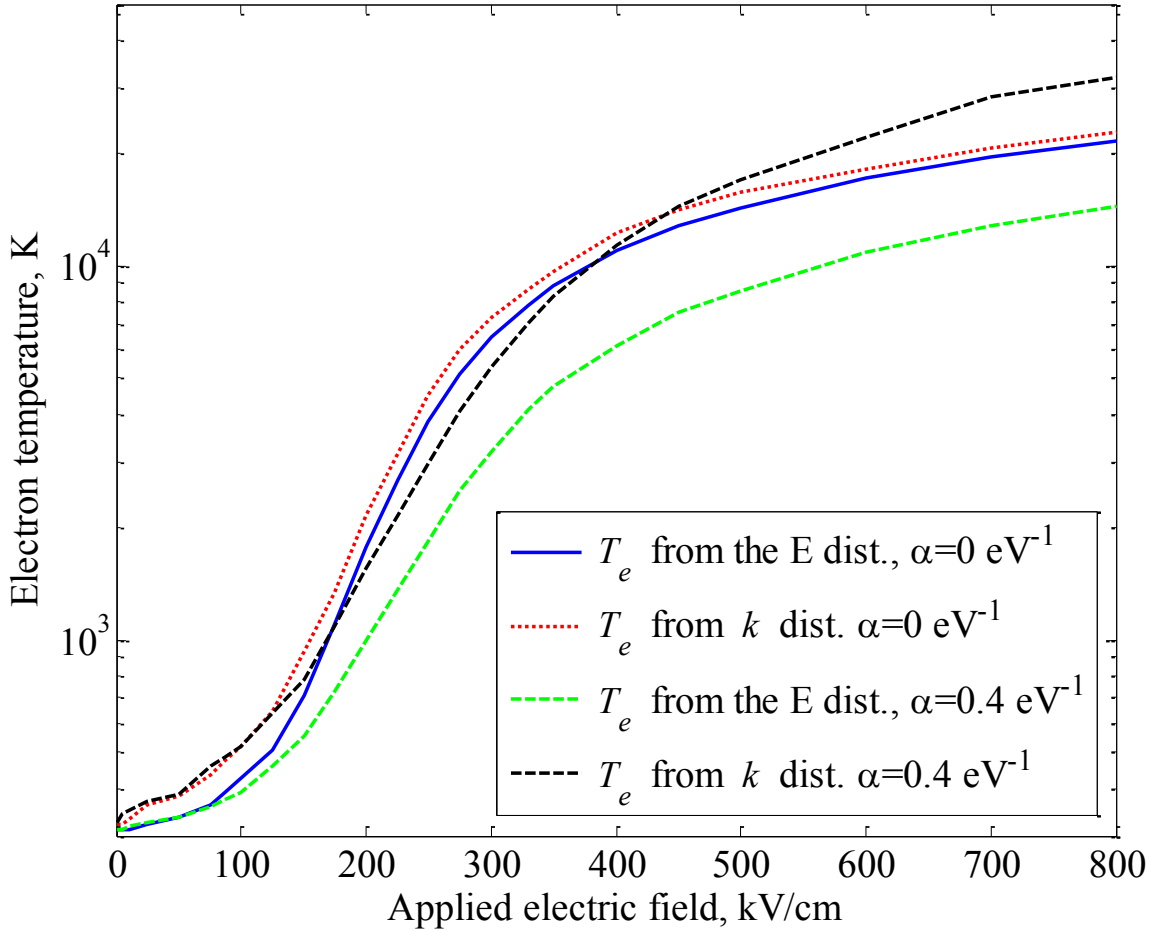
$$f(k_i) = \sqrt{\frac{\hbar^2}{2 m_n^* \pi k_B T}}\,\exp\left(-\frac{\hbar^2 k_i^2}{2 m_n^* k_B T}\right)$$

$$\sigma^2 = \frac{m_n^* k_B T_e}{\hbar^2} \quad \rightarrow \quad T_e = \frac{\hbar^2 \sigma^2}{m_n^* k_B}$$

5. Limits of the drifted Gaussian

Disadvantages of the HD/EB models:

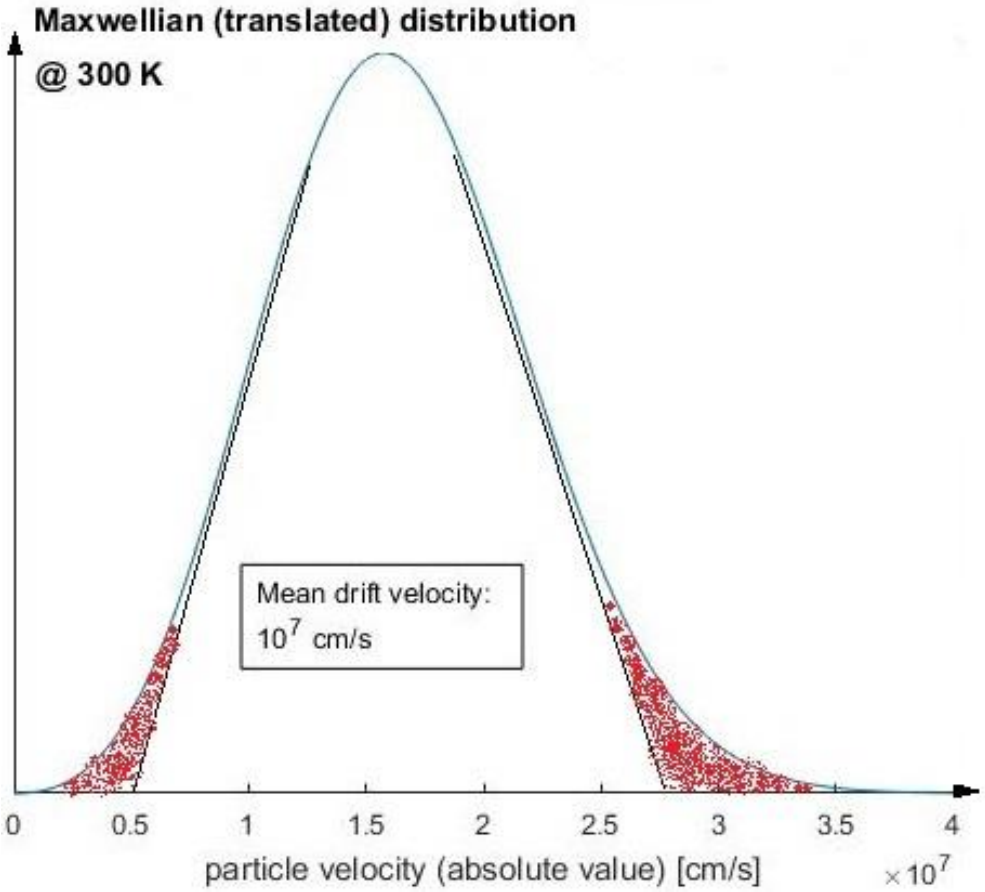
iii. The definition of a carrier temperature is unequivocal only for classical particles with a perfectly parabolic dispersion relation: for realistic electrons/holes, one gets different T_e values from the Maxwellian-like *f(E)* and from the Gaussian-like *f(k):* here is an example for ZnO when nonparabolicity is taken into account



[Solid-State Electron. **52**, 1796, 2008]

5. Limits of the drifted Gaussian

What's worse, there are several important cases where the HD model does not provide a satisfactory solution of the BTE, e.g.:

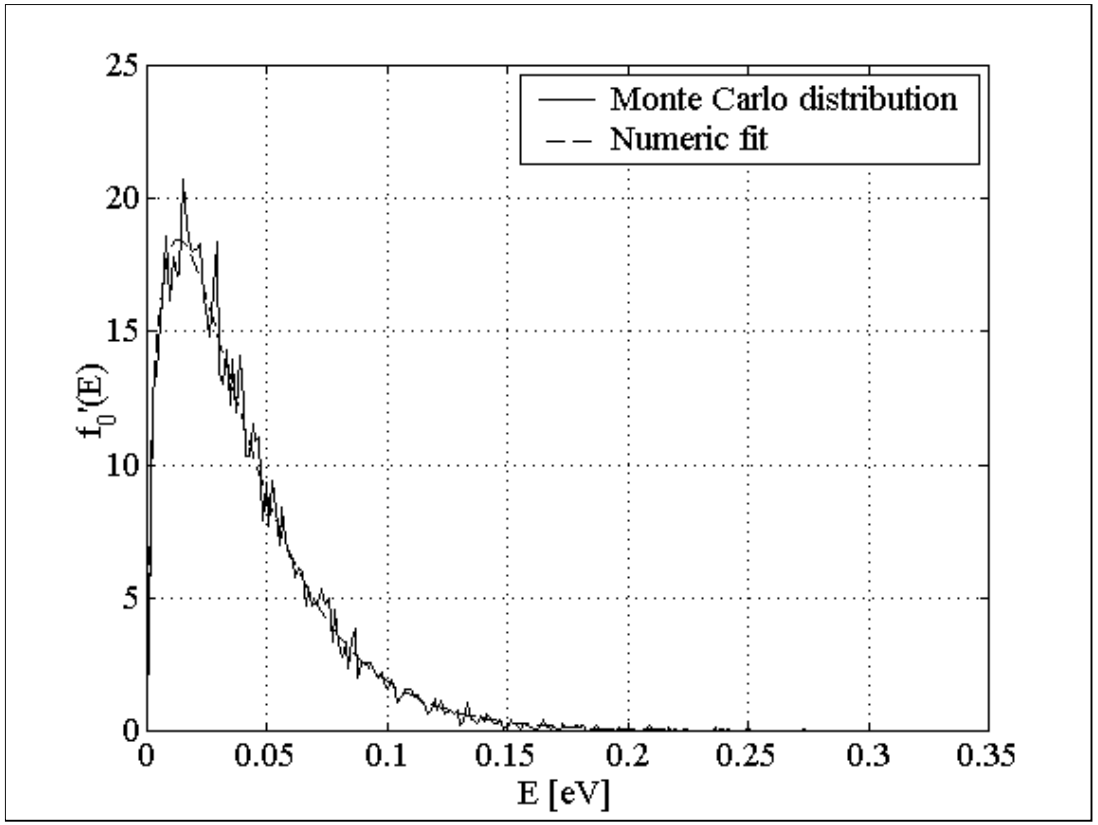


- when phenomena due to high energy tails are relevant, as in the analysis of avalanche breakdown (or tunneling through the oxide of a MOSFET)
- when the carrier distribution is very different from a Maxwellian

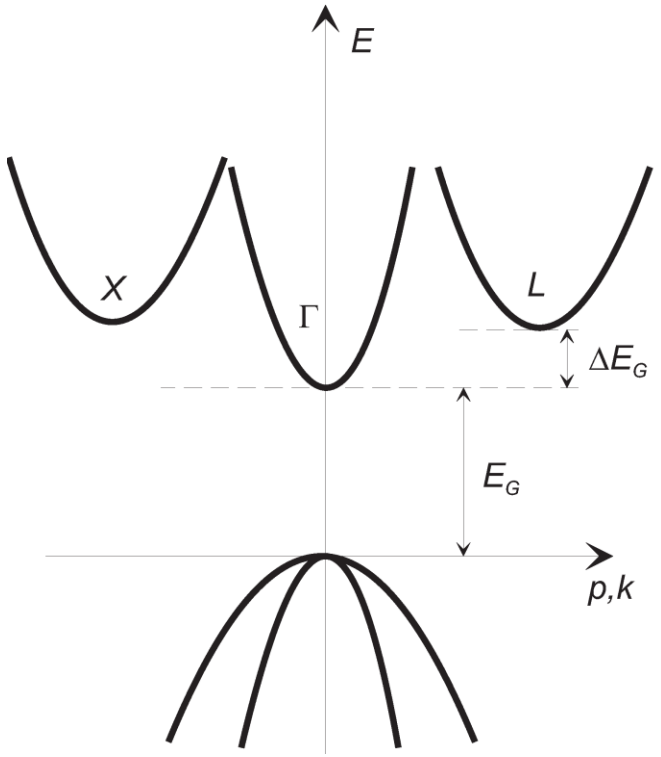
5. Limits of the drifted Gaussian

The shape of the distribution function may be significantly different from a Maxwellian in several circumstances, e.g. near heterojunctions, or under high fields in multivalley semiconductors: when intervalley scattering becomes significant, the distribution becomes bimodal, as shown in the following Monte Carlo simulations.

Energy distribution in GaAs vs. applied field



- 0 kV/cm



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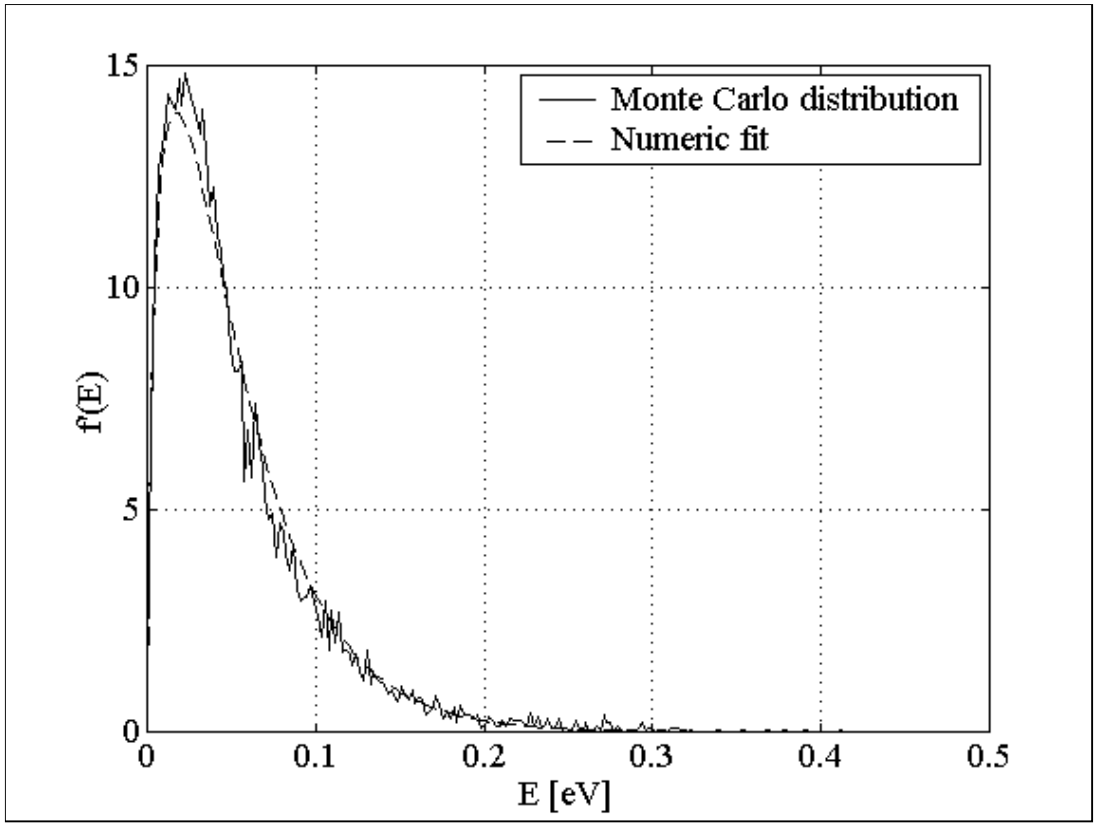
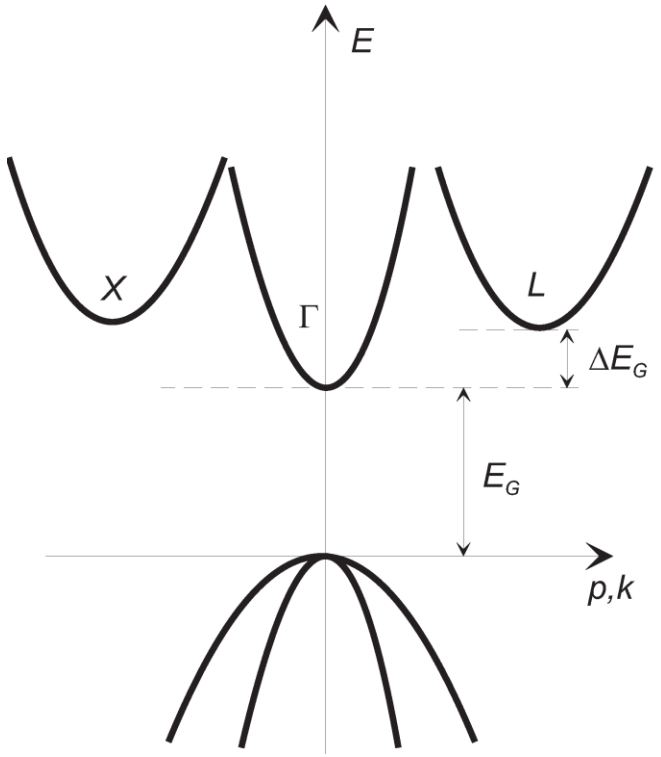


- 2 kV/cm



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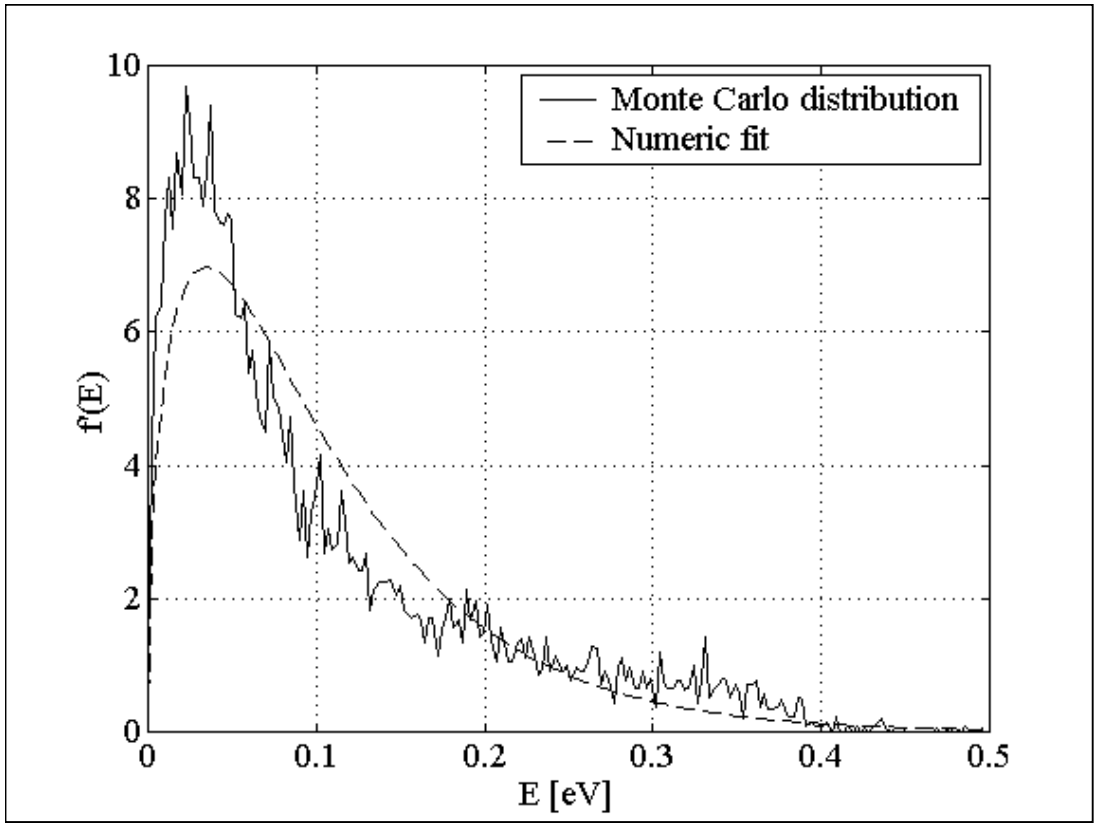
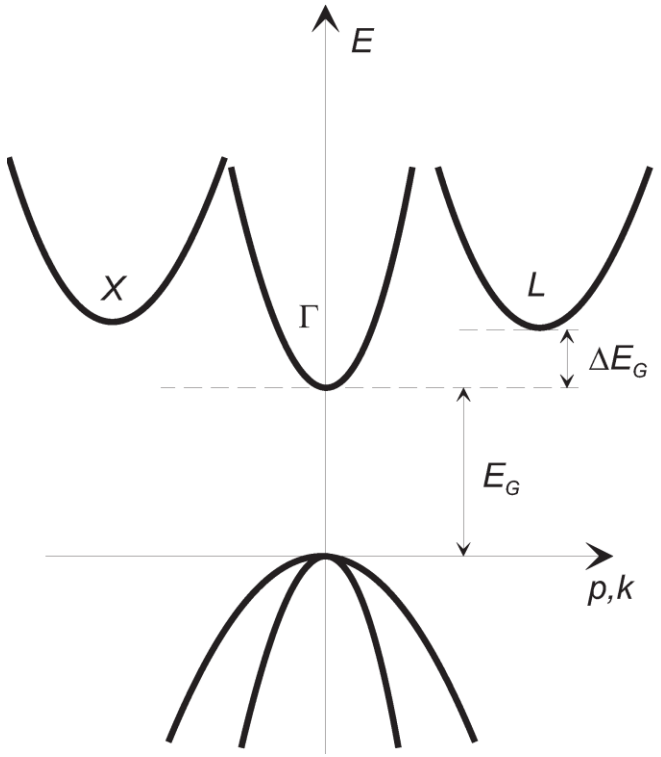


- 4 kV/cm



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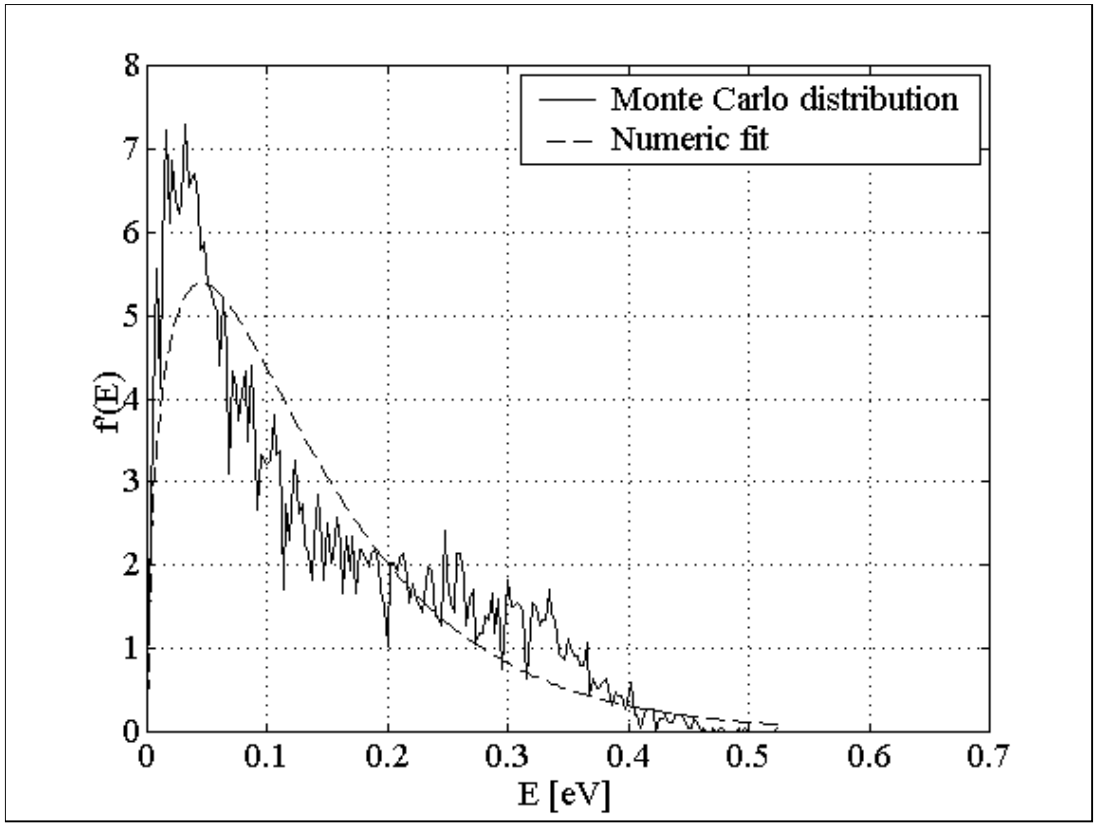
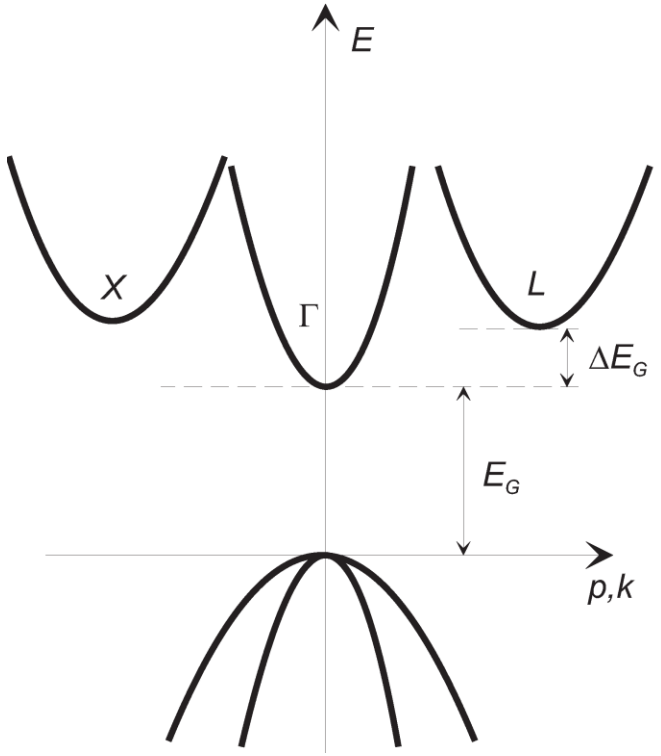


- 5 kV/cm



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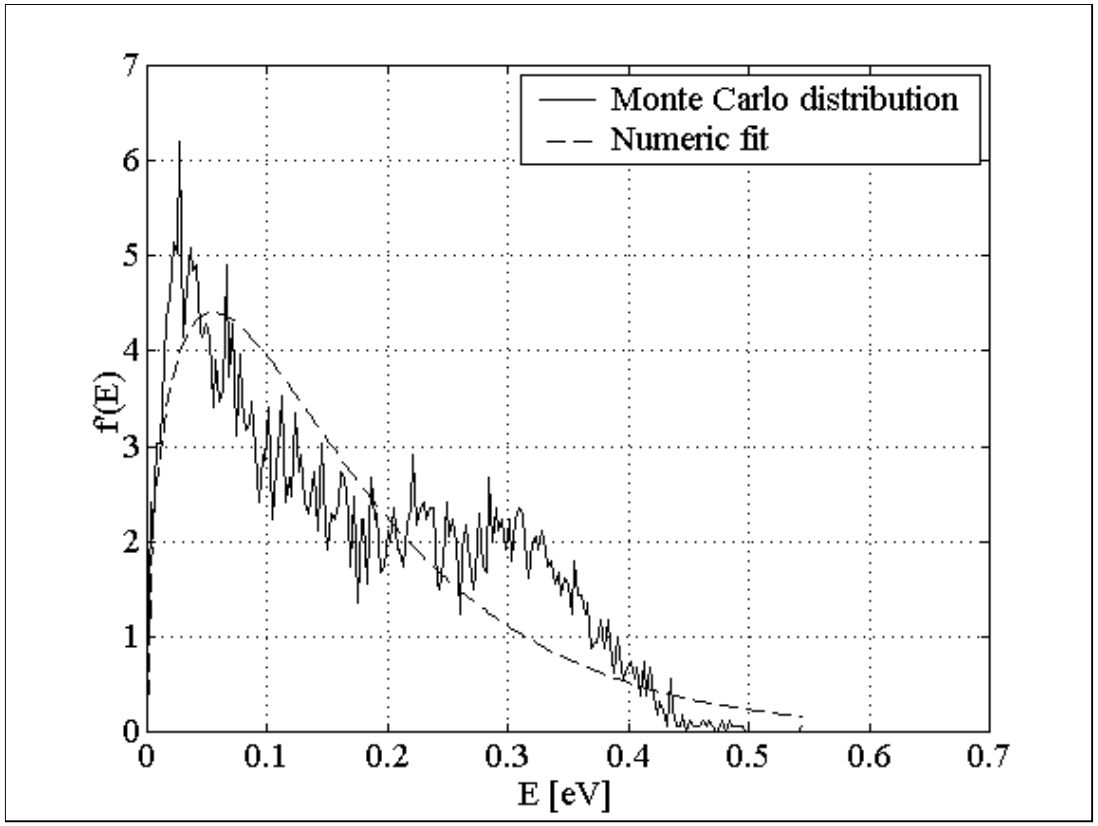
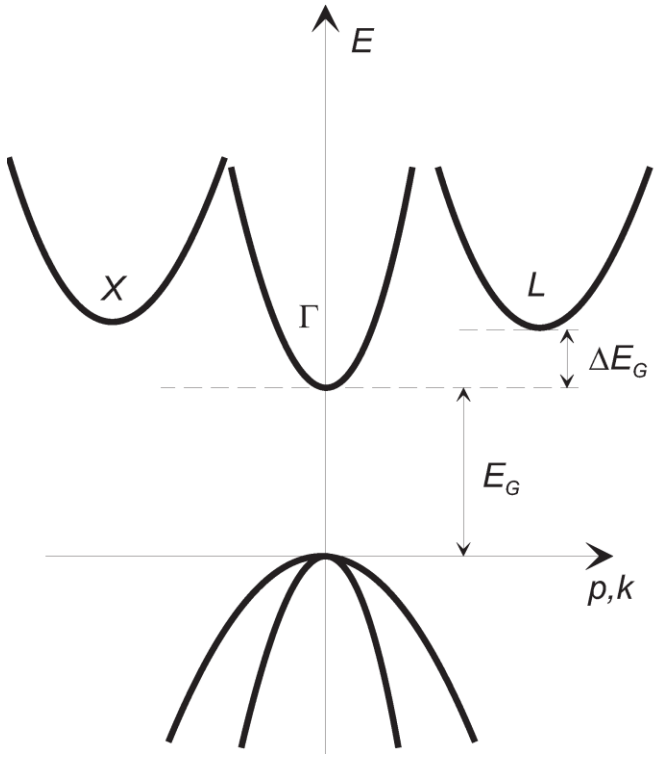


- 6 kV/cm



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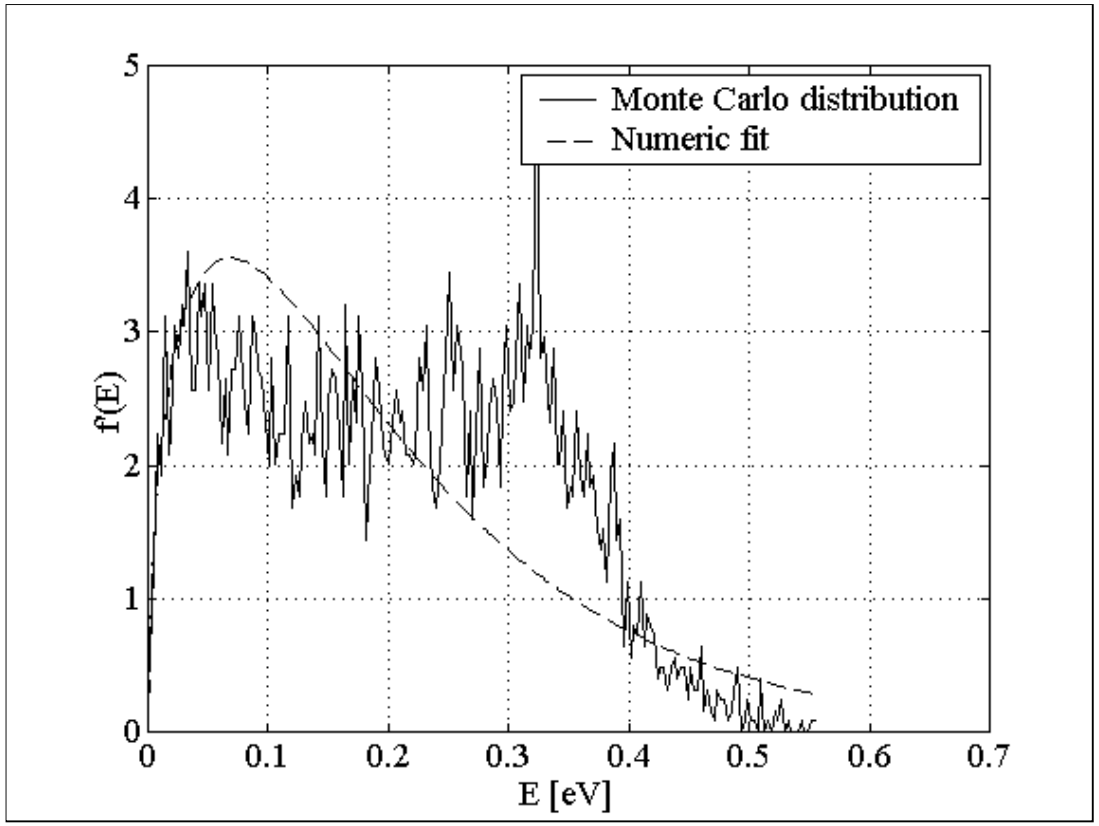
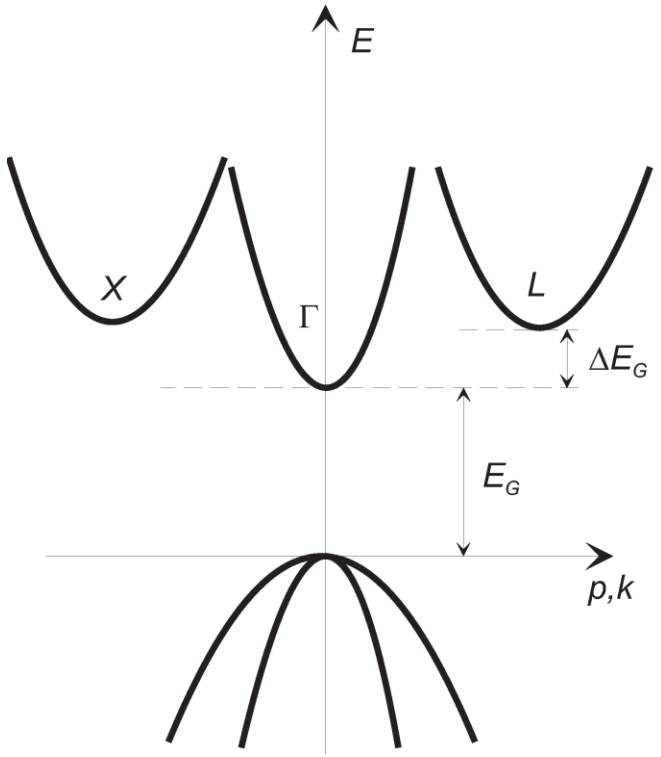


- 8 kV/cm



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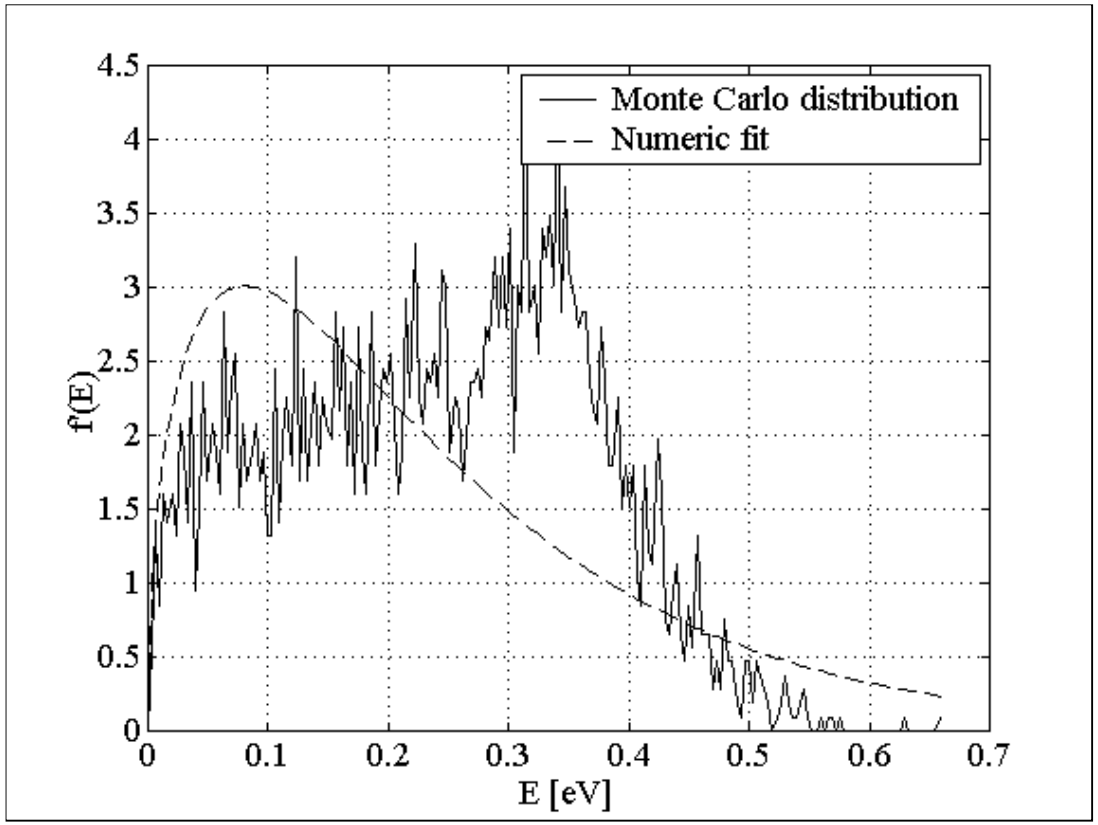
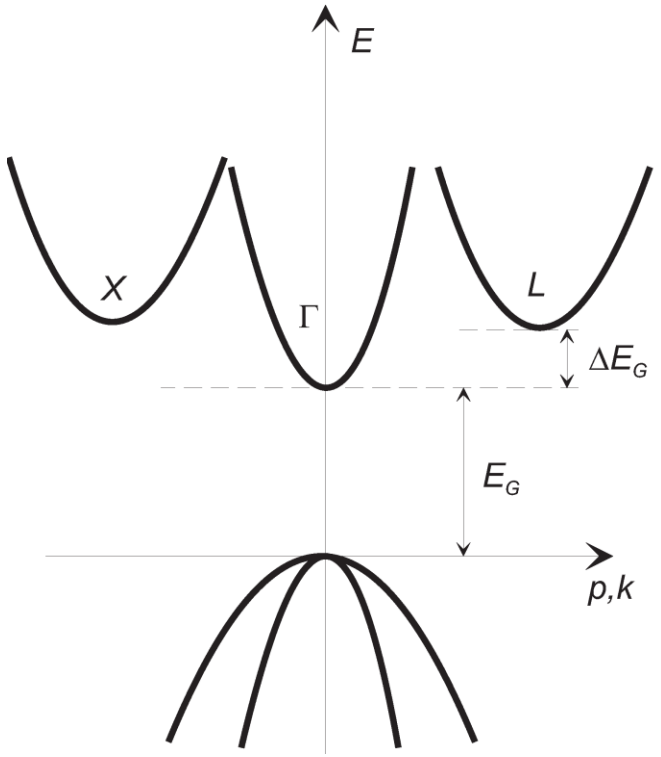


- 12 kV/cm



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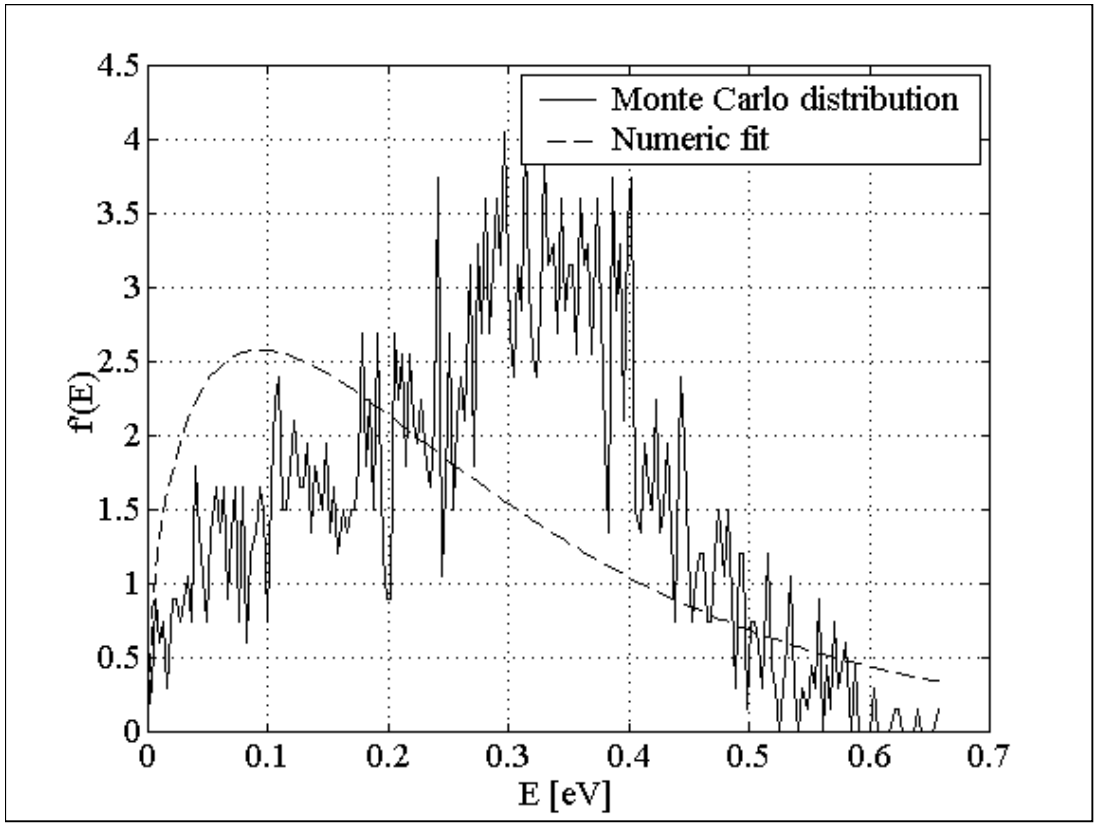


- 20 kV/cm

Intervalley scattering

Non-Maxwellian distributions

The T_e concept (heated Maxwellian) becomes questionable...

5. Limits of the drifted Gaussian

The verdict about HD/EB:

- probably unsuited for most direct-gap compound semiconductors, because of many-valley effects (e.g. GaAs) and nonparabolicity (e.g. ZnO)
- could be worth considering for indirect-gap semiconductors (e.g., Si and Ge)
- validation against Monte Carlo simulations is always highly recommended

Outline

1. Introduction
2. The basics
3. Hot electrons and the drift-diffusion model
4. Beyond drift-diffusion
5. Limits of the drifted Gaussian
6. Monte Carlo transport simulation
7. Conclusions

6. Monte Carlo transport simulation

Advantages:

- Many physicists are already familiar with Monte Carlo techniques devised for the simulation of trajectories in solids to describe the radiation-matter interaction (did we mention MCNP, Geant, etc?)

- Direct solution of the BTE: no simplifying assumptions on the distribution function

- Ability to perform numerical experiments starting with arbitrary distributions: ideally suited for matching e.g. the results of time-resolved photoluminescence spectroscopy, where carriers are excited by high energy optical probes. (The analogy with other high energy excitations is obvious ;-)

6. Monte Carlo transport simulation: taxonomy

Possible classification of Monte Carlo approaches for transport in semiconductors:

- Single particle: applicable if the history of a particle is equivalent to the history of any other particle in the system $\Leftrightarrow$ ergodicity

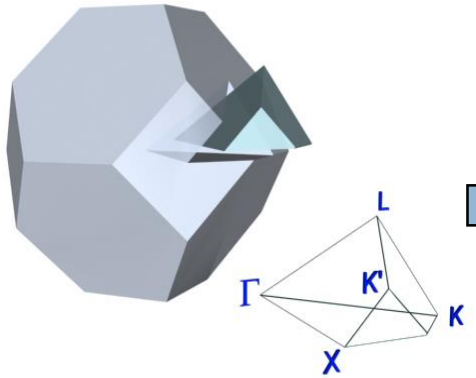
- Ensemble: allows for the selfconsistent solution of Poisson's equation $\Rightarrow$ usually required for device-level simulation

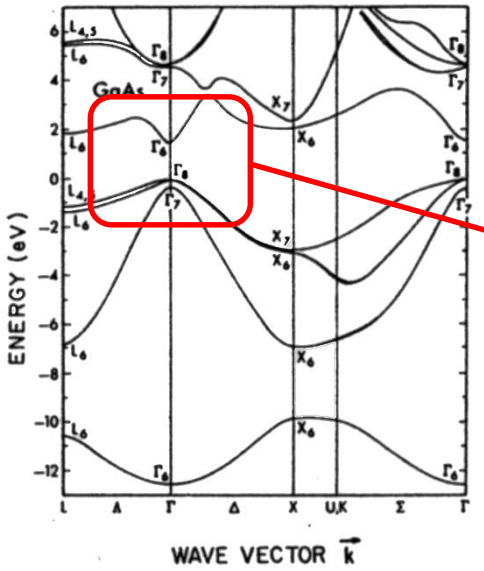
6. Monte Carlo transport simulation: taxonomy

Possible classification of Monte Carlo approaches for transport in semiconductors:

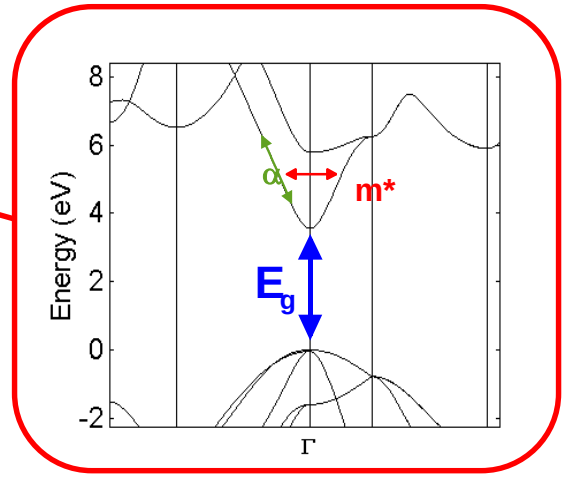
- Analytic-band: effective mass approximation in a number of nonparabolic valleys

Irreducible wedge

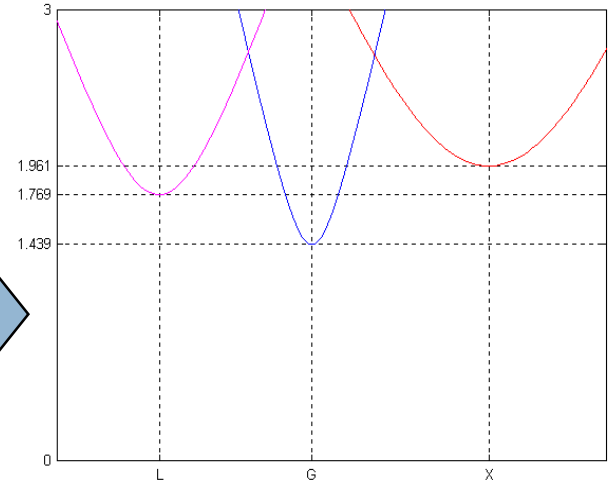




Parameter extraction for each valley



Approximate electronic structure

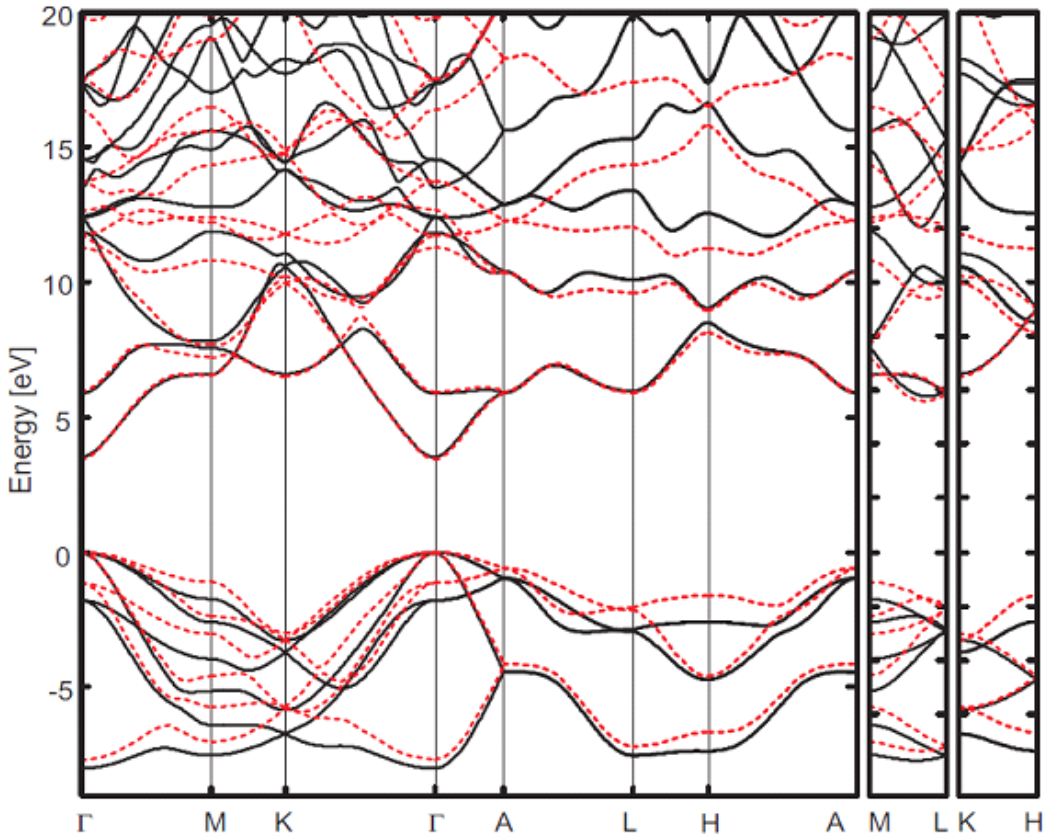


$$E(1+\alpha E) = \frac{h^2 k^2}{2m^*}$$

6. Monte Carlo transport simulation: taxonomy

Possible classification of Monte Carlo approaches for transport in semiconductors:

- Analytic-band: effective mass approximation in a number of nonparabolic valleys
- Full-band (FBMC): the electron dispersion relation E(k) in the entire Brillouin zone is taken into account



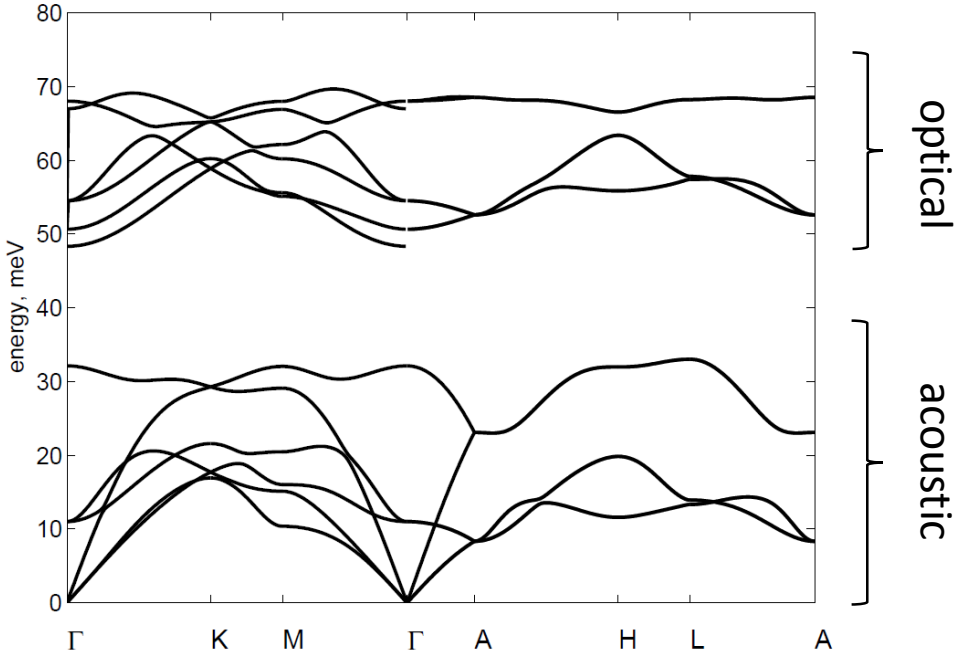
[GaN, IEEE Trans. Electron. Devices **60**, 3204 (2013)]

6. Monte Carlo transport simulation: taxonomy

Possible classification of Monte Carlo approaches for transport in semiconductors:

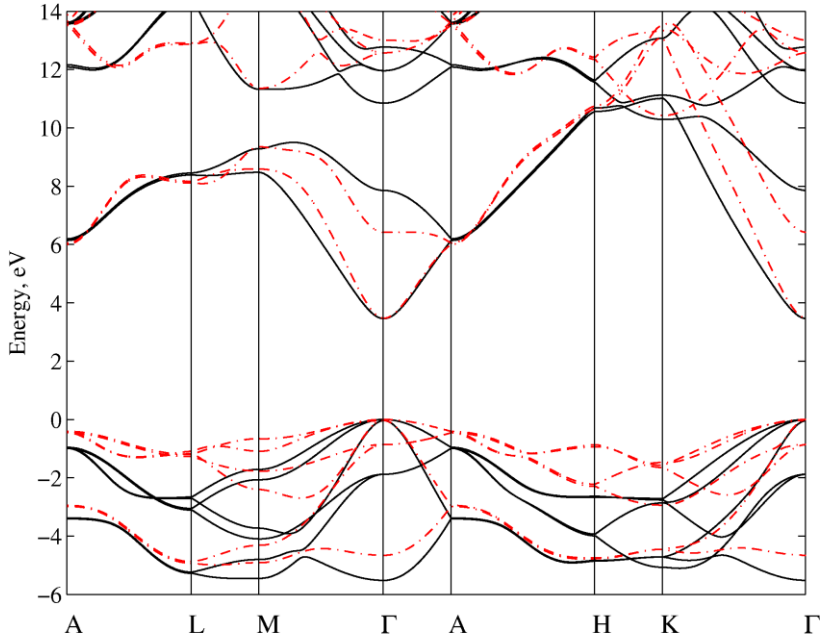
- Within FBMC, a subtler distinction is between the use of
  - energy-dependent scattering rates (semiempirical deformation potentials)
  - *k*-dependent scattering rates (a full BZ description of the phonon dispersion relation is also required)

6. Monte Carlo transport simulation: bulk ZnO



phonons

+



electrons

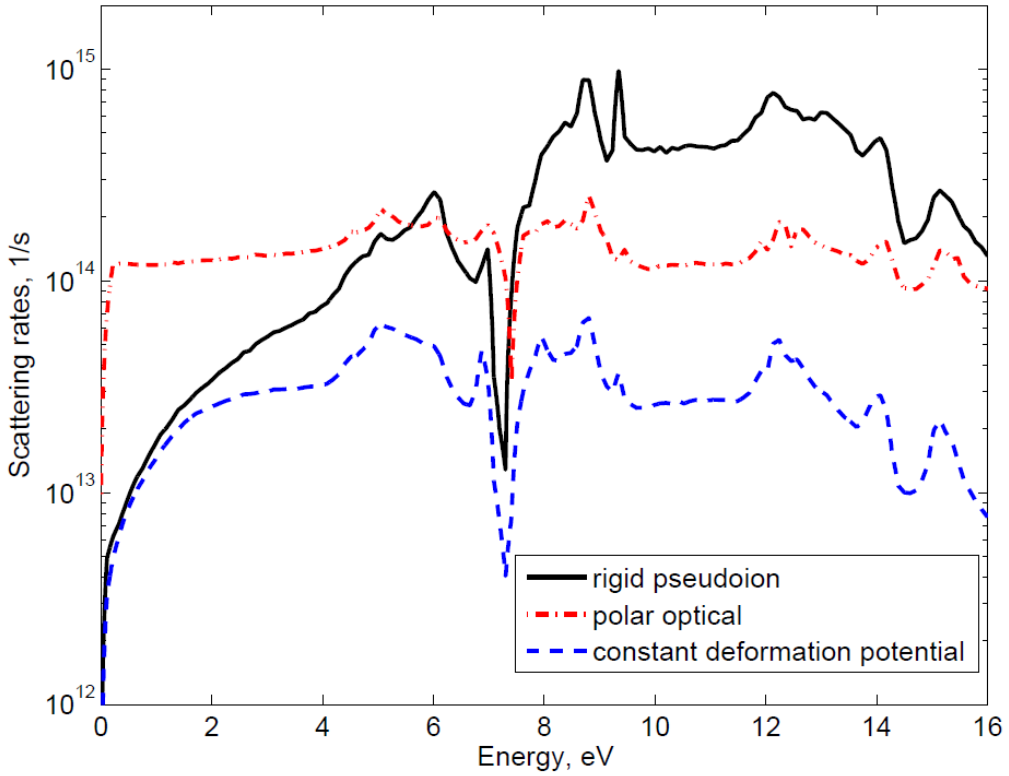
Rigid pseudo-ion model

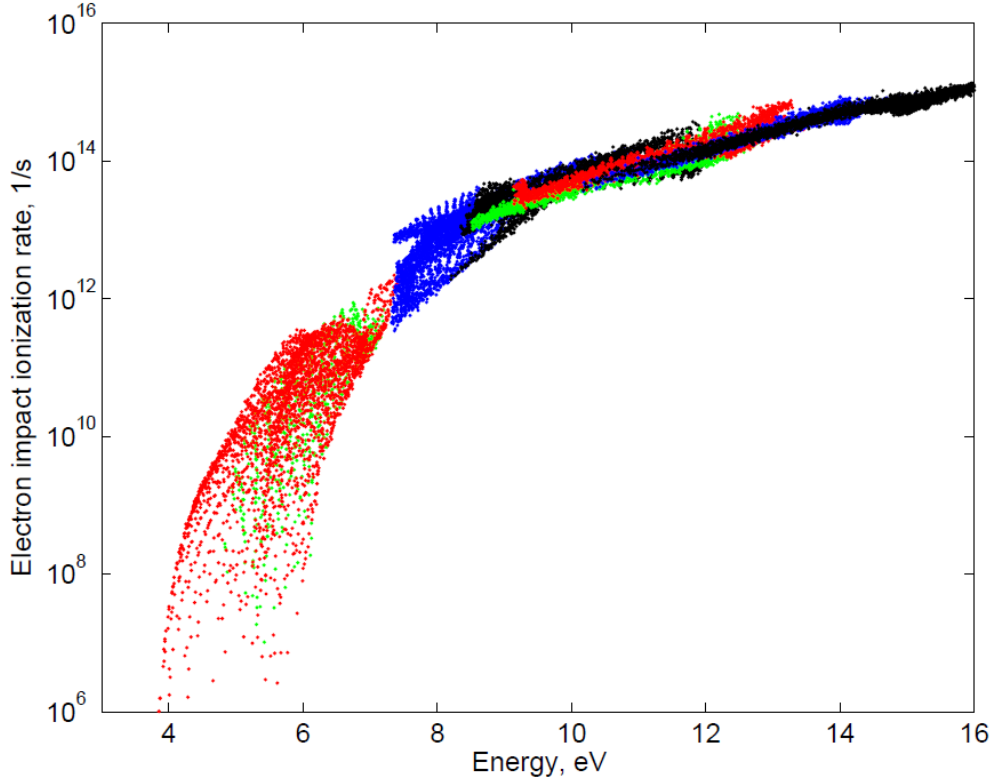
calculation of the deformation potentials from first principles using information from the electronic structure and the lattice dynamics

no fitting parameters, fully anisotropic

6. Monte Carlo transport simulation: bulk ZnO

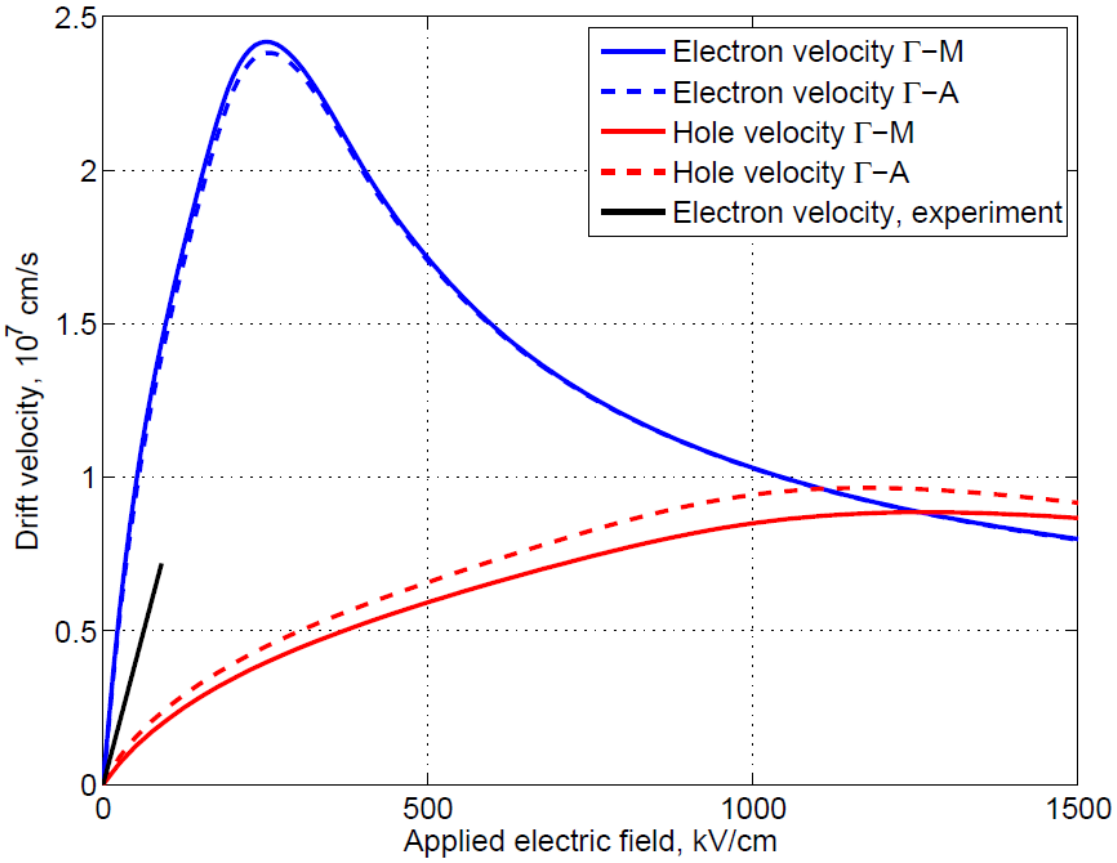
First, Monte Carlo integrations are performed to compute vast databases of k-dependent scattering rates…



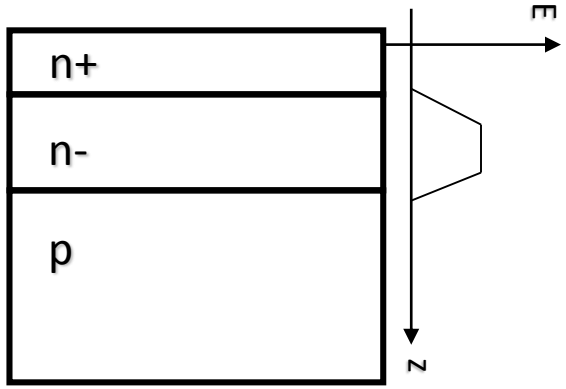


6. Monte Carlo transport simulation: bulk ZnO

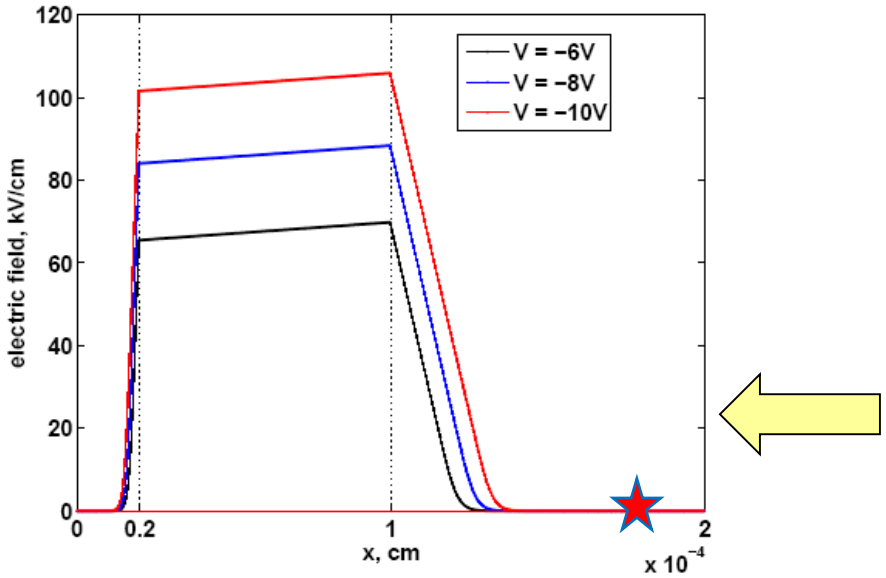
Then, using the k-dependent information on scattering mechanisms, Monte Carlo transport simulations can be performed e.g. to predict the direction-dependent transport properties



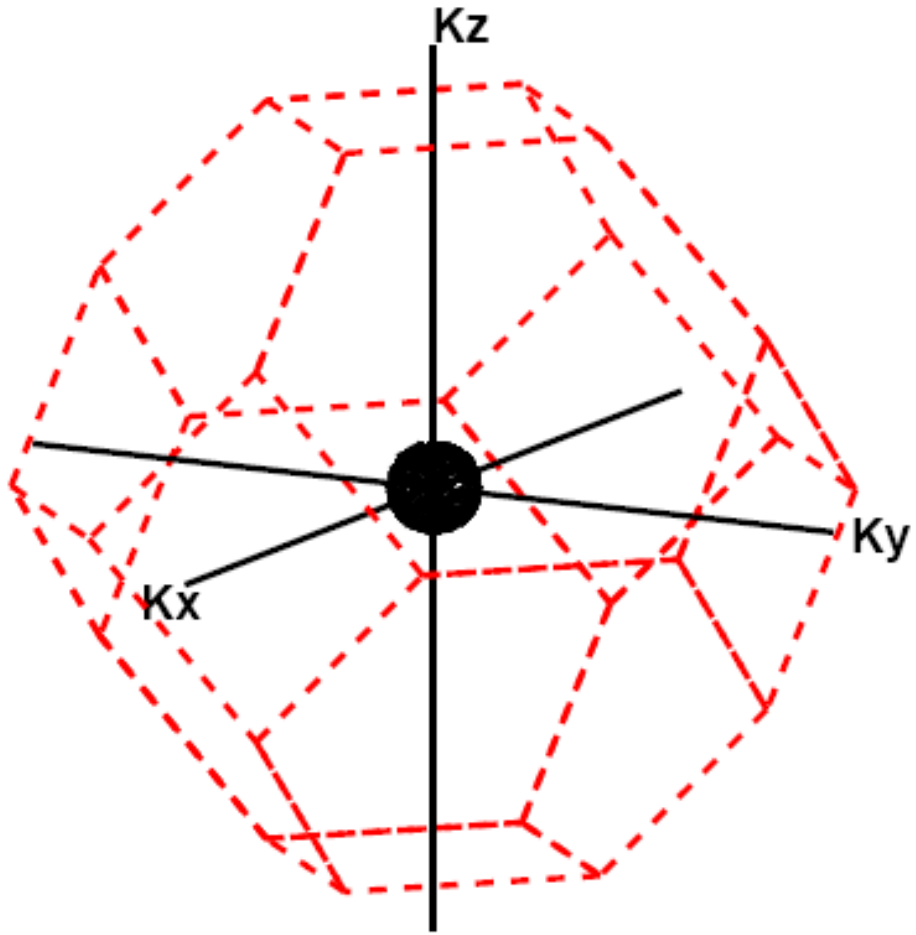
6. Monte Carlo transport simulation: HgCdTe APDs



Back illumination
(injected electrons @ 1550 nm)



The APD gain is computed simulating the multiplication process with the Monte Carlo model, see J. Appl. Phys. **106**, 063719 (2009)



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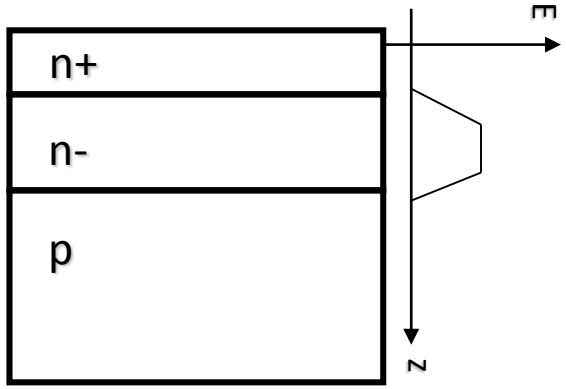

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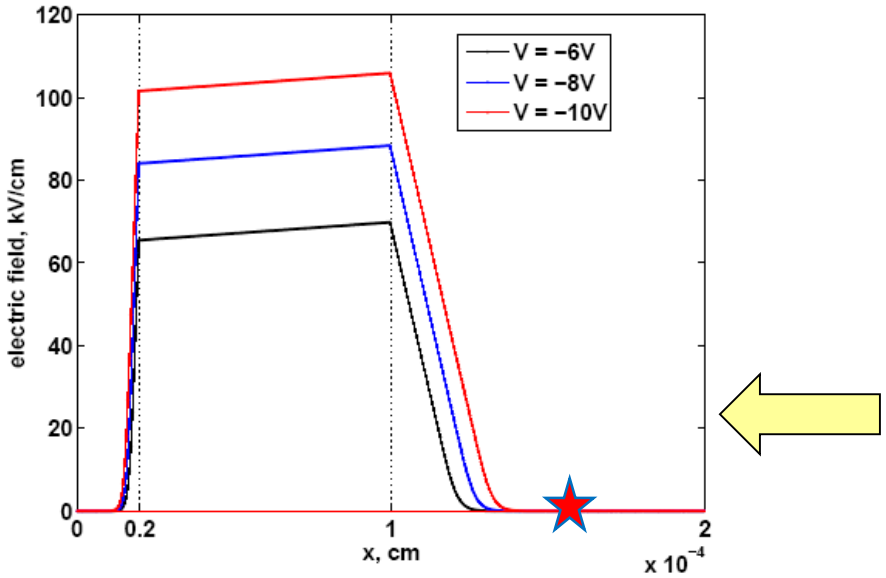

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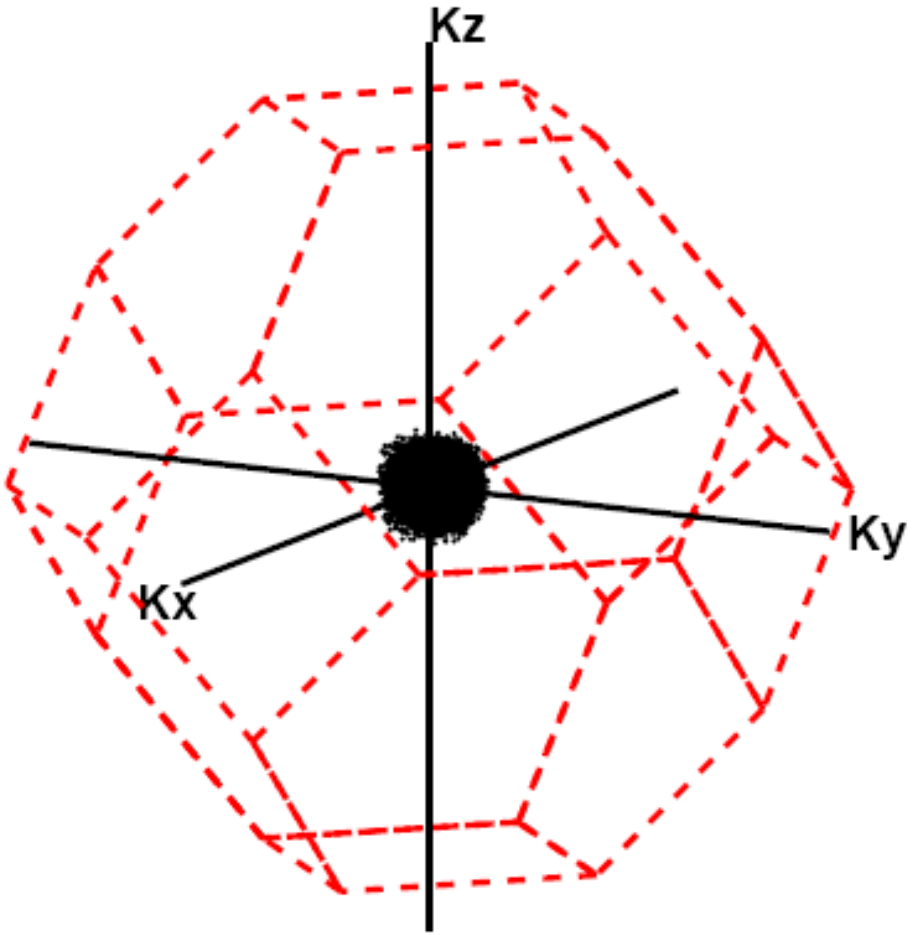

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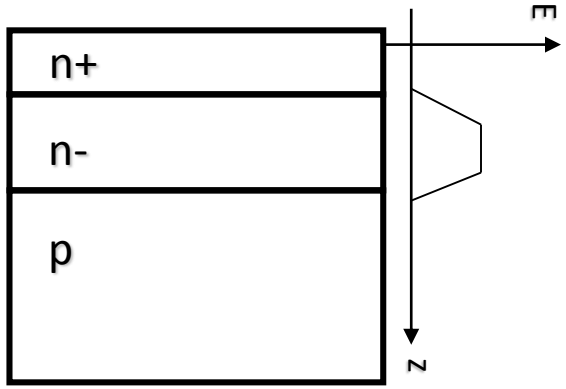

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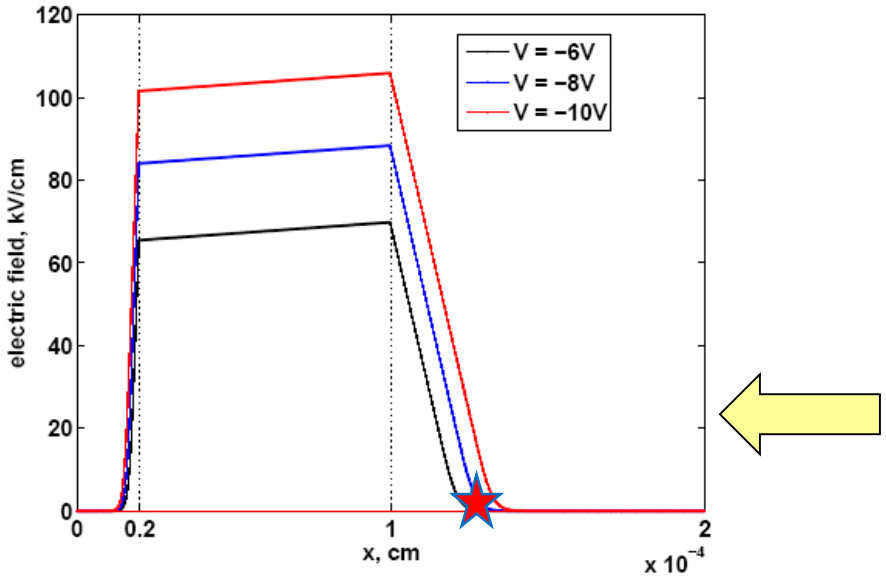

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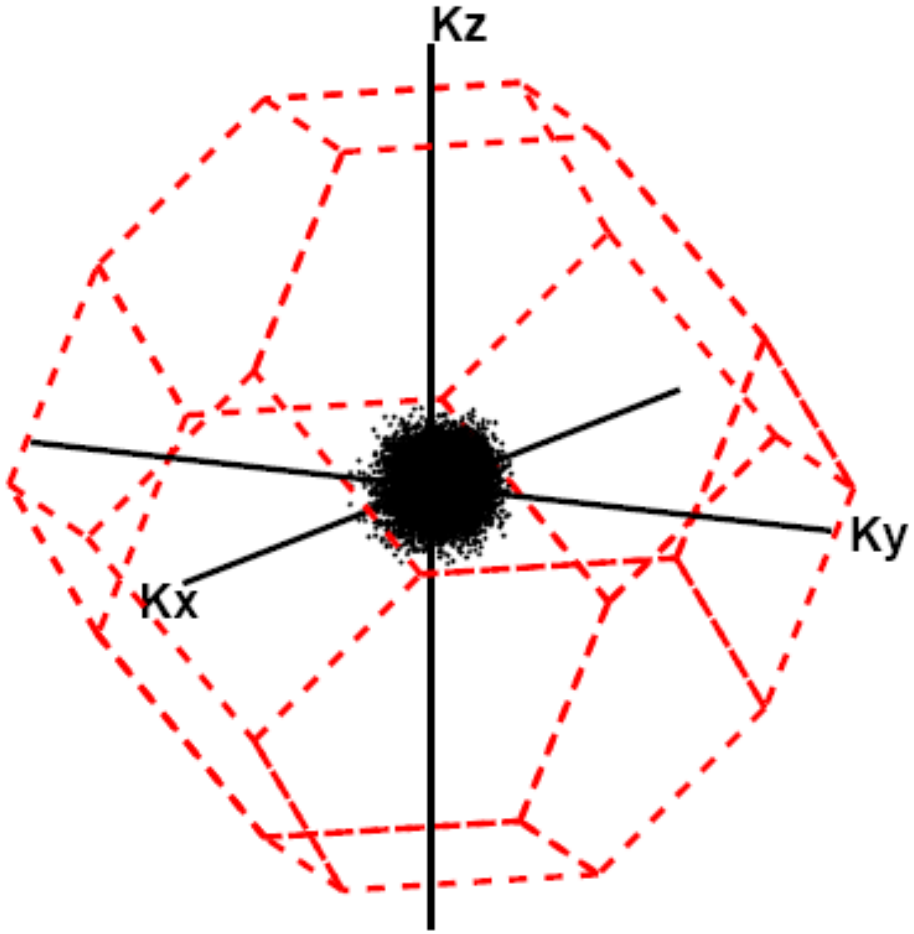

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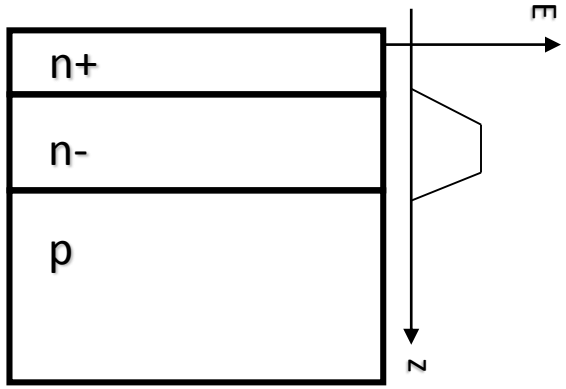

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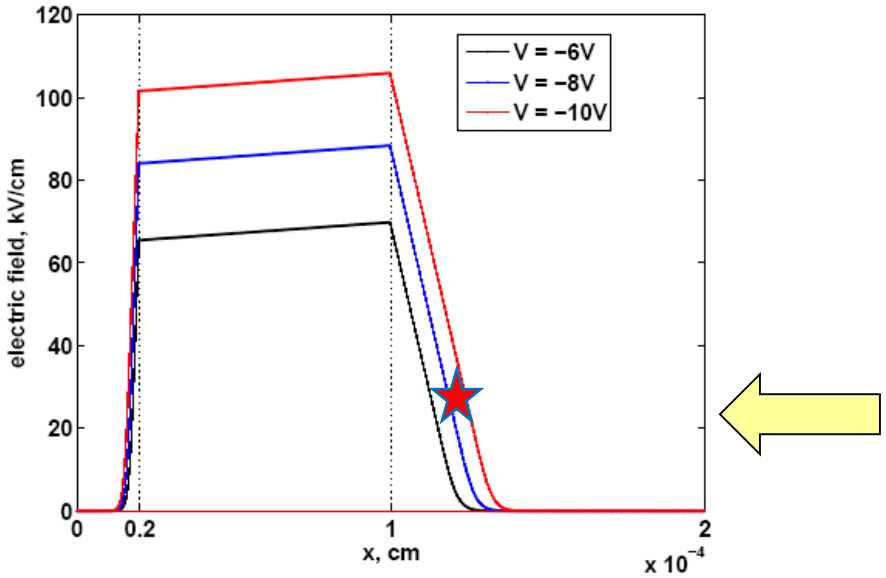

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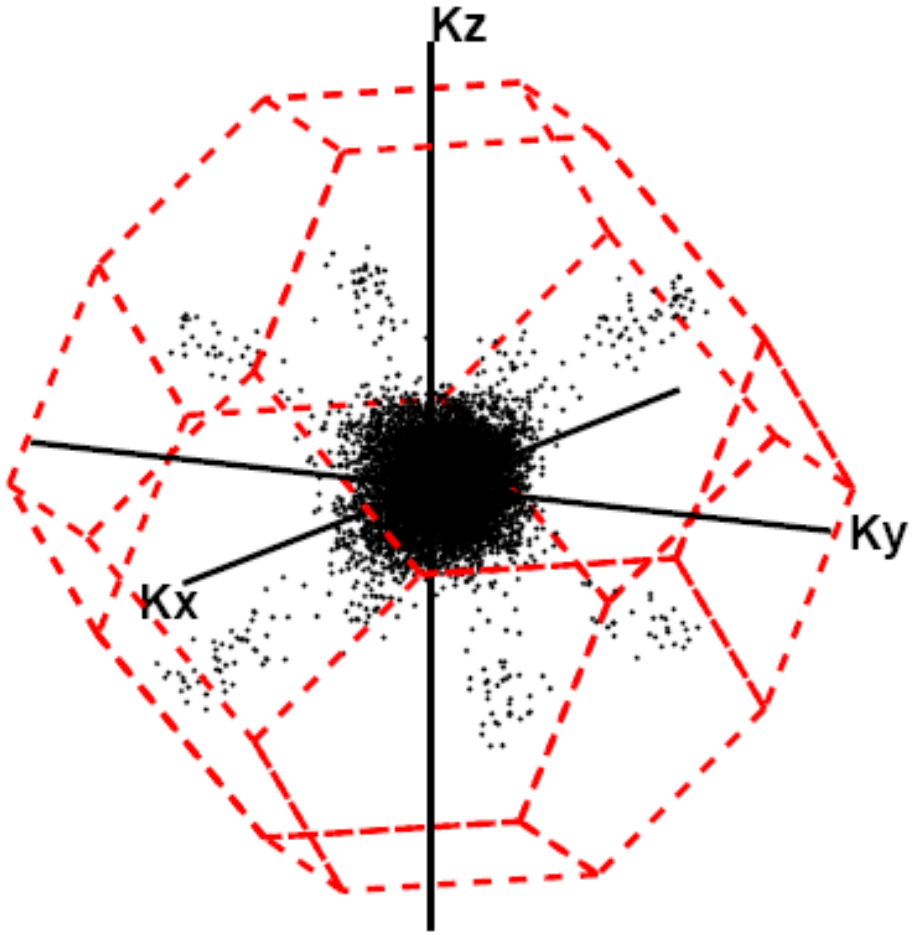

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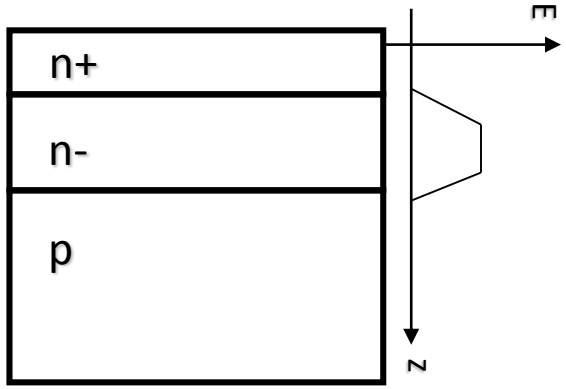

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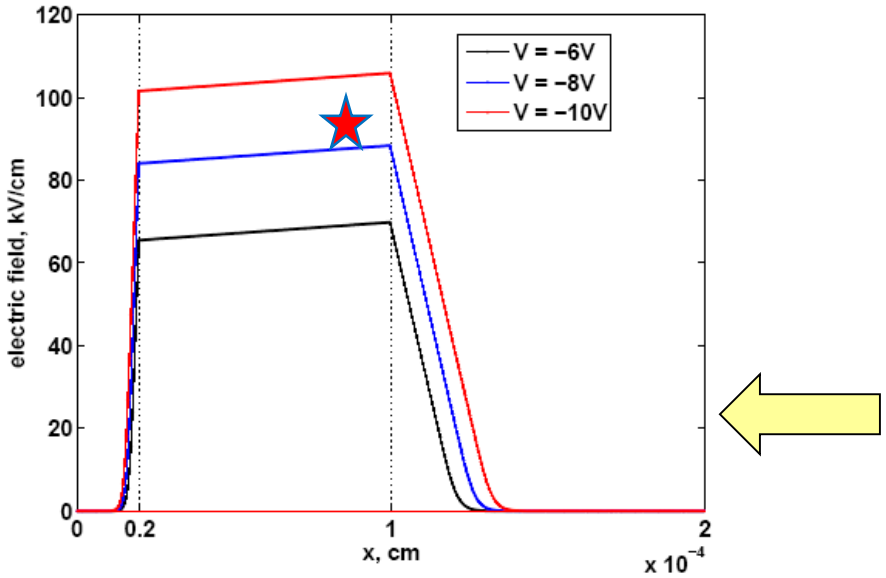

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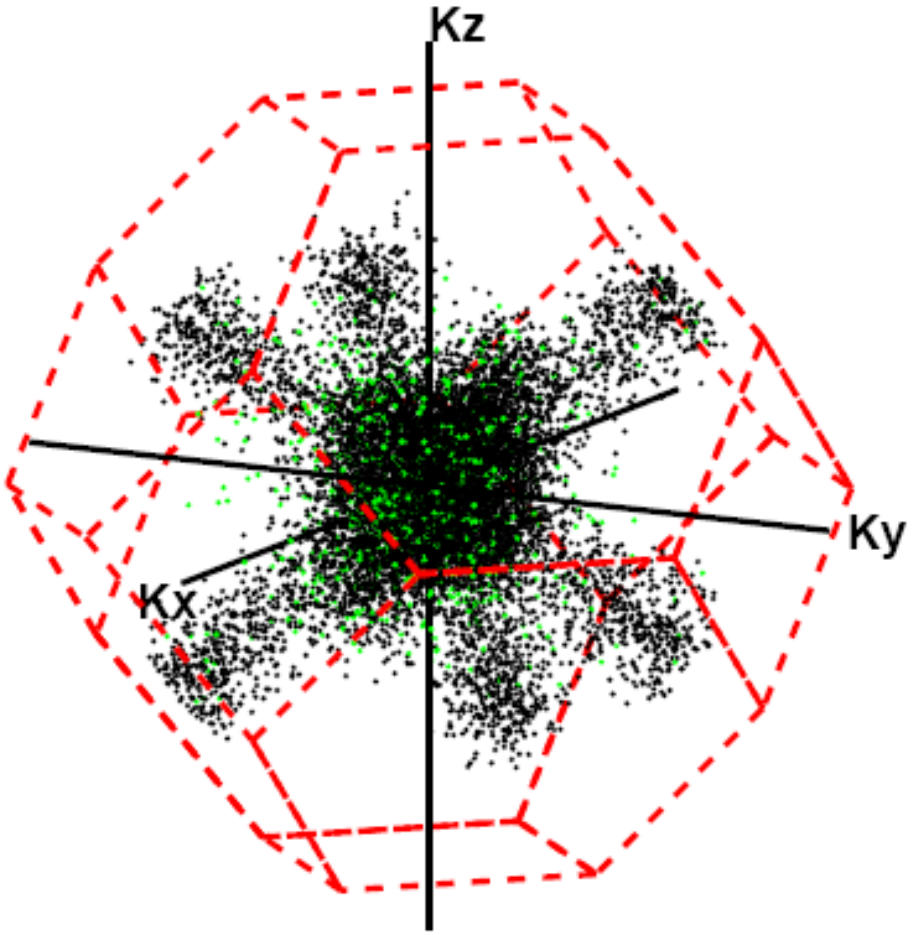
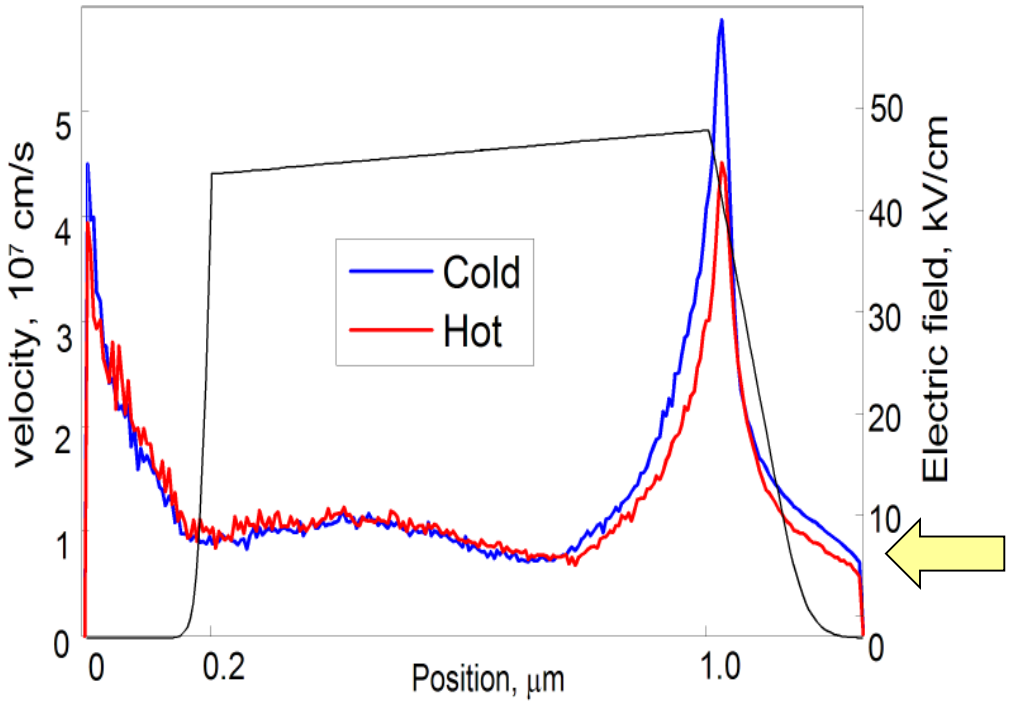
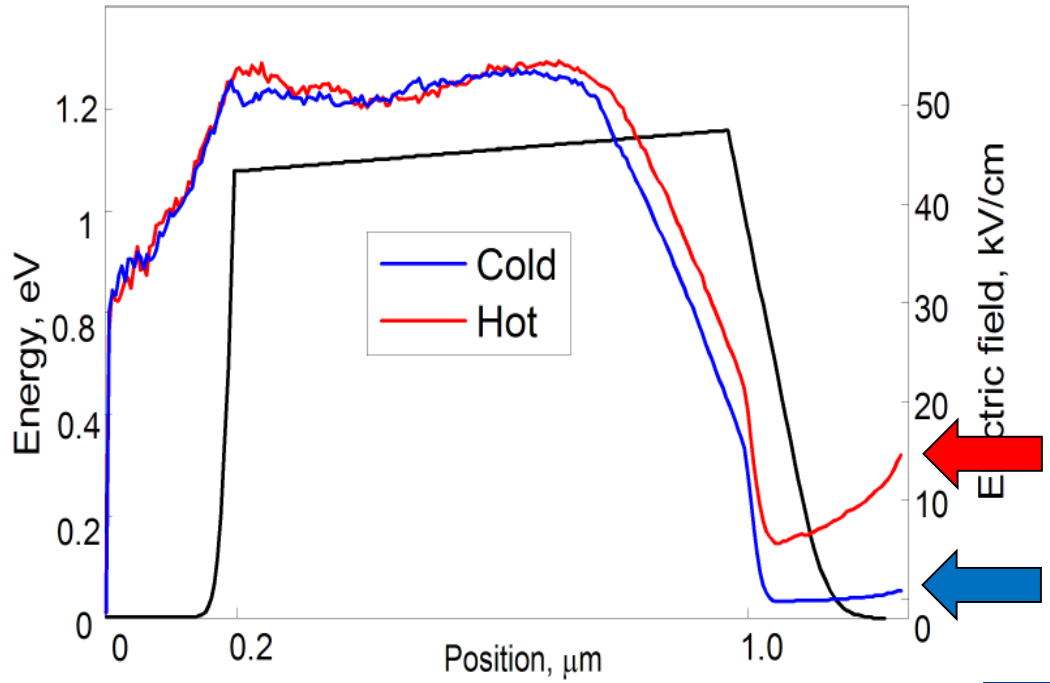


6. Monte Carlo transport simulation: HgCdTe APDs

- Electrons are injected in the *p*-side and relax while diffusing to the multiplication region
- Significant velocity overshoot is observed at the beginning of the multiplication region
- Multiplication gain may depend on the laser wavelength if photo-generated carriers are injected close to the multiplication region



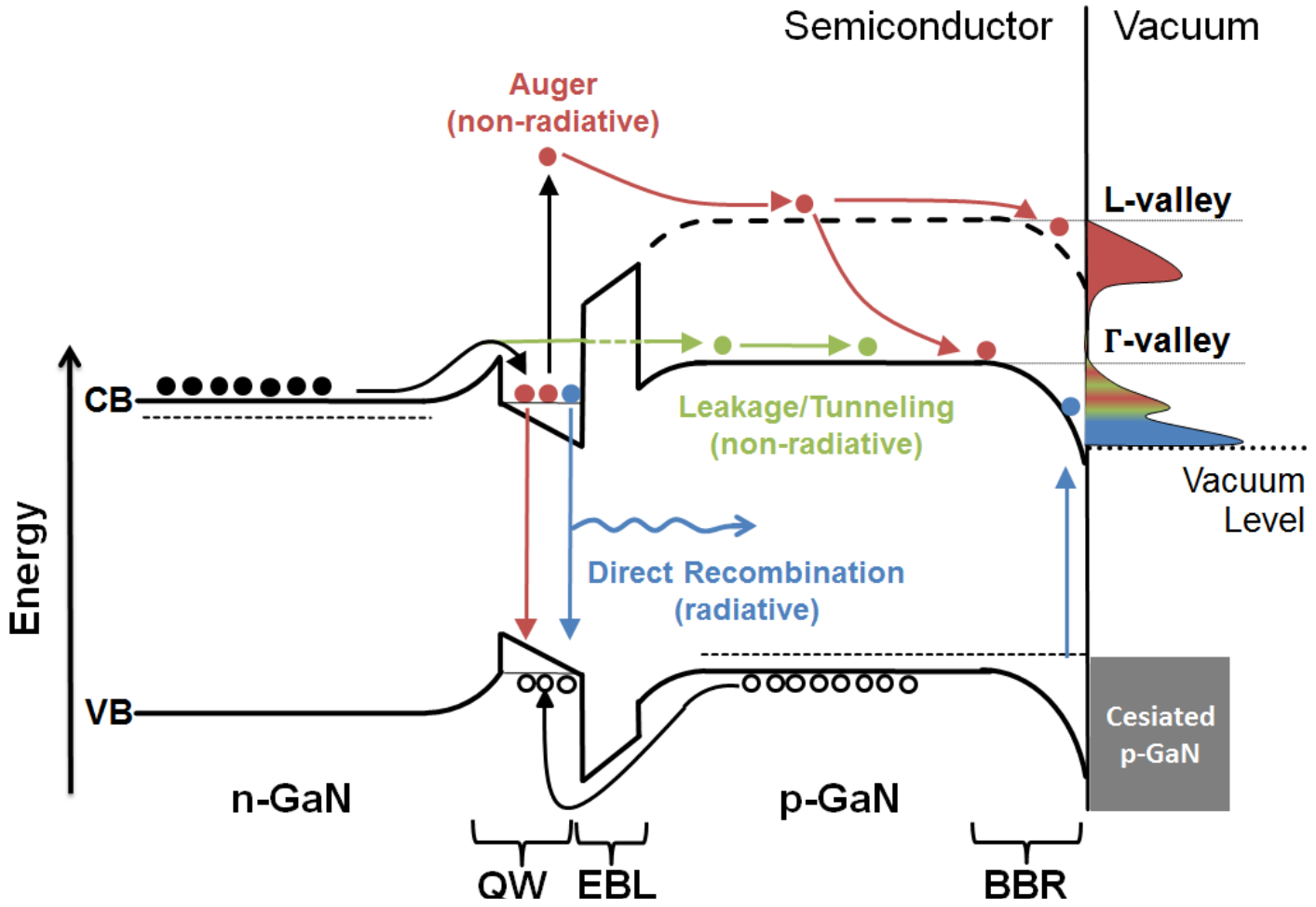


- Injection @ 1550 nm
- Injection at band edge

6. Monte Carlo transport simulation: GaN LEDs

The electron distribution can differ substantially from a Maxwellian also in InGaN/GaN LEDs. Recently, our group discussed a proposed «demonstration» of the role of Auger recombination in LED droop.

A spectroscopic study of the electrons emitted from the thick p-cap of a forward-biased LED revealed a high-energy peak, attributed to hot electrons generated by Auger recombination in the active region and quickly thermalized at the bottom of the L valley, a satellite valley supposedly located 0.9 eV above the bottom of the conduction band (Γ valley) [Phys. Rev. Lett. 110, 177406, 2013]

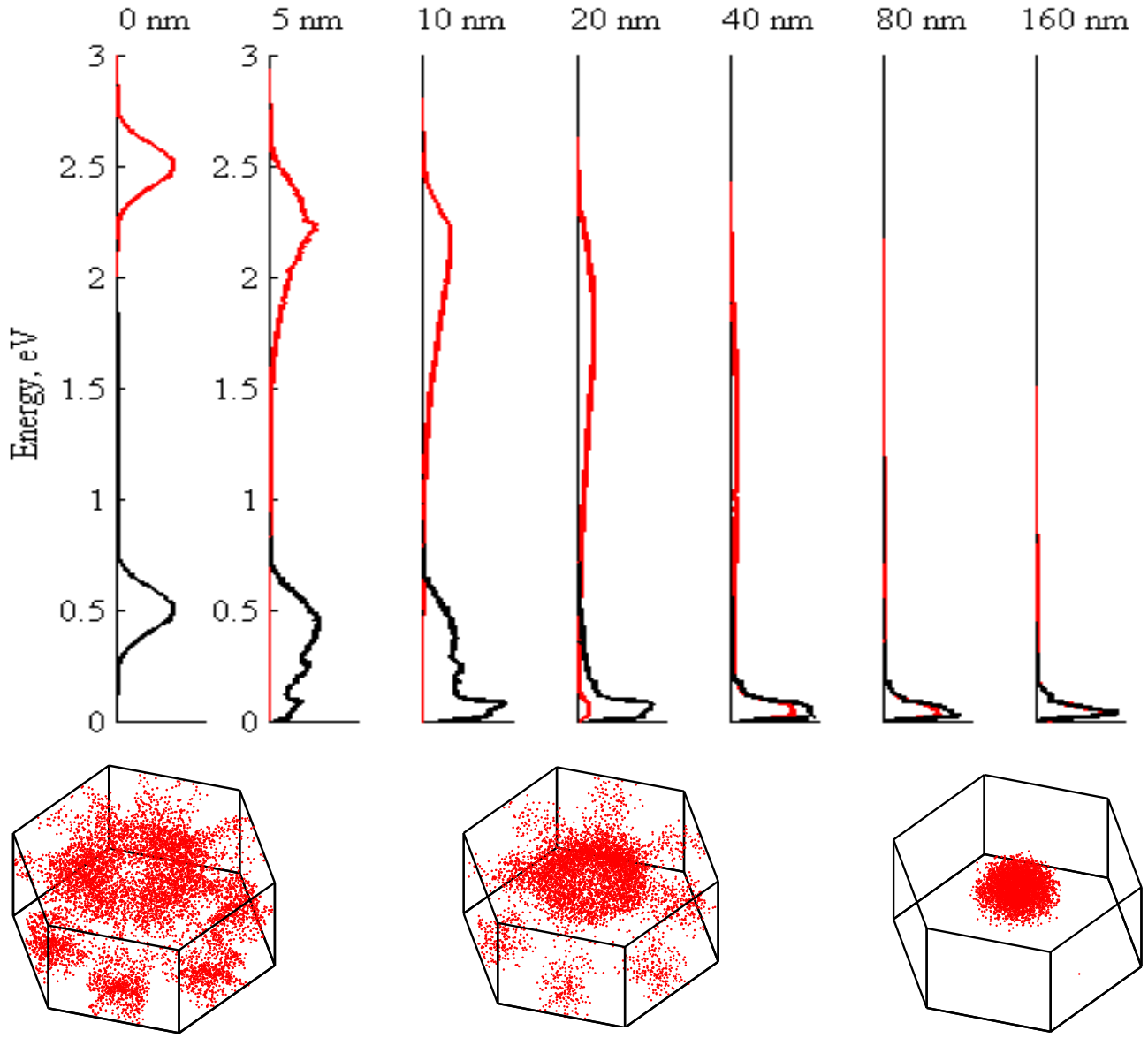


6. Monte Carlo transport simulation: GaN LEDs

To test this explanation, transport through the GaN p-cap was studied by simulating the injection of

- electrons leaking just above the blocking layer (black)
- hot electrons with energies higher than the satellite valleys of the GaN CB, as generated by Auger processes (red)

Monte Carlo results reveal that, after just 80 nm, electrons due to leakage and to Auger cannot be distinguished.



[Appl. Phys. Lett. **106**, 061112 (2015)]

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7. Conclusions

- drift-diffusion: essential starting point, to be used responsibly ☺
- HD/EB models: possibly worth considering for Si devices
- Monte Carlo: definitely the most promising approach
  - already included in some commercial suites for the prediction of transport parameters
  - no commercial/open source version available yet for device-level simulation
  - could be ideally integrated in the «low-energy extension» of existing particle-based simulators for radiation detectors
  - FBMC requires multidisciplinary cooperation

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