

Boltzmann equation and MC simulation:

1. Boltzmann transport equation

- derivation
- collision integral
- scattering theory

2. Description of various scattering mechanisms

- elastic scattering mechanisms
- inelastic scattering mechanisms

3. Monte Carlo method for the solution of the BTE

- Monte Carlo integration
- Generation of random flight times
- Choice of scattering event
- Choice of final state
- Ensemble Monte Carlo simulation
- Monte Carlo flow-chart
- Inclusion of Pauli exclusion principle
- Carrier-carrier scattering

4. Monte Carlo device simulation

- Charge assignment and force interpolation
- Motion in real space
- Monte Carlo device simulation results
- Short-range Coulomb force treatment in PB-simulations

1. Boltzmann Transport Equation

1.1 Derivation of the Boltzmann Transport Equation

Kinetic theory: We need to derive an equation for the single particle distribution function $f(\mathbf{v}, \mathbf{r}, t)$ (classical) which gives the probability of finding a particle with 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 which neglects quantum mechanical nature of particles.
- $f(\mathbf{v}, \mathbf{r}, t)$ allows us to calculate ensemble averages over velocity and space (particle density, current density, energy density, etc.):

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

- For this to give the proper average, f is normalized as follows:

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

- To derive an equation of motion for $f(\mathbf{v}, \mathbf{r}, t)$, it is somewhat easier to consider the particle density

$$n(\mathbf{v}, \mathbf{r}, t) = Nf(\mathbf{v}, \mathbf{r}, t)$$

where

$$N = \int d\mathbf{r} \int d\mathbf{v} n(\mathbf{v}, \mathbf{r}, t) = \text{Total \# of particles}$$

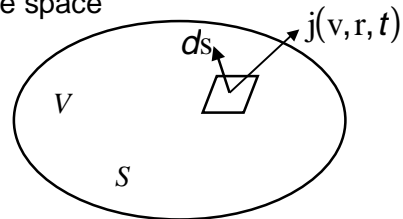
- The density $n(\mathbf{v}, \mathbf{r}, t)$ should satisfy a continuity equation in the 6D phase space defined by

$$x, y, z, v_x, v_y, v_z \rightarrow \text{Independent } t \text{ variables}$$

- Consider a hypervolume in phase space

$\mathbf{j}(\mathbf{r}, \mathbf{v}, t)$ is the flux density

$\mathbf{j}(\mathbf{r}, \mathbf{v}, t) \cdot d\mathbf{s}$ is flux through hypersurface $d\mathbf{s}$



- Consider the particle balance through the hyper-volume V

$$\frac{\partial}{\partial t} \int_V d\mathbf{r} d\mathbf{v} n(\mathbf{v}, \mathbf{r}, t) = - \int_S \mathbf{j}(\mathbf{v}, \mathbf{r}, t) \cdot d\mathbf{s} + \int_V d\mathbf{r} d\mathbf{v} \left. \frac{\partial n}{\partial t} \right|_{\text{Coll}} +$$

Time rate of change
of # particles in V

Leakage
through S

Time rate of change
due to collisions

$$+ \int_V d\mathbf{r} d\mathbf{v} \{G(\mathbf{r}, \mathbf{v}, t) - R(\mathbf{r}, \mathbf{v}, t)\}$$

Time rate of change due to G-R mechanisms

- The flux density is written in terms of the time derivatives of the 'position' variables in 6D:

$$\mathbf{j}(x, y, z, v_x, v_y, v_z) = v_x n(v, r, t) \hat{\mathbf{a}}_x + v_y n \hat{\mathbf{a}}_y + v_z n \hat{\mathbf{a}}_z + \frac{F_x}{m} n \hat{\mathbf{b}}_{v_x} + \frac{F_y}{m} n \hat{\mathbf{b}}_{v_y} + \frac{F_z}{m} n \hat{\mathbf{b}}_{v_z} \text{ with } \dot{\mathbf{v}} = \frac{\mathbf{F}}{m}$$

- Applying the divergence theorem in 6D

$$\int_S \mathbf{j}(v, r, t) \cdot d\mathbf{s} = \int_V d\mathbf{r} d\mathbf{v} \nabla \cdot \mathbf{j}(v, r, t)$$

where the divergence of \mathbf{j} is

$$\nabla \cdot \mathbf{j} = v_x \frac{\partial n}{\partial x} + v_y \frac{\partial n}{\partial y} + v_z \frac{\partial n}{\partial z} + \frac{F_x}{m} \frac{\partial n}{\partial v_x} + \frac{F_y}{m} \frac{\partial n}{\partial v_y} + \frac{F_z}{m} \frac{\partial n}{\partial v_z}$$

which is written more compactly as:

$$\nabla \cdot \mathbf{j} = \mathbf{v} \cdot \nabla_r n + \frac{\mathbf{F}}{m} \cdot \nabla_v n$$

- Particle balance is therefore:

$$\int_V d\mathbf{r} d\mathbf{v} \left(\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla_r n + \frac{\mathbf{F}}{m} \cdot \nabla_v n - \frac{\partial n}{\partial t} \Big|_{\text{Coll}} - \frac{\partial n}{\partial t} \Big|_{G-R} \right) = 0$$

Normalizing, we get the classical form of the Boltzmann transport equation:

$$\frac{\partial f(\mathbf{r}, \mathbf{v}, t)}{\partial t} = \underbrace{-\mathbf{v} \cdot \nabla_r f - \frac{\mathbf{F}}{m} \cdot \nabla_v f}_{\text{streaming terms}} + \frac{\partial f}{\partial t} \Big|_{\text{Coll}} + \frac{\partial f}{\partial t} \Big|_{G-R}$$

First two terms on the rhs are the streaming terms

- For Bloch electrons in a semiconductor, we could have considered a 6D space x, y, z, k_x, k_y, k_z where \mathbf{k} is the wavevector and

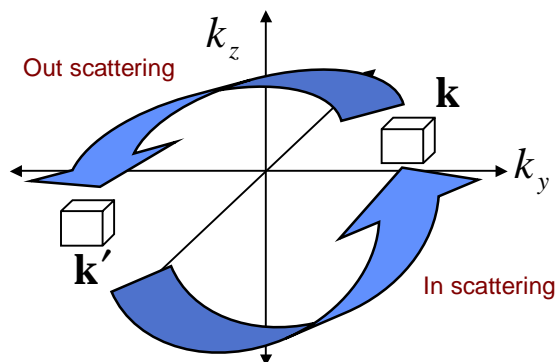
$$\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} E(\mathbf{k})$$

- The semi-classical BTE for transport of Bloch electrons is therefore

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

1.2 Collisional Integral

Assume instantaneous, single collisions which are independent of the driving force and take particles from \mathbf{k} to \mathbf{k}' (out scattering) or from \mathbf{k}' to \mathbf{k} (in scattering).



(A) Out Scattering

$$\Delta n(\mathbf{r}, \mathbf{k}, t) = -n(\mathbf{r}, \mathbf{k}, t)\Gamma_{\mathbf{k}\mathbf{k}'}\Delta t$$

where $\Gamma_{\mathbf{k}\mathbf{k}'}$ is the transition rate per particle from \mathbf{k} to \mathbf{k}'

Distribution function is: $f(\mathbf{r}, \mathbf{k}, t) = \frac{n(\mathbf{r}, \mathbf{k}, t)}{N}$

Take limit as $\Delta t \rightarrow 0$

$$\left. \frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} \right|_{OUT} = -f(\mathbf{r}, \mathbf{k}, t)\Gamma_{\mathbf{k}\mathbf{k}'}[1 - f(\mathbf{r}, \mathbf{k}', t)]$$

where the last term in brackets accounts for the **Pauli exclusions principle** (degeneracy of the final state after scattering).

(B) In Scattering

By an analogous argument, the rate of change of the distribution function due to in scattering is:

$$\left. \frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} \right|_{IN} = f(\mathbf{r}, \mathbf{k}', t)\Gamma_{\mathbf{k}'\mathbf{k}}[1 - f(\mathbf{r}, \mathbf{k}, t)]$$

Total rate of change of $f(\mathbf{r}, \mathbf{k}, t)$ around \mathbf{k} is a sum over all possible initial and final states \mathbf{k}' :

$$\left. \frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} \right|_{Coll} = \sum_{\mathbf{k}'} \{ \overset{\text{In scattering}}{f(\mathbf{r}, \mathbf{k}', t)[1 - f(\mathbf{r}, \mathbf{k}, t)]\Gamma_{\mathbf{k}'\mathbf{k}} - \underset{\text{Out scattering}}{f(\mathbf{r}, \mathbf{k}, t)[1 - f(\mathbf{r}, \mathbf{k}', t)]\Gamma_{\mathbf{k}\mathbf{k}'}} \}$$

(C) Boltzmann Equation with Collision Integral

The sum over final states \mathbf{k}' may be converted to an integral due to the small volume of k-space associated with each state:

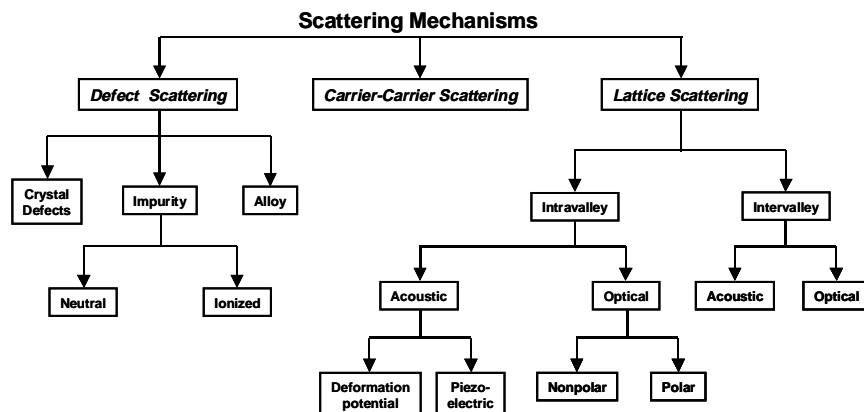
$$\sum_{\mathbf{k}'} \rightarrow \frac{V}{8\pi^3} \int d\mathbf{k}'$$

The BTE becomes:

$$\frac{\partial f_{\mathbf{k}}}{\partial t} + \frac{1}{\hbar} \nabla_{\mathbf{k}} E \cdot \nabla_{\mathbf{r}} f_{\mathbf{k}} + \frac{F}{\hbar} \nabla_{\mathbf{k}} f_{\mathbf{k}} = \frac{V}{8\pi^3} \int d\mathbf{k}' \{ f_{\mathbf{k}'} [1 - f_{\mathbf{k}}] \Gamma_{\mathbf{k}'\mathbf{k}} - f_{\mathbf{k}} [1 - f_{\mathbf{k}'}] \Gamma_{\mathbf{k}\mathbf{k}'} \}$$

1.3 Scattering Theory

What contributes to $\Gamma_{\mathbf{k}\mathbf{k}'}$?



Time dependent perturbation theory

- Assume the Hamiltonian may be decomposed as $H=H_0+V_s$, where H_0 is the Hamiltonian of the perfect crystal (described by Bloch states), $V_s(\mathbf{r},t)$ is a small random potential. If $V_s \ll H_0$, then it is a good approximation to expand the solution (with random part) in terms of unperturbed eigenstates:

$$H_0 \psi_k = E_k \psi_k; \quad \psi_k^0(\mathbf{r}, t) = \psi_k(\mathbf{r}) e^{-iE_k t / \hbar}$$

- Expand actual solution in terms of these orthonormal functions:

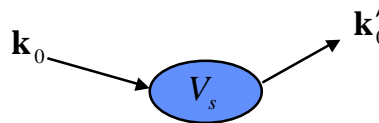
$$\psi(\mathbf{r}, t) = \sum_k c_k(t) \psi_k(\mathbf{r}) e^{-iE_k t / \hbar}$$

- If the initial wave packet is centered around \mathbf{k}_0 , so that

$$c_{k_0}(t) \approx 1 \quad c_{k \neq k_0}(t) \approx 0$$

- In the limit at $t \rightarrow \infty$, the probability of finding the particle in another state \mathbf{k}'_0 is

$$P_{k_0 k'_0} = \lim_{t \rightarrow \infty} |c_{k'_0}(t)|^2$$



- Define the transition rate

$$\Gamma_{k_0 k'_0} = \lim_{t \rightarrow \infty} \frac{|c_{k'_0}(t)|^2}{t}$$

- Solve for $c_{k'_0}$ using the S.E. and the previous expansion

$$\{H_0 + V_s\} \sum_k c_k(t) \psi_k(\mathbf{r}) e^{-iE_k t / \hbar} = i\hbar \frac{\partial}{\partial t} \sum_k c_k(t) \psi_k(\mathbf{r}) e^{-iE_k t / \hbar}$$

H_0 part cancels with phase factor on RHS

$$V_s \sum_k c_k(t) \psi_k(\mathbf{r}) e^{-iE_k t/\hbar} = i\hbar \sum_k \frac{\partial c_k(t)}{\partial t} \psi_k(\mathbf{r}) e^{-iE_k t/\hbar}$$

- Multiply both sides by $\psi_{k_0}^*(\mathbf{r}) e^{-iE_{k_0} t/\hbar}$ and integrate

$$i\hbar \frac{\partial c_{k_0}(t)}{\partial t} = \sum_k c_k(t) \langle k_0 | V_s | k \rangle e^{-i(E_{k_0} - E_k)t/\hbar}$$

where the *matrix element*, using Dirac notation, is defined as

$$\langle k_0 | V_s | k \rangle = \int d\mathbf{r} \psi_{k_0}^* V_s(\mathbf{r}, t) \psi_k$$

- Assume *sufficiently weak scattering* that $c_{k_0} \approx 1$, and $c_{k \neq k_0} \approx 0$ for all time. The dominant term in the sum is:

$$i\hbar \frac{\partial c_{k_0}(t)}{\partial t} = c_{k_0}(t) \langle k_0 | V_s | k_0 \rangle e^{-i(E_{k_0} - E_{k_0})t/\hbar}$$

which integrates to

$$c_{k_0}(t) = \frac{1}{i\hbar} \int_0^t dt' \langle k_0 | V_s | k_0 \rangle e^{-i(E_{k_0} - E_{k_0})t'/\hbar} + c_{k_0}(0)$$

- Suppose $V(\mathbf{r}, t)$ may be Fourier decomposed, so that

$$V_s(\mathbf{r}, t) = V_s(\mathbf{r}) e^{\mp i\omega t}$$

Note that this form of $V(\mathbf{r}, t)$ may correspond to interaction with lattice vibrations or with optical excitation.

- Then substituting

$$c_{k'_0}(t) = \frac{1}{i\hbar} \langle k'_0 | V_s | k_0 \rangle \int_0^t dt' e^{-i\Lambda t'}; \quad \Lambda = (E_{k'_0} - E_{k_0} \mp \hbar\omega) / \hbar$$

and integrating this last expression leads to

$$c_{k'_0}(t) = \frac{1}{i\hbar} V_s^{k_0 k'_0} \frac{e^{-i\Lambda t} - 1}{i\Lambda}$$

$$c_{k'_0}(t) = \frac{1}{i\hbar} V_s^{k_0 k'_0} e^{-i\Lambda t/2} \left(\frac{\sin(\Lambda t)}{\Lambda t} \right) t$$

- Since the probability of being in k'_0 is given by

$$P_{k_0 k'_0} = \lim_{t \rightarrow \infty} |c_{k'_0}(t)|^2$$

- Substituting for c and taking the magnitude squared gives

$$P_{k_0 k'_0} = \lim_{t \rightarrow \infty} \frac{1}{\hbar^2} |V_s^{k_0 k'_0}|^2 \left(\frac{\sin(\Lambda t)}{\Lambda t} \right)^2 t^2$$

where asymptotically

$$\lim_{t \rightarrow \infty} \left(\frac{\sin(\Lambda t)}{\Lambda t} \right)^2 = 2\pi\delta(\Lambda) / t = 2\pi\hbar\delta(E_{k'_0} - E_{k_0} \mp \hbar\omega) / t$$

This gives the famous **Fermi's Golden Rule** (dropping 0s index)

$$\Gamma_{kk'} = \frac{P_{kk'}}{t} = \frac{2\pi}{\hbar} |V_s^{kk'}|^2 \delta(E_{k'} - E_k \mp \hbar\omega)$$

- Assumptions made:

- (1) Long time between scattering (no multiple scattering events)
- (2) Neglect contribution of other c 's (Collision broadening ignored)

2. Description of various scattering mechanisms

2.1 Elastic Scattering Mechanisms

(A) Ionized Impurities scattering

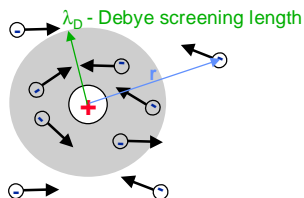
(Ionized donors/acceptors, substitutional impurities, charged surface states, etc.)

- The potential due to a single ionized impurity with net charge Ze is:

$$V_i^0(\mathbf{r}) = -\frac{Ze^2}{4\pi\epsilon r} \quad \text{mks units}$$

- In the one electron picture, the actual potential seen by electrons is *screened* by the other electrons in the system.

What is Screening?



Example:

$$\mathbf{3D:} \quad \frac{1}{r} \xrightarrow{\text{screening cloud}} \frac{1}{r} \exp\left(-\frac{r}{\lambda_D}\right)$$

Ways of treating screening:

- Thomas-Fermi Method
static potentials + slowly varying in space
- Mean-Field Approximation (Random Phase Approximation)
time-dependent and not slowly varying in space

- Considering the induced charge caused by the change in the electron gas by the impurity, the net potential seen is

$$V_i(\mathbf{q}) = \frac{V^0_i(\mathbf{q})}{\epsilon(\mathbf{q}, \omega)}$$

In the above expression, \mathbf{q} is the wavevector associated with Fourier transforming the potential (and Poisson's equation), $V_i(\mathbf{q})$ is the total potential seen by an electron due to an impurity, and $\epsilon(\mathbf{q}, \omega)$ is the *dielectric function* characterizing the polarization of the electron gas to the impurity potential.

- In linear response theory, this may be calculated in the random phase approximation (RPA) to give the Lindhard dielectric function

$$\epsilon(\mathbf{q}, \omega) = 1 - \lim_{s \rightarrow \infty} \frac{e^2}{\epsilon_{sc} q^2} \sum_{\mathbf{k}} \frac{f_0(E_{\mathbf{k}+\mathbf{q}}) - f_0(E_{\mathbf{k}})}{E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + \hbar\omega + i\delta}$$

ASU Computational Electronics

- Assuming low frequencies, and assuming long wavelengths, the Thomas-Fermi function is obtained to be of the form:

$$\lim_{\omega, q \rightarrow 0} \epsilon(\mathbf{q}, \omega) \approx 1 + \frac{\lambda^2}{q^2}$$

where the inverse screening length λ^2 is given as (3D):

$$\lambda^2 = \frac{e^2 n}{\epsilon_{sc} k_B T} \quad \text{high temperature}; \quad \lambda^2 = \frac{3e^2 n}{2\epsilon_{sc} E_F}; \quad T = 0K$$

In here, n is the carrier density and E_F is the Fermi energy.

- Assuming the Fermi Thomas form, inverse Fourier transforming gives the form of the screened potential in real space as:

$$V_i(r) = -\frac{Zq^2}{4\pi\epsilon r} e^{-\lambda r}$$

ASU Computational Electronics

- For the scattering rate due to impurities, we need for Fermi's rule the matrix element between initial and final Bloch states

$$\langle n', k' | V_i(\mathbf{r}) | n, k \rangle = V^{-1} \int d\mathbf{r} u_{n', k'}^* e^{-i\mathbf{k}' \cdot \mathbf{r}} V_i(\mathbf{r}) u_{n, k} e^{i\mathbf{k} \cdot \mathbf{r}}$$

Since the u 's have periodicity of lattice, expand in reciprocal space

$$\begin{aligned} &= \sum_{\mathbf{G}} V^{-1} \int d\mathbf{r} e^{-i\mathbf{k}' \cdot \mathbf{r}} V_i(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} e^{-i\mathbf{G} \cdot \mathbf{r}} U_{nn'kk'}(\mathbf{G}) \\ &= \sum_{\mathbf{G}} V^{-1} \int d\mathbf{r} e^{-i\mathbf{k}' \cdot \mathbf{r}} V_i(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} e^{-i\mathbf{G} \cdot \mathbf{r}} \int_{\Omega} d\mathbf{r}' u_{n', k'}^*(\mathbf{r}') u_{n, k}(\mathbf{r}') e^{i\mathbf{G} \cdot \mathbf{r}'} \end{aligned}$$

- For impurity scattering, the matrix element has a $1/q$ type dependence which usually means $\mathbf{G} \neq 0$ terms are small

$$= V^{-1} \int d\mathbf{r} e^{-i\mathbf{k}' \cdot \mathbf{r}} V_i(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \int_{\Omega} d\mathbf{r}' u_{n', k'}^*(\mathbf{r}') u_{n, k}(\mathbf{r}') = V_i(\mathbf{q}) I_{kk'}^{nn'}$$

ASU Computational Electronics

- The usual argument is that since the u 's are normalized within a unit cell (i.e. equal to 1), the Bloch overlap integral I , is approximately 1 for $n' = n$ [interband(valley)]. Therefore, for impurity scattering, the matrix element for scattering is approximately

$$|\langle \mathbf{k}' | V_i(\mathbf{r}) | \mathbf{k} \rangle|^2 = |V_i(\mathbf{q})|^2 \cong \frac{Z^2 e^4}{V^2 (q^2 + \lambda^2) \epsilon_{sc}^2}; \quad V = \text{volume}$$

where the scattered wavevector is: $\mathbf{q} = \mathbf{k} - \mathbf{k}'$

- This is the scattering rate for a single impurity. If we assume that there are N_i impurities in the whole crystal, and that scattering is completely uncorrelated between impurities:

$$V_i^{kk'} \cong \frac{N_i Z^2 e^4}{V^2 (q^2 + \lambda^2) \epsilon_{sc}^2} = \frac{n_i Z^2 e^4}{V (q^2 + \lambda^2) \epsilon_{sc}^2}$$

where n_i is the impurity density (per unit volume).

ASU Computational Electronics

- The total scattering rate from \mathbf{k} to \mathbf{k}' is given from Fermi's golden rule as:

$$\Gamma_{kk'}^i = \frac{2\pi n_i Z^2 e^4}{V\hbar(q^2 + \lambda^2)\epsilon_{sc}^2} \delta(E_{k'} - E_k)$$

If θ is the angle between \mathbf{k} and \mathbf{k}' , then:

$$q = |\mathbf{k} - \mathbf{k}'| = k^2 + k'^2 - 2kk' \cos \theta = 2k^2(1 - \cos \theta)$$

- Comments on the behavior of this scattering mechanism:
 - Increases linearly with impurity concentration
 - Decreases with increasing energy (k^2), favors lower T
 - Favors small angle scattering
 - Ionized Impurity-Dominates at low temperature, or room temperature in impure samples (highly doped regions)
- Integration over all \mathbf{k}' gives the total scattering rate Γ_k :

$$\Gamma_k^i = \frac{n_i Z^2 e^4 m^*}{8\pi\epsilon_{sc}^2 \hbar^3 k^3} \left[\frac{4k^2}{q_D^2(4k^2 + q_D^2)} \right]; \quad q_D = 1/\lambda$$

ASU Computational Electronics

(A1) Neutral Impurities scattering

- This scattering mechanism is due to unionized donors, neutral defects; short range, point-like potential.
- May be modeled as bound hydrogenic potential.
- Usually not strong unless very high concentrations ($>1 \times 10^{19}/\text{cm}^3$).

(B) Alloy Disorder Scattering

- This is short-range type of interaction as well.
- It is calculated in the virtual crystal approximation or coherent potential approximation.
- Limits mobility of ternary and quaternary compounds, particularly at low temperature.
- The total scattering rate out of state \mathbf{k} for this scattering mechanism is of the form:

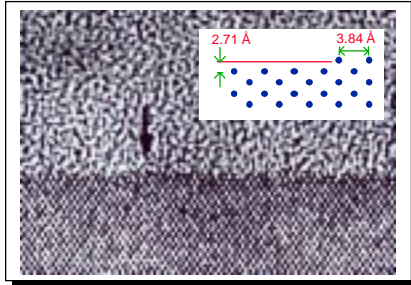
$$\Gamma_k^{alloy} = \frac{(\delta E)^2}{2\pi\hbar} \left(\frac{2m^*}{\hbar^2} \right)^{3/2} E^{1/2}$$

ASU Computational Electronics

(C) Surface Roughness Scattering

- This is a short range interaction due to fluctuations of heterojunction or oxide-semiconductor interface.
- Limits mobility in MOS devices at high effective surface fields.

High-resolution transmission electron micrograph of the interface between Si and SiO₂ (Goodnick et al., Phys. Rev. B 32, pp. 8171, 1985)



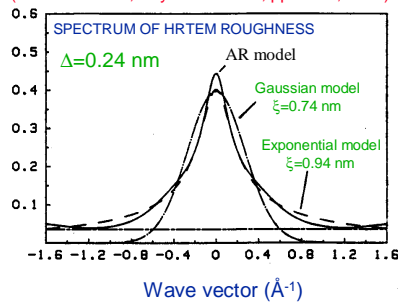
Modeling surface-roughness scattering potential:

$$H'(r, z) = V_0\theta[-z + \Delta(r)] - V_0\theta[-z] \approx V_0\delta(z)\Delta(r)$$

random function that describes the deviation from an atomically flat interface

- Extensive experimental studies have led to two commonly used forms for the autocovariance function.
- The power spectrum of the autocovariance function is found to be either Gaussian or exponentially correlated.

Comparison of the fourth-order AR spectrum with the fits arising from the Exponential and Gaussian models (Goodnick et al., Phys. Rev. B 32, pp. 8171, 1985)



Commonly assumed power spectrums for the autocovariance function :

- Gaussian: $S_G(q) = \pi\Delta^2\zeta^2 \exp\left(-\frac{q^2\zeta^2}{4}\right)$
- Exponential: $S_E(q) = \frac{\pi\Delta^2\zeta^2}{(1+q^2\zeta^2/2)^{3/2}}$

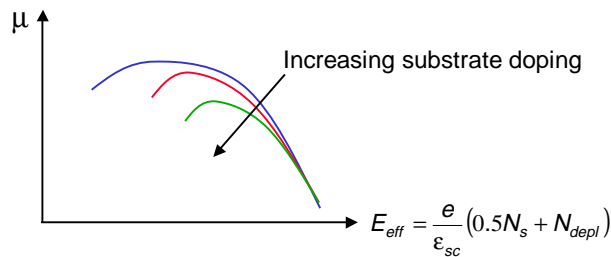
- Note that Δ is the r.m.s of the roughness and ζ is the roughness correlation length.

- The total scattering rate out of state k for surface-roughness scattering is of the form:

$$\Gamma_k^{sr} = \frac{m^* \Delta^2 \zeta^2 e^4}{\hbar^3 \epsilon_{sc}^2} (N_{depl} + 0.5N_s) \frac{1}{\sqrt{1 + k^2 \zeta^2}} E\left(\frac{k\zeta}{\sqrt{1 + k^2 \zeta^2}}\right)$$

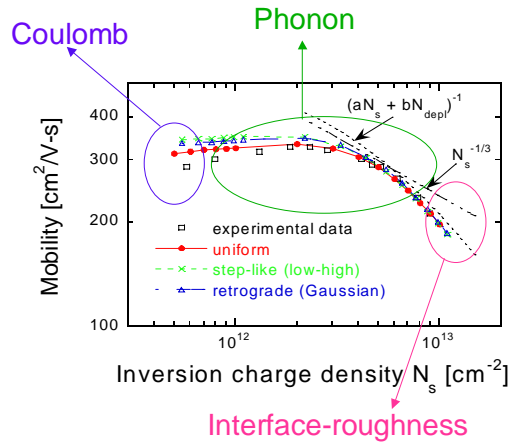
where E is a complete elliptic integral, N_{depl} is the depletion charge density and N_s is the sheet electron density.

- It is interesting to note that this scattering mechanism leads to what is known as the *universal mobility behavior*, used in mobility models described earlier.



The Role of Interface Roughness:

D. Vasileska and D. K. Ferry, "Scaled silicon MOSFET's: Part I - Universal mobility behavior," *IEEE Trans. Electron Devices* **44**, 577-83 (1997).



2.2 Inelastic Scattering Mechanisms

2.2.1 Some general considerations

- The **Electron Lattice Hamiltonian** is of the following form:

$$H = H_e + H_l + H_{ep}$$

$H_e = \text{Electron Hamiltonian}; H_l = \text{lattice Hamiltonian}$

$H_{ep} = \text{Electron – Phonon coupling}$

where $H_e \psi_{n,k} = E_{n,k} \psi_{n,k}$ $\psi_{n,k} = e^{ik \cdot r} u_{n,k}$ Bloch states

- For the lattice Hamiltonian we have:

$$H_l \phi_l = E_l \phi_l \quad \phi_l \Rightarrow |n_{q1} n_{q2} n_{q3} \dots\rangle$$

$$E_l = \sum_{\xi, q} \hbar \omega_q^\xi \left(n_q^\xi + \frac{1}{2} \right) \quad \text{Second quantized representation, where } n_q \text{ is the number of phonons with wave-vector } \mathbf{q}, \text{ mode } \xi.$$

- Phonons:**

The Fourier expansion in reciprocal space of the coupled vibrational motion of the lattice decouples into *normal modes* which look like an independent set of Harmonic oscillators with frequency ω_q^ξ

ξ labels the mode index, acoustic (longitudinal, 2 transverse modes) or optical (1 longitudinal, 2 transverse)

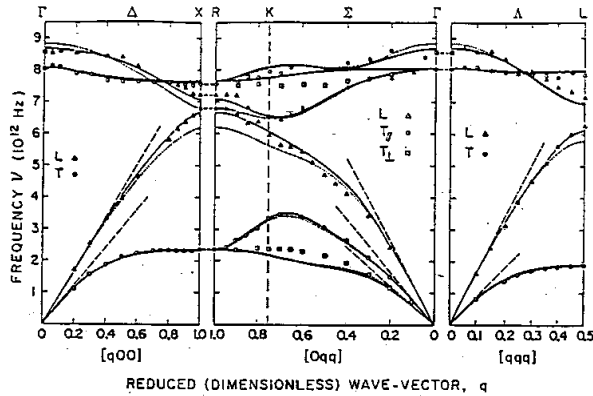
\mathbf{q} labels the wavevector corresponding to traveling wave solutions for individual components,

- The velocity and the occupancy of a given mode are given by:

$$v_q^\xi = \frac{\partial \omega_q^\xi}{\partial q}$$

$$n_q^\xi = \frac{1}{e^{\hbar \omega_q^\xi / k_B T_i} - 1}; \quad \text{Bose – Einstein distribution}$$

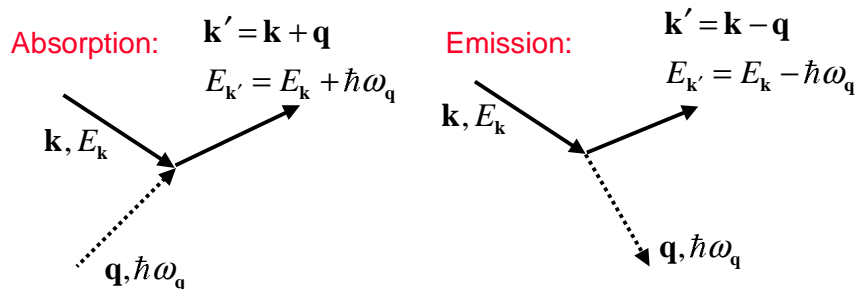
- (1) For **acoustic modes**, $\lim_{q \rightarrow 0} v_q^{\xi} = \frac{\partial \omega_q^{\xi}}{\partial q} = u^{\xi}$, acoustic velocity.
- (2) For **optical modes**, velocity approaches zero as q goes to zero.



Room temperature dispersion curves for the acoustic and the optical branches. Note that phonon energies range between 0 and 60-70 meV.

- The **Electron-Phonon Interaction** is categorized as to mode (acoustic or optical), polarization (transverse or longitudinal), and mechanism (deformation potential, polar, piezoelectric).

During scattering processes between electrons and phonon, both wavevector and energy are conserved to lowest order in the perturbation theory. This is shown diagrammatically in the figures below.



- For emission, $E_{k'} \geq \hbar\omega_q$ must hold, otherwise it is prohibited by conservation of energy. Therefore, there is an emission threshold in energy
- Emission: $n'_q = n_q + 1$ Absorption: $n'_q = n_q - 1$

2.2.2 Deformation Potential Scattering

Replace H_{ep} with the shift of the band edge energy produced by a homogeneous strain equal to the local strain at position \mathbf{r} resulting from a lattice mode of wavevector \mathbf{q}

(A) Acoustic deformation potential scattering

- Expand $E(\mathbf{k})$ in terms of the strain. For spherical constant energy surface

$$E(\mathbf{k}) = E^0(\mathbf{k}) + E_1\Delta + \mathcal{O}(\epsilon^2)$$

where:

$$\Delta = \nabla \cdot \mathbf{u}(\mathbf{r}) = \text{dilation of volume of unit cell}$$

$$E_1 = \text{Deformation potential const.}$$

$$E_1\Delta = \text{Deformation potential}$$

and \mathbf{u} is the displacement operator of the lattice

$$\mathbf{u}^\xi(\mathbf{r}) = \sum_{\mathbf{q}} \left(\frac{\hbar}{2NM\omega_{\mathbf{q}}^\xi} \right)^{1/2} \bar{\mathbf{e}}_{\mathbf{q},\xi} \left(a_{\mathbf{q},\xi} e^{i\mathbf{q}\cdot\mathbf{r}} + a_{\mathbf{q},\xi}^* e^{-i\mathbf{q}\cdot\mathbf{r}} \right)$$

$$\bar{\mathbf{e}}_{\mathbf{q},\xi} = \text{polarization vector}$$

- Taking the divergence gives factor of $\mathbf{e}\cdot\mathbf{q}$ of the form:

$$\bar{\mathbf{e}}_{\mathbf{q},\xi} \cdot \mathbf{q} = q \text{ for longitudinal modes}$$

$$\bar{\mathbf{e}}_{\mathbf{q},\xi} \cdot \mathbf{q} = 0 \text{ for transverse modes}$$

Therefore, only longitudinal modes contribute.

- For ellipsoidal valleys (i.e. Si, Ge), shear strains may contribute to the scattering potential

$$E(\mathbf{k}) \cong E^0(\mathbf{k}) + E_d \Delta + E_u e_{zz}$$

$$e_{zz} \cong \frac{\partial u}{\partial z} \cdot \hat{z}; \quad e_{zz} \text{ is component of the strain tensor}$$

Scattering Matrix Element:

Assuming $\omega_q = u_l q$, then:

$$|V_{ac}|^2 = \frac{\hbar E_1^2 q_{\pm} (n_q + 1 \mp 1)}{2V\rho u_l} \begin{pmatrix} \text{upper absorption} \\ \text{lower emission} \end{pmatrix}$$

- At sufficient high temperature, (equipartition approximation):

$$n_q \approx n_q + 1 \approx \frac{k_B T_l}{\hbar \omega_q}$$

- Substituting and assuming linear dispersion relation, Fermi's rule becomes

$$\Gamma_{kk'}^{ac} = \frac{2\pi}{\hbar} |V_{ac}|^2 \delta(E_{k'} - E_k \mp \hbar \omega_q) = \frac{2\pi E_1^2 k_B T_l}{\hbar V \rho u_l^2} \delta(E_{k'} - E_k \mp \hbar \omega_q)$$

- The total scattering rate due to acoustic modes is found by integrating over all possible final states \mathbf{k}'

$$\Gamma_k^{ac} = \frac{2\pi E_1^2 k_B T_l}{\hbar V \rho u_l^2} \frac{V}{8\pi^3} (4\pi) \int_0^{\infty} dk' k'^2 \delta(E_{k'} - E_k \mp \hbar \omega_q)$$

where the integral over the polar and azimuthal angles just gives 4π .

- For acoustic modes, the phonon energies are relatively small since

$$\omega_q \rightarrow 0 \text{ as } q \rightarrow 0$$

- Integrating gives (assuming a parabolic band model)

$$\Gamma_k^{ac} = \frac{m^* k E_1^2 (k_B T)_l}{\pi \hbar^3 c_l}; \quad c_l = \rho u_l^2$$

where c_l is the longitudinal elastic constant. Replacing k , using parabolic band approximation, finally leads to:

$$\Gamma_k^{ac} = \frac{\sqrt{2} m^{*3/2} E_1^2 (k_B T)_l}{\pi \hbar^4 c_l} E^{1/2}$$

- Assumptions made in these derivations:

- spherical parabolic bands*
- equipartition (not valid at low temperatures)*
- quasi-elastic process (non-dissipative)*
- deformation potential Ansatz*

(B) Optical deformation potential scattering

(Due to symmetry of CB states, forbidden for Γ -minimas)

- Assume no dispersion:

$$\omega_q \rightarrow \omega_0 \text{ as } q \rightarrow 0$$

Out of phase motion of basis atoms creates a strain called the optical strain.

- This takes the form (D_0 is optical deformation potential field)

$$V_{do} = \vec{D}_0 \cdot \mathbf{u}(\mathbf{r}); \quad D_0 \approx \vec{D}_0 \cdot \vec{e}_q \quad \text{zeroth order}$$

The matrix element for spherical bands is given by

$$|V_{kk'}^{ac}|^2 = \left(\frac{\hbar D_0^2}{2\rho V\omega_0} \right) \left\{ n_{\omega_0} \delta(\mathbf{k} - \mathbf{k}' + \mathbf{q}) + [n_{\omega_0} + 1] \delta(\mathbf{k} - \mathbf{k}' - \mathbf{q}) \right\}$$

which is independent of \mathbf{q} .

- The total scattering rate is obtained by integrating over all \mathbf{k}' for both absorption and emission

$$\Gamma_k^{do} = \frac{1}{\tau_{do}} = \frac{m^{*3/2} D_0^2}{\sqrt{2\pi\rho\hbar^3\omega_0}} \left\{ n_{\omega_0} (E + \hbar\omega_0)^{1/2} + [n_{\omega_0} + 1] (E - \hbar\omega_0)^{1/2} \Theta(E - \hbar\omega_0) \right\}$$

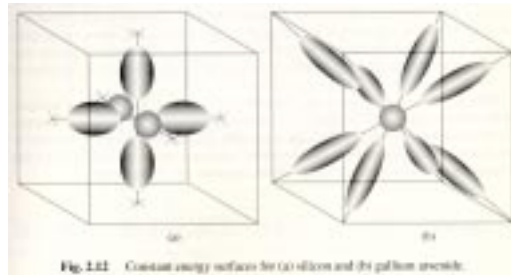
where the first term in brackets is the contribution due to absorption and the second term is that due to emission

- For non-spherical valleys, replace $m^{*3/2} \Rightarrow m_t m_l^{1/2}$
- The non-polar scattering rate is basically proportional to density of states

$$\Gamma_k^{do} \propto \rho(E \pm \hbar\omega_0)$$

(C) Intervalley scattering

- May occur between equivalent or nonequivalent sets of valleys



- Intervalley scattering is important in explaining room temperature mobility in multi-valley semiconductors, and the NDR observed (Gunn effect) in III-V compounds
- Crystal momentum conservation requires that $\mathbf{q} \approx \Delta\mathbf{k}$ where \mathbf{k} is the vector joining the two valley minima

- Since $\Delta \mathbf{k}$ is large compared to \mathbf{k} , assume $\omega_{\mathbf{q}} \rightarrow \omega_{\Delta \mathbf{q}}$ and treat the scattering the same as non-polar optical scattering replacing D_0 with D_{ij} the intervalley deformation potential field, and the phonon coupling valleys i and j

$$\omega_{\mathbf{q}} \rightarrow \omega_{ij}$$

- Conservation of energy also requires that the difference in initial and final valley energy be accounted for, giving

$$\Gamma_k^{iv} = \sum_j \frac{m_{d_j}^{3/2} D_{ij}^2}{\sqrt{2\pi} \rho \hbar^3 \omega_{ij}} \left\{ n_{\omega_{ij}} (E - \Delta E_{ij} + \hbar \omega_{ij})^{1/2} + [n_{\omega_{ij}} + 1] (E - \Delta E_{ij} - \hbar \omega_{ij})^{1/2} \Theta(E - \Delta E_{ij} - \hbar \omega_{ij}) \right\}$$

where the sum is over all the final valleys, j and

$$\Delta E_{ij} = E_{\min j} - E_{\min i}$$

2.2.3 Phonon Scattering in Polar Semiconductors

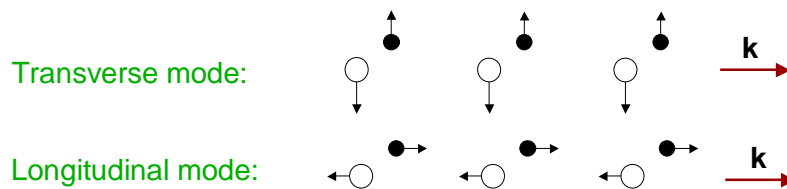
- Zinc-blend crystals: one atom has $Z > 4$, other has $Z < 4$.
- The small charge transfer leads to an effective dipole which, in turn, leads to lattice contribution to the dielectric function.
- Deformation of the lattice by phonons perturbs the dipole moment between the atoms, which results in electric field that scatters carriers.
- Polar scattering may be due to:
 - optical phonons \Rightarrow polar optical phonon scattering (very strong scattering mechanism for compound semiconductors such as GaAs)
 - acoustic phonons \Rightarrow piezoelectric scattering (important at low temperatures in very pure semiconductors)

(A) Polar Optical Phonon Scattering (POP)

Scattering Potential:

Microscopic model is difficult. A simpler approach is to consider the contribution of this dipole to the polarization of the crystal and its effect on the high- and low-frequency dielectric constants.

- Consider a diatomic lattice in the long-wavelength limit ($\mathbf{k} \approx 0$), for which identical atoms are displaced by a same amount.
- For optical modes, the oppositely charged ions in each primitive cell undergo oppositely directed displacements, which gives rise to nonvanishing polarization density \mathbf{P} .



- Associated with this polarization are macroscopic electric field \mathbf{E} and electric displacement \mathbf{D} , related by:

$$\mathbf{D} = \epsilon_{\infty} \mathbf{E} + \mathbf{P}$$



Here, we have taken into account the contribution to the dielectric function due to valence electrons

- Assume $\mathbf{D}, \mathbf{E}, \mathbf{P} \propto e^{i\mathbf{k}\cdot\mathbf{r}}$. Then, in the absence of free charge:

$$\nabla \cdot \mathbf{D} = i\mathbf{k} \cdot \mathbf{D} = 0 \quad \text{and} \quad \nabla \times \mathbf{E} = i\mathbf{k} \times \mathbf{E} = 0$$



$$\mathbf{k} \perp \mathbf{D} \quad \text{or} \quad \mathbf{D} = 0$$

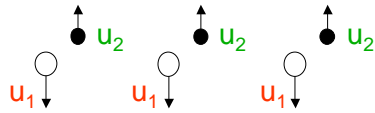


$$\mathbf{k} \parallel \mathbf{E} \quad \text{or} \quad \mathbf{E} = 0$$

- Longitudinal modes: $\mathbf{P} \parallel \mathbf{k} \Rightarrow \mathbf{D} = 0, \epsilon(\omega_{LO}) = 0$
- Transverse modes: $\mathbf{P} \perp \mathbf{k} \Rightarrow \mathbf{E} = 0, \epsilon(\omega_{TO}) = \infty$

- The equations of motion of the two modes (in the $k \rightarrow 0$ limit), for the relative displacement of the two atoms in the unit cell $w = u_1 - u_2$ are:

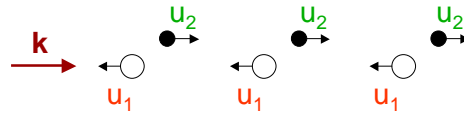
Transverse mode:



$$\frac{d^2 w}{dt^2} + \omega_{TO}^2 w = 0$$

$$\omega_{TO}^2 = 2C \left(\frac{1}{M_1} + \frac{1}{M_2} \right) = \frac{2C}{\bar{M}}$$

Longitudinal mode:



$$\frac{d^2 w}{dt^2} + \omega_{TO}^2 w = \frac{1}{\bar{M}} e^* E$$

$$E(t) = E e^{j\omega t}$$

$$w = \frac{e^* E / \bar{M}}{\omega_{TO}^2 - \omega^2}$$

ASU Computational Electronics

- The longitudinal displacement of the two atoms in the unit cell leads to a polarization dipole:

$$\mathbf{P} = \frac{N}{2V} e^* \mathbf{w} = \frac{N e^{*2} / 2V \bar{M}}{\omega_{TO}^2 - \omega^2} \mathbf{E}$$

- The existence of a finite polarization dipole modifies the dielectric function:

$$\mathbf{D} = \epsilon_\infty \mathbf{E} + \mathbf{P} = \epsilon_\infty \mathbf{E} + \frac{N e^{*2} / 2V \bar{M}}{\omega_{TO}^2 - \omega^2} \mathbf{E} = \epsilon(\omega) \mathbf{E}$$

$$\epsilon(\omega) = \epsilon_\infty \left(1 + \frac{S}{\omega_{TO}^2 - \omega^2} \right) = \epsilon_\infty \left(1 + \frac{\omega_{LO}^2 - \omega_{TO}^2}{\omega_{TO}^2 - \omega^2} \right)$$

Polarization constant $\longrightarrow S = \frac{N e^{*2}}{2V \epsilon_\infty \bar{M}} = \omega_{LO}^2 \epsilon_\infty \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon(0)} \right)$

ASU Computational Electronics

- The electric field associated with the perturbed dipole moment is obtained from the condition that, in the absence of macroscopic free charge:

$$\nabla \cdot \mathbf{D} = \nabla \cdot (\epsilon_\infty \mathbf{E}_{ind} + \mathbf{P}) = 0 \Rightarrow \mathbf{D} = 0 \text{ and } \mathbf{E}_{ind} = -\frac{\mathbf{P}}{\epsilon_\infty}$$

- Consider only one Fourier component:

$$\mathbf{E}_{ind} = -\nabla \varphi_{ind} = \frac{1}{e} \nabla V(q) = \frac{1}{e} \nabla [V_q e^{i\mathbf{q}\cdot\mathbf{r}}] = i \frac{1}{e} \mathbf{q} V(q)$$

$$V(q) = i \frac{e}{\epsilon_\infty q^2} \mathbf{q} \cdot \mathbf{P} \Rightarrow V(q) = i \frac{e}{\epsilon_\infty q} P$$

$$V(\mathbf{r}) = i \frac{e}{\epsilon_\infty} \frac{N}{2V} e^* \sqrt{\frac{\hbar}{2M(N/2)\omega_{LO}}} \sum_q \frac{1}{q} (a_q e^{i\mathbf{q}\cdot\mathbf{r}} + a_q^+ e^{-i\mathbf{q}\cdot\mathbf{r}})$$

$$= i \left(\frac{\hbar e^2}{2V\gamma\omega_{LO}} \right)^{1/2} \sum_q \frac{1}{q} (a_q e^{i\mathbf{q}\cdot\mathbf{r}} + a_q^+ e^{-i\mathbf{q}\cdot\mathbf{r}}), \quad \frac{1}{\gamma} = \omega_{LO}^2 \left[\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon(0)} \right]$$

ASU Computational Electronics

Scattering Rate Calculation:

- Matrix element squared for this interaction:

$$|V_{k,k'}|^2 = \frac{\hbar e^2}{2V\gamma\omega_{LO}} \frac{1}{q^2} (N_0 + \frac{1}{2} \mp \frac{1}{2}) \delta(\mathbf{k}' - \mathbf{k} \mp \mathbf{q})$$

- Transition rate per unit time from state \mathbf{k} to state \mathbf{k}' :

$$\Gamma_{k,k'} = \frac{2\pi}{\hbar} |V_{k,k'}|^2 \delta(\epsilon_{k'} - \epsilon_k \mp \hbar\omega_{LO})$$

$$= \frac{\pi e^2}{V\gamma\omega_{LO}} \frac{1}{q^2} (N_0 + \frac{1}{2} \mp \frac{1}{2}) \delta(\mathbf{k}' - \mathbf{k} \mp \mathbf{q}) \delta(\epsilon_{k'} - \epsilon_k \mp \hbar\omega_{LO})$$

- Total scattering rate per unit time out of state \mathbf{k} :

$$\Gamma_k = \sum_{k'} \Gamma_{k,k'} = \sum_q \Gamma_{k,q} = \frac{V}{(2\pi)^3} \int_0^{2\pi} d\varphi \int_{-1}^1 d(\cos\theta) \int_0^\infty q^2 \Gamma_{k,q} dq$$

ASU Computational Electronics

- Momentum and energy conservation delta-functions limit the values of q in the range $[q_{\min}, q_{\max}]$:

$$\text{absorption: } q_{\min} = -k + k\sqrt{1 + \hbar\omega_{LO}/E(k)}$$

$$q_{\max} = k + k\sqrt{1 + \hbar\omega_{LO}/E(k)}$$

$$\text{emission: } q_{\min} = k - k\sqrt{1 - \hbar\omega_{LO}/E(k)}$$

$$q_{\max} = k + k\sqrt{1 - \hbar\omega_{LO}/E(k)}$$

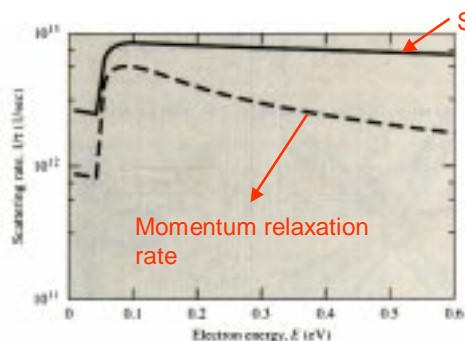
$$E(k) \geq \hbar\omega_{LO}, \text{ emission threshold}$$

- Final expression for Γ_k

$$\Gamma_k = \frac{m^* e^2}{2\pi\hbar^2 k \gamma \omega_{LO}} \left[N_0 \sinh^{-1} \left(\sqrt{\frac{E(k)}{\hbar\omega_{LO}}} \right) + (N_0 + 1) \sinh^{-1} \left(\sqrt{\frac{E(k)}{\hbar\omega_{LO}} - 1} \right) \right]$$

Discussion:

1. The $1/q^2$ dependence of $\Gamma_{k,k'}$ implies that polar optical phonon scattering is anisotropic, i.e. favors small angle scattering
2. It is inelastic scattering process
3. Γ_k is nearly constant at high energies
4. Important for GaAs at room-temperature and II-VI compounds (dominates over non-polar)



Scattering rate

Momentum relaxation rate

The larger momentum relaxation time is a consequence of the fact that POP scattering favors small angle scattering events that have smaller influence on the momentum relaxation.

(B) Piezoelectric scattering

- Since the polarization is proportional to the acoustic strain, we have

$$\mathbf{P} = e_{pz} \nabla \cdot \mathbf{u}$$

- Following the same arguments as for the polar optical phonon scattering, one finds that the matrix element squared for this mechanism is:

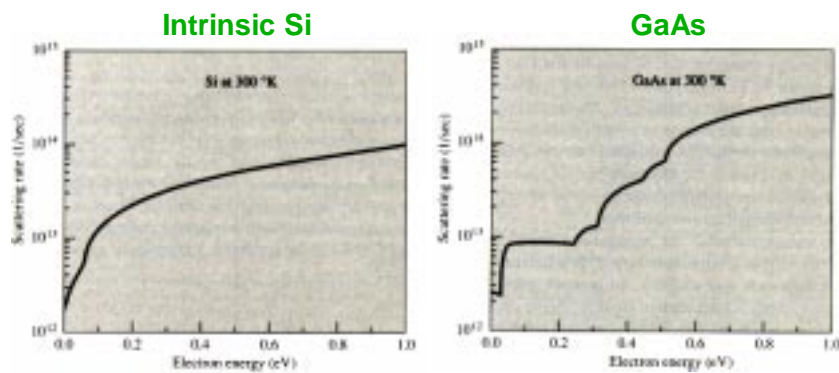
$$|V_{kk'}|^2 = \frac{\hbar}{2\rho V\omega_{qv}} \left(\frac{ee_{pz}}{\epsilon_\infty} \right)^2 \left(N_q + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\mathbf{k} - \mathbf{k}' \pm \mathbf{q})$$

- The scattering rate, in the elastic and the equipartition approximation, is then of the form;

$$\Gamma_k = \frac{m^* k_B T}{4\pi\hbar^3 k\rho} \left(\frac{ee_{pz}}{\epsilon_\infty v_s} \right)^2 \ln \left(1 + 4 \frac{k^2}{q_D^2} \right)$$

where q_D is the screening wavevector.

Total Electron Scattering Rate Versus Energy:



In both cases the electron scattering rates were calculated by assuming non-parabolic energy bands.

3. Monte Carlo method for the solution of the BTE

- The Monte Carlo method is a stochastic method for solving the Boltzmann Transport equation.
- Semiclassical particle motion is assumed to be decomposed into:

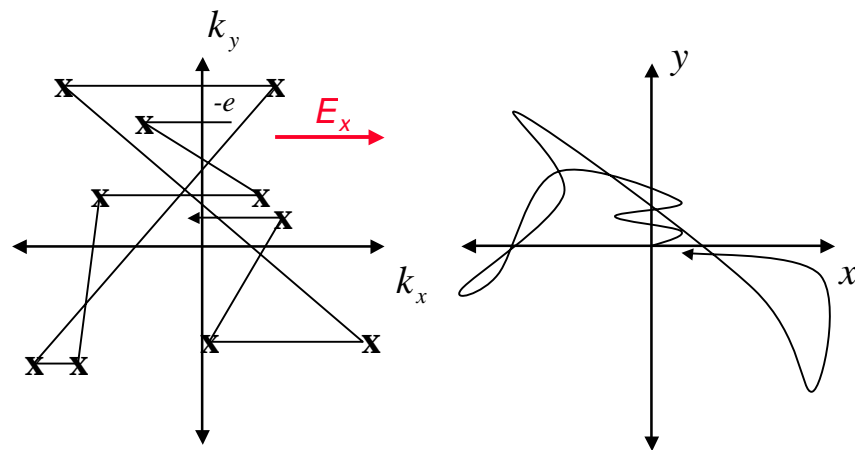
– free flights (subject to external forces)

$$\mathbf{k}(t) = \mathbf{k}(0) - e(\mathbf{v} \times \mathbf{B} + \mathbf{E})t/\hbar$$

– Instantaneous, memory-less, scattering events
(Elastic, inelastic, intercarrier, electron-photon, etc.)

References:

- 1) C. Jacoboni and L. Reggiani, *Rev. Mod. Phys.* 55, no. 3, pp. 645-705, 1983
- 2) C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation*, 1990



Particle trajectories in k-space and real space

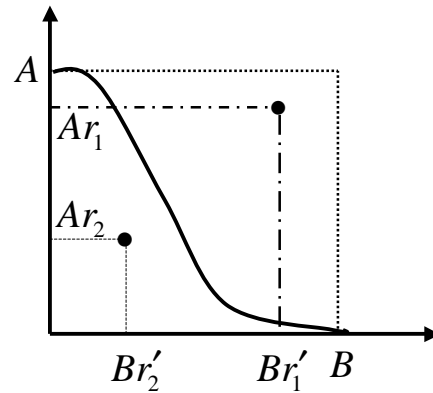
3.1 Monte Carlo Integration

(M. H. Kalas and P. A. Whitlock, "Monte Carlo Methods," John Wiley, 1986)

Suppose we want to integrate: $g(x) = Ae^{-(x/L)^2}$ $0 < x < B$

Monte Carlo Algorithm:

- Define ceiling function
 $g(x) = A$
- Generate pairs of random numbers: r_1, r_1'
If $Ar_1 > g(Br_1')$ reject
If $Ar_2 < g(Br_2')$ accept
- Ratio of accepted to total times area AB is integral



Typical algorithm for accomplishing this goal is:

```
acceptnum=0
do 10 i=1,nsampltot
  xval=rand()*Bmax
  yval=rand()*Amax
  gy=Amax*exp(-(xval/Lg)**2)
  if (gy.gt.yval) acceptnum=acceptnum+1
10 continue
area=Amax*Bmax*acceptnum/nsampltot
```

Here `rand()` is a generic call to a random number generator (either intrinsic or subroutine). Ideally it produces a uniformly distributed random number between 0 and 1

3.2 Generation of Random Flight Times

- The probability of an electron scattering in a small time interval dt is $\Gamma(\mathbf{k})dt$, where $\Gamma(\mathbf{k})$ is the total transition rate per unit time. Time dependence originates from the change in $\mathbf{k}(t)$ during acceleration by external forces

$$\mathbf{k}(t) = \mathbf{k}(0) - e(\mathbf{E} + \mathbf{v} \times \mathbf{B})t / \hbar$$

where \mathbf{v} is the velocity of the particle.

- The probability that an electron has not scattered after scattering at $t = 0$ is:

$$P_n(t) = e^{-\int_0^t dt \Gamma(\mathbf{k}(t))}$$

- The probability therefore that an electron will suffer its next collision during dt around t is

$$P(t)dt = \Gamma(\mathbf{k}(t))e^{-\int_0^t dt \Gamma(\mathbf{k}(t))} dt$$

$P(t)$ represents a non-uniform distribution of *free flight times* over a semi-infinite interval 0 to ∞ . We want to sample random flight times from this non-uniform distribution using uniformly distributed random numbers over the interval 0 to 1, corresponding to typical numerical random number generators.

- To calculate the carrier free-flight time, it is necessary to generate random numbers x with a given probability distribution $f(x)$ over an interval (a,b) from evenly distributed numbers r .

(A) Direct Technique

- If $P(r)$ is a uniform distribution between 0 and 1 then:

$$r = \int_0^r dr' P(r') = F = \int_a^{x_r} f(x) dx / \int_a^b f(x) dx$$

where x_r is a random number sampled from $f(x)$. x_r is found by inverting this integration.

- Example, for constant $f(x)$ is given below:

$$r = (x_r - a)/(b - a) \quad \text{or} \quad x_r = a + r(b - a)$$

(B) Rejection Technique

- For most cases of interest, the integral cannot be easily inverted. As in the case of Monte Carlo integration, a *rejection* technique may be employed.
- Choose a maximum value C , such that $C > f(x)$ for all x in the interval (a,b) .
- As in the case of Monte Carlo integration, pairs of random numbers are chosen, one between a and b

$$x_1 = a + r_1(b - a)$$

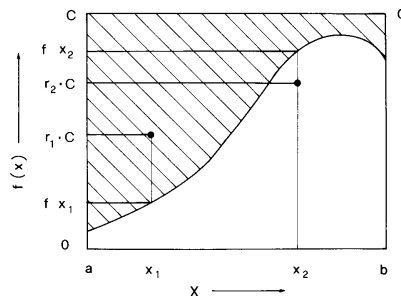
and another between 0 and C :

$$f_1 = r_1' C$$

- If

$$f_1 \leq f(x_1)$$

the number x_1 is accepted as a suitable sample, otherwise it is rejected.



(C) Combined Technique

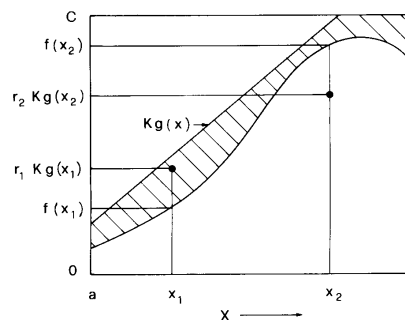
- If the probability function is singular in nature, the simple rejection technique with a constant ceiling function may be inefficient. If a ceiling function may be defined such that

$$Kg(x) \geq f(x)$$

over the range of interest, and random numbers may be sample from g using the direct technique, then a combined technique may be used, where if:

$$r_1 Kg(x_1) \leq f(x_1)$$

the random number x_1 is accepted.



(D) Self-Scattering

- The use of the full integral form of the free-flight probability density function is tedious (unless \mathbf{k} is invariant during the free flight).
- The introduction of *self-scattering* (Rees, *J. Phys. Chem. Solids* **30**, 643, 1969) simplifies the procedure considerably.
- The properties of the self-scattering mechanism are that it does not change either the energy or the momentum of the particle.
- The self-scattering rate adjusts itself in time so that the total scattering rate is constant. Under these circumstances, one has that:

$$\Gamma = \Gamma(\mathbf{k}(t)) + \Gamma_{\text{self}}(\mathbf{k}(t)) \quad P(t)dt = \Gamma e^{-\int_0^t dt \Gamma} dt = \Gamma e^{-\Gamma t} dt$$

- Random flight times t_r may be generated from $P(t)$ above using the direct method to get:

$$r = e^{-\Gamma t_r} \quad t_r = -\frac{1}{\Gamma} \ln(1-r) = -\frac{1}{\Gamma} \ln(r)$$

where r is a uniform random between 0 and 1 (and therefore r and $1-r$ are the same).

- Γ must be chosen (a priori) such that $\Gamma > \Gamma(\mathbf{k}(t))$ during the entire flight.
- Choosing a new t_r after every collision generates a random walk in \mathbf{k} -space over which statistics concerning the occupancy of the various states \mathbf{k} are collected.

3.3 Choice of Scattering Event Terminating Free Flight

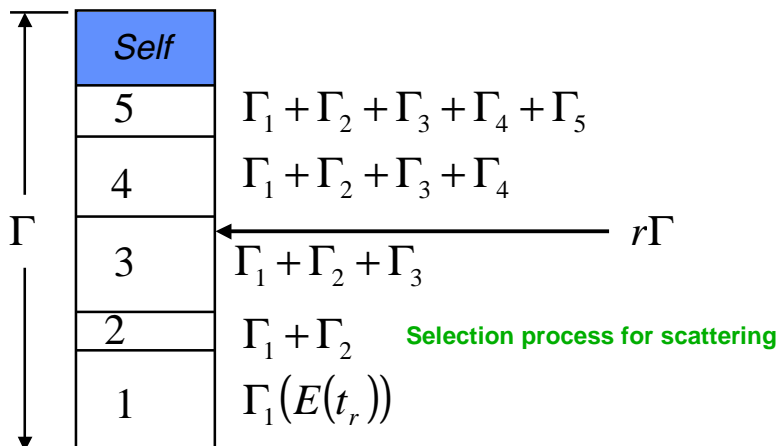
- At the end of the free flight t_r , the type of scattering which ends the flight (either real or self-scattering) must be chosen according to the relative probabilities for each mechanism.
- Assume that the total scattering rate for each scattering mechanism is a function only of the energy, E , of the particle at the end of the free flight

$$\Gamma = \Gamma_{self}(E) + \Gamma_i(E) + \Gamma_{ac}(E) + \Gamma_{pop}(E) + \dots$$

where the rates due to the real scattering mechanisms are typically stored in a lookup table.

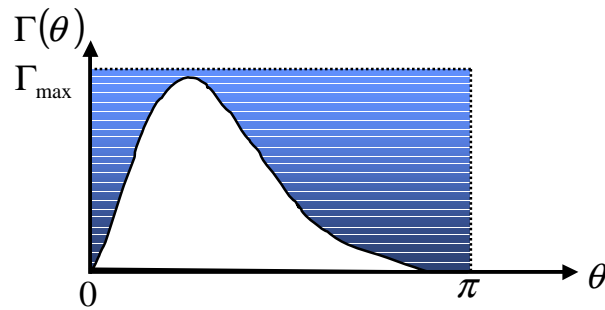
- A histogram is formed of the scattering rates, and a random number $r\Gamma$ is used as a pointer to select the right mechanism. This is schematically shown on the next slide.

Choice of Scattering Event Terminating Free Flight:



- Below is an example given for the choice of the polar angle for POP scattering:

$$\Gamma_{POP}(\theta)d\theta \sim \frac{\sin(\theta)d\theta}{(E + E' - 2\sqrt{EE'} \cos \theta)}$$



Angular dependence for POP scattering
(A rejection technique may be used to choose final polar angle)

3.5 Ensemble Monte Carlo Simulation

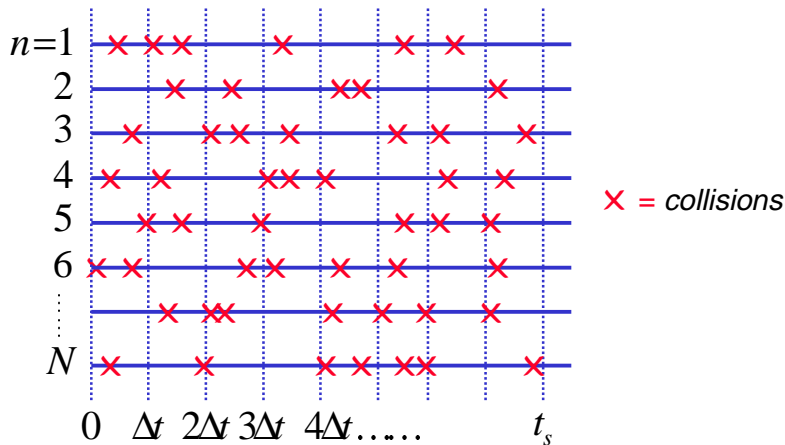
- For **stationary problems**, a single electron may be followed and statistics collected from time averages of the particle motion.
- Estimators may be derived for the average drift velocity, energy, and particle distribution function (e.g.):

$$\bar{v}_z \cong \frac{1}{N_s} \sum_{i=1}^{N_s} v_z(t_i) \quad s = \frac{\sigma}{\sqrt{N_s}}$$

where t_i is the i th free flight and s is the **standard error**, with σ^2 the variance of v_z estimated by:

$$\sigma^2 \cong \frac{N_s}{N_s - 1} \left\{ \frac{1}{N_s} \sum_{i=1}^{N_s} v_z^2(t_i) - \left(\frac{1}{N_s} \sum_{i=1}^{N_s} v_z(t_i) \right)^2 \right\}$$

- For **non-stationary** (e.g. transient) problems, an ensemble Monte Carlo approach is used by considering N particles simultaneously, and introducing a time step, Δt , at which the motion of all the particles is synchronized



- Estimates of the observable quantities are given by averages over the ensemble of particles at each time step (or multiples thereof)

$$\bar{v}_z(n\Delta t) \cong \frac{1}{N} \sum_{j=1}^N v_z^j(n\Delta t); \quad s = \frac{\sigma}{\sqrt{N}}$$

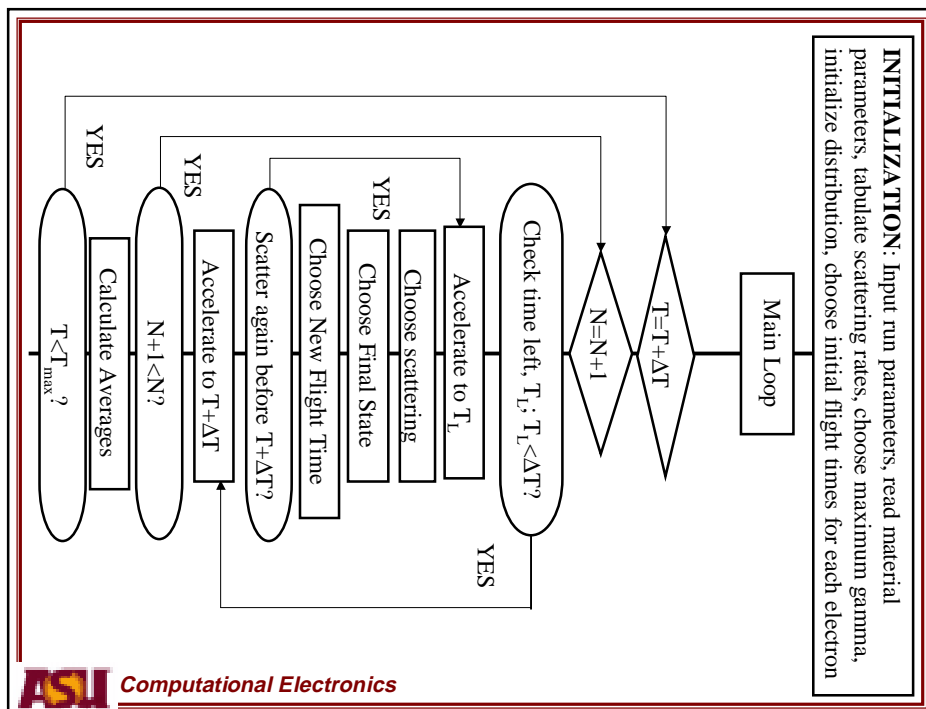
with the variance at each time step estimated as

$$\sigma^2 \cong \frac{N}{N-1} \left\{ \frac{1}{N} \sum_{j=1}^N (v_z^j)^2 - \bar{v}_z^2 \right\}$$

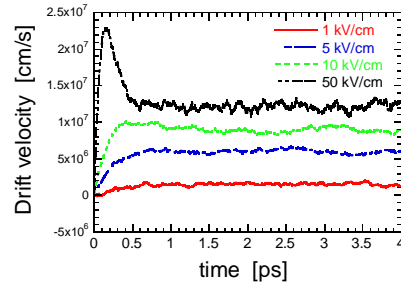
- In steady-state, both ensemble and time averaging may be used to further reduce the error, and this is usually done in practice.

3.6 Monte Carlo Flowchart and Simulation Results

- Constant Γ method: Choose maximum Γ at beginning of simulation, check whether the actual scattering rate ever exceeds this value.
- Input material parameters, maximum energy, tabulate scattering rates, choose Γ_{\max} , choose maximum time for simulation (T_{\max}), time step (ΔT), number of particles, etc.
- After every time step (or multiples of time steps), calculate averages of interest, distribution functions, etc.

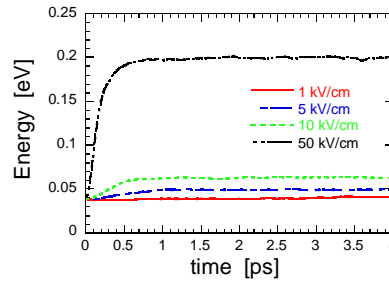


Transient simulation results for Si bulk:

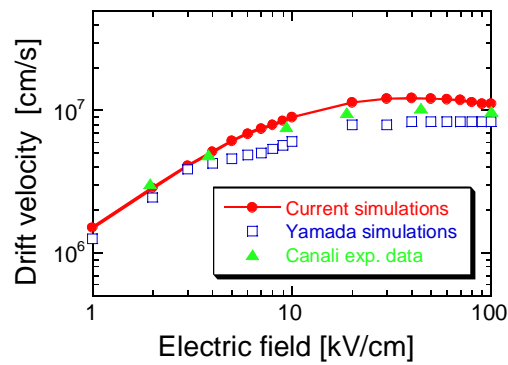


Time evolution of mean drift velocity. Electric field is: (a) 1.0 kV/cm, (b) 5.0 kV/cm, (c) 10 kV/cm, and (d) 50 kV/cm, respectively.

Time evolution of the average electron kinetic energy. The electric field equals: (a) 1 kV/cm, (b) 5 kV/cm, (c) 10 kV/cm, and (d) 50 kV/cm, respectively.



Steady-state simulation results for Si bulk:



Mean drift velocity characteristics with respect to applied electric field. Also shown in this figure are the simulation results by Yamada *et al.* [1] and Canali [2] experimental data.

[1] T. Yamada, J.-R. Zhou, H. Miyata and D. K. Ferry, *Phys. Rev. B*, Vol. **49**, 1875 (1994).
 [2] C. Canali, G. Ottaviani, and A. Alberigi-Quaranta, *J. Phys. Chem. Solids*, Vol. **32**, 1707 (1971).

3.7 Inclusion of the Pauli Exclusion Principle

- The influence of the final state on the scattering rate is important at low temperatures and high carrier densities.
- This effect may be included via a self-scattering rejection method (Bosi and Jacoboni, *J. Phys. C* **9**, 315 (1976); Lugli and Ferry, *IEEE Trans. Elec. Dev.* **32**, 2431 (1985)).
- The electron (hole) distribution function $f(k_x, k_y, k_z)$ is updated in \mathbf{k} -space (on a 2D or a 3D grid).
- Once the final state has been selected, a new random number is generated:
 - If $0 < r < f(\mathbf{k})$, then self-scattering is assumed to occur with no change of momentum or energy
 - If $f(\mathbf{k}) < r < 1$, then accept the scattering event

Let $\frac{N}{n_{2d}} = A = L^2$

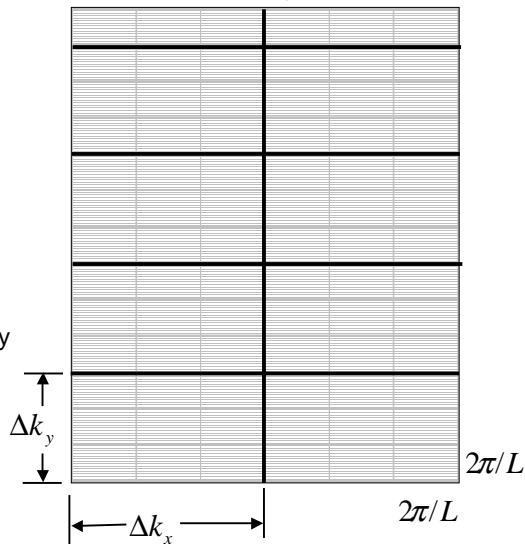
The area per state in k -space is

$$A_k = \left(\frac{2\pi}{L}\right)^2$$

Some important notes:

- The size of the grid in \mathbf{k} -space determines how many electrons may occupy the grid.
- The accuracy improves as the number of particles increases.

Two-Dimensional System Example



3.8 Carrier-Carrier Scattering

- For two-particle interactions, the electron-electron (hole-hole, electron-hole) scattering rate may be treated as a screened Coulomb interaction (impurity scattering in a relative coordinate system). The total scattering rate depends on the instantaneous distribution function, and is of the form:

$$\Gamma_{ee}(k_0) = \frac{m_n e^4}{\hbar^3 V \epsilon_\infty^2} \sum_k f(k) \frac{|k - k_0|}{\beta^2 (|k - k_0|^2 + \beta^2)}$$

β = Screening constant

There are three methods commonly used for the treatment of the electron-electron interaction:

- A. Method due to Lugli and Ferry
- B. Rejection algorithm
- C. Real-space molecular dynamics

(A) Method due to Lugli and Ferry

- This method starts from the assumption that the sum over the distribution function is simply an ensemble average of a given quantity.
- In other words, the scattering rate is defined to be of the form:

$$\Gamma_{ee}(k_0) = \frac{nm_n e^4 L_D^2}{4\pi\hbar^3 \epsilon_\infty^2} \sum_{i=1}^N \frac{|k - k_i|}{|k - k_i|^2 + 1/L_D^2}$$

- The advantages of this method are:
 1. The scattering rate does not require any assumption on the form of the distribution function
 2. The method is not limited to steady-state situations, but it is also applicable for transient phenomena, such as femtosecond laser excitations
- The main limitation of the method is the computational cost, since it involves 3D sums over all carriers and the rate depends on \mathbf{k} rather on its magnitude.

(B) Rejection algorithm

- Within this algorithm, a self-scattering mechanism, internal to the interparticle scattering is introduced by the following substitution:

$$\frac{|k - k_0|}{|k - k_0|^2 + 1/L_D^2} \rightarrow \frac{1}{2L_D}$$

- When carrier-carrier collision is selected, a counterpart electron is chosen at random from the ensemble.
- Internal rejection is performed by comparing the random number with:

$$\frac{|k - k_0|}{|k - k_0|^2 + 1/L_D^2}$$

- If the collision is accepted, then the final state is calculated using:

$$\cos \theta_r = 1 - \frac{2r}{1 + g^2(1-r)L_D^2}, \quad \text{where } \theta_r = \text{angle}(\mathbf{g}, \mathbf{g}')$$

where:

$$\mathbf{g} = \mathbf{k} - \mathbf{k}_0; \quad \mathbf{g}' = \mathbf{k}' - \mathbf{k}_0'$$

The azimuthal angle is then taken at random between 0 and 2π .

- The final states of the two particles are then calculated using:

$$\mathbf{k}'_0 = \mathbf{k}_0 - \frac{1}{2}(\mathbf{g}' - \mathbf{g})$$

$$\mathbf{k}' = \mathbf{k}_0 + \frac{1}{2}(\mathbf{g}' - \mathbf{g})$$

(C) Real-space molecular dynamics

- An alternative to the previously described methods is the real-space treatment proposed by Jacoboni.
- According to this method, at the observation time instant $t_i = i\Delta t$, the total force on the electron equals the sum of the interparticle coulomb interaction between a particular electron and the other $(N-1)$ electrons in the ensemble.
- When implementing this method, several things need to be taken into account:
 1. The fact that N electrons are used to represent a carrier density $n = N/V$ means that a simulation volume equals $V = N/n$.
 2. Periodic boundary conditions are imposed on this volume, and because of that, care must be taken that the simulated volume and the number of particles are sufficiently large that artificial application from periodic replication of this volume do not appear in the calculation results.

- Using Newtonian kinematics, the real-space trajectories of each particle are represented as:

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}\Delta t + \frac{1}{2} \frac{\mathbf{F}(t)}{m^*} \Delta t^2$$

and:

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \frac{\mathbf{F}(t)}{m^*} \Delta t$$

Here, $\mathbf{F}(t)$ is the force arising from the applied field as well as that of the Coulomb interaction:

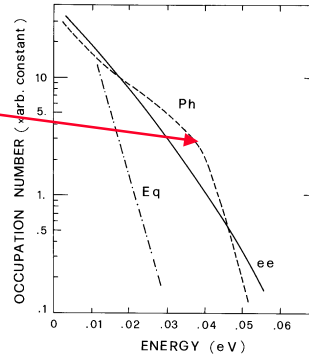
$$\mathbf{F}(t) = q \left[\mathbf{E} - \sum_i \nabla \phi(\mathbf{r}(t)_i) \right]$$

- The contributions due to the periodic replication of the particles inside V in cells outside is represented with the Ewald sum:

$$\mathbf{F}(t) = -\frac{e^2}{4\pi\epsilon} \sum_{i=1}^N \left(\frac{1}{r_i^2} \mathbf{a}_i + \frac{2\pi}{3V} \mathbf{r}_i \right)$$

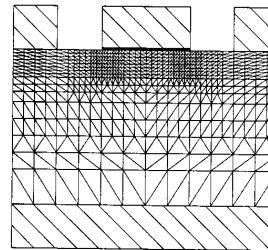
Simulation example of the role of the electron-electron interaction:

- The effect of the e-e scattering allows equilibrium distribution function to approach Fermi-Dirac or Maxwell Boltzmann distribution.
- Without e-e, there is a phonon 'kink' due to the finite energy of the phonon



4. Monte Carlo Device Simulation

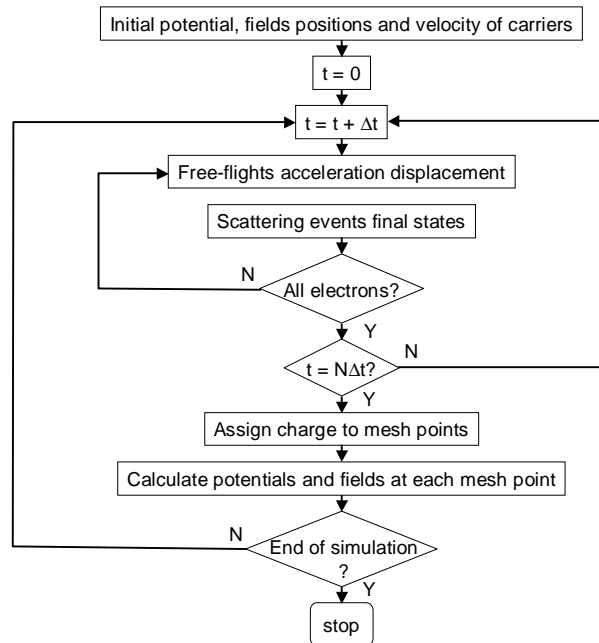
- The extension of the k -space Monte Carlo to simulate semiconductor devices requires that the real space position of each carrier be calculated, and the resulting charge used to solve Poisson's equation simultaneously with the particle dynamics.*
- The semiconductor is discretized using either the finite difference or the finite elements approach for the solution of Poisson's eq.
- The charge of the particles (super particles) is then assigned to the grid points.



*R.W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, McGraw-Hill, 1981

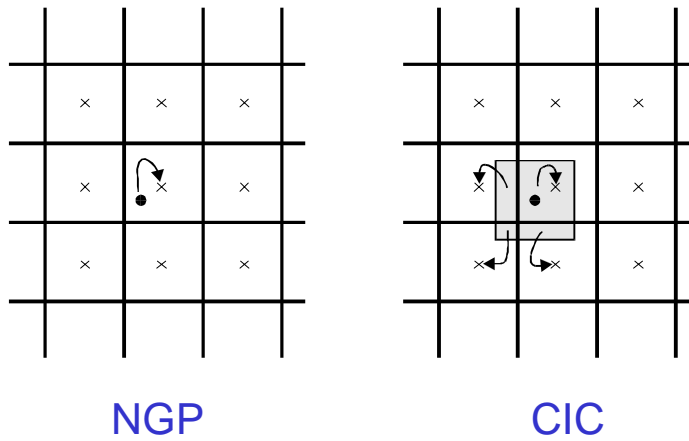
- In the usual algorithm, the Monte Carlo particle dynamics are de-coupled from Poisson's equation over the interval of one time step.
- The particles are accelerated by the interpolated forces derived from the solution of Poisson's equation from the previous time-step.
- The **particle-mesh coupling scheme** consists of the following steps:
 - Assign charge to the Poisson solver mesh
 - Solve Poisson's equation for $V(\mathbf{r})$
 - Calculate the force $q\mathbf{E}(\mathbf{r}) = -q\nabla V(\mathbf{r})$, and interpolate it to the particle locations (q is the charge of the particle)
 - Solve the equations of motion:

$$\frac{d\mathbf{r}}{dt} = \frac{1}{\hbar} \nabla_{\mathbf{k}} E(\mathbf{k}(t)); \quad \frac{d\mathbf{k}}{dt} = \frac{q\mathbf{E}(\mathbf{r})}{\hbar}$$



4.1 Charge Assignment and force interpolation

- There are two methods most commonly used for the charge assignment: Nearest Grid Point (NGP) and Cloud in Cell (CIC) scheme (see figures below):



- In general, the charge on the p_{th} grid point is written as:

$$\rho(r_p) = \frac{q}{V_{cell}} \sum_{i=1}^N W(r_i - r_p)$$

where r_i is the position of the i th particle, V_{cell} is the volume of the p_{th} cell, q is the super-particle charge, and W is the weight function.

- In the NGP scheme*, the weighting function is of the following form:

$$W(r) = \begin{cases} 1 & -H/2 \leq r < H/2 \\ 0 & \text{otherwise} \end{cases}$$

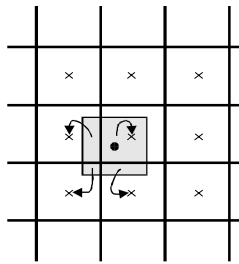
where:

$$\mathbf{H} = (H_1, H_2, H_3) \rightarrow \text{Vector describing cell dimensions}$$

- In the CIC scheme(3D), the weighting function is of the form:

$$W(\mathbf{r}) = \begin{cases} \left(1 - \frac{|x|}{H_1}\right) \left(1 - \frac{|y|}{H_2}\right) \left(1 - \frac{|z|}{H_3}\right) & -H \leq r < H \\ 0 & \text{otherwise} \end{cases}$$

Schematic description
of the CIC scheme



CIC

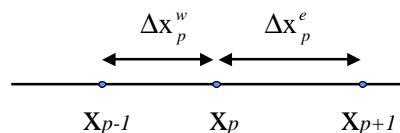
ASU Computational Electronics

- When the Poisson equation is solved, the force acting on the i -th particle in the p -th cell is given by:

$$\mathbf{F}(\mathbf{r}_i) = q \sum_p W(\mathbf{r}_i - \mathbf{r}_p) \mathbf{E}(\mathbf{r}_p)$$

where the electric field at the p -th grid point is:

$$\mathbf{E}_p = -\frac{1}{2} \left[\frac{V_{p+1} - V_p}{\Delta x_p^e} + \frac{V_p - V_{p-1}}{\Delta x_p^w} \right]$$



ASU Computational Electronics

4.2 Motion in Real Space

- The position in real space between collisions is determined by the coupled set of equations:

$$\frac{d\mathbf{r}}{dt} = \frac{1}{\hbar} \nabla_{\mathbf{k}} E(\mathbf{k}(t)) \quad \frac{d\mathbf{k}}{dt} = \frac{q\mathbf{E}(\mathbf{r})}{\hbar}$$

- In the full band case, they are solved via Runge-Kutta numerical integration¹. For parabolic bands:

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \frac{\hbar\mathbf{k}}{m^*} \quad \frac{d\mathbf{k}}{dt} = \frac{q\mathbf{E}(\mathbf{r})}{\hbar}$$

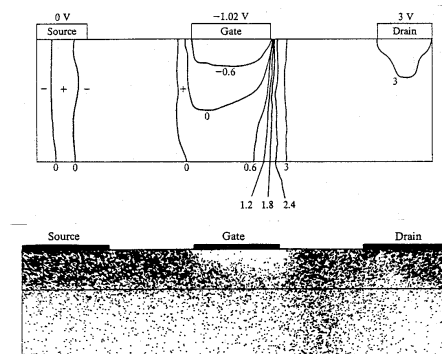
$$x(t) = x(0) + v_x(0)t + \frac{qE_x^0 t^2}{2m^*}$$

¹S.E. Laux and M.Fischetti, in *Monte Carlo Device Simulation..*(ed. K. Hess, Kluwer 1991), 1-27.

4.3 Monte Carlo Device Simulation Results

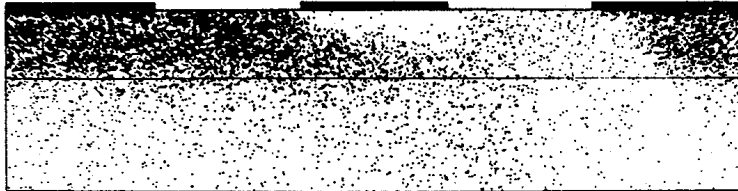
- To start the simulation, it is usual to assume that the device is charge neutral, in equilibrium.
- For transient simulations it is necessary to establish steady state conditions

(A) MESFET Example



*Hockney and Eastwood, *Computer Simulation Using Particles*

Gamma and L-valley distributions of the electrons in a MESFET:



Gamma - valley distribution of electrons

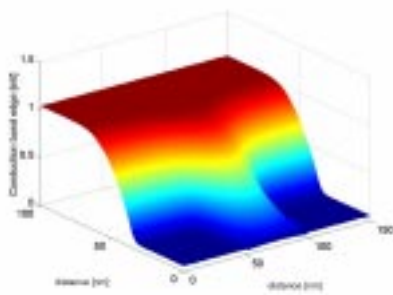


L - valley distribution of electrons

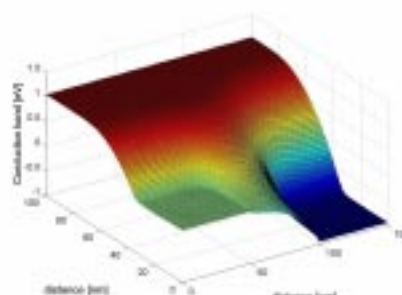
ASU Computational Electronics

(B) MOSFET Example (50nm channel length):

Conduction Band Edge



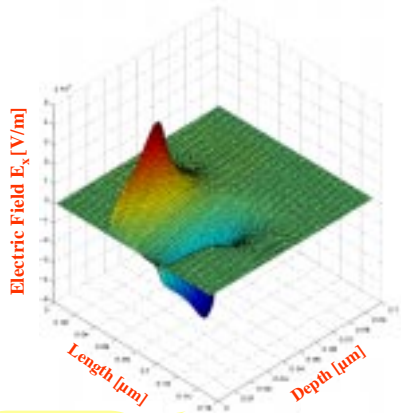
Initial State
Equilibrium



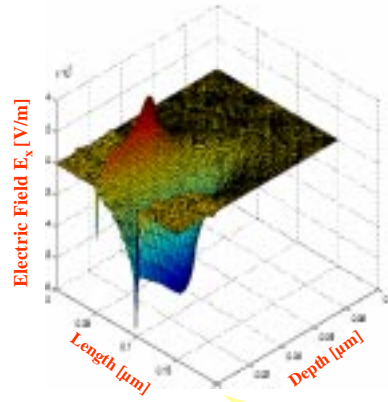
Final State
 $V_D = 1$ V, $V_G = 1$ V

ASU Computational Electronics

Electric field profile along the channel (x-axis)



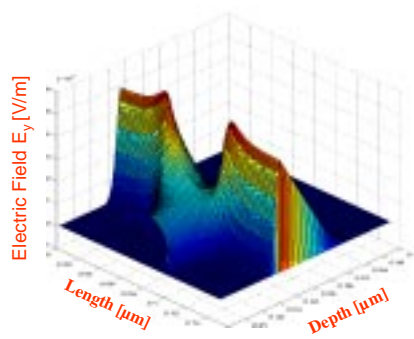
Initial State
Equilibrium



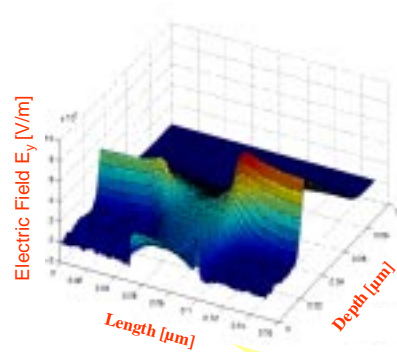
Final State
 $V_D = 1 \text{ V}$, $V_G = 1 \text{ V}$

ASU Computational Electronics

Electric field profile along the depth (y-axis)



Initial State
Equilibrium

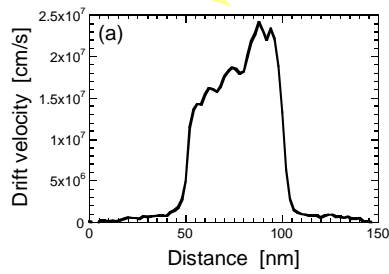


Final State
 $V_D = 1 \text{ V}$, $V_G = 1 \text{ V}$

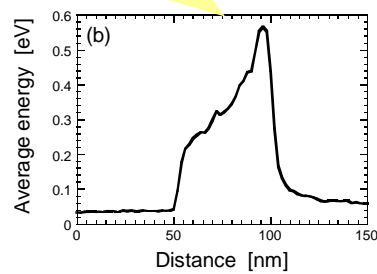
ASU Computational Electronics

Velocity and energy along the channel

Mean Drift Velocity Along the Channel



Average Kinetic Energy Along the Channel

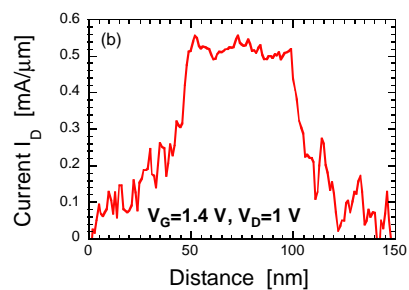
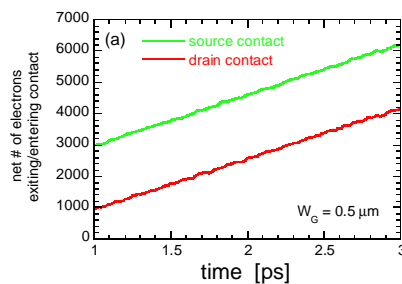


$V_D = 1 \text{ V}, V_G = 1.2 \text{ V}$

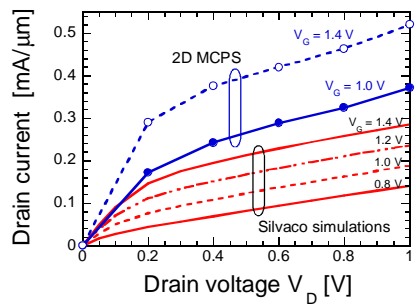
Current calculation

Two different methods can be used for the calculation of the current:

- Counting the net charge entering/exiting a contact
- Evaluating the current via electron drift velocity along the x-axis



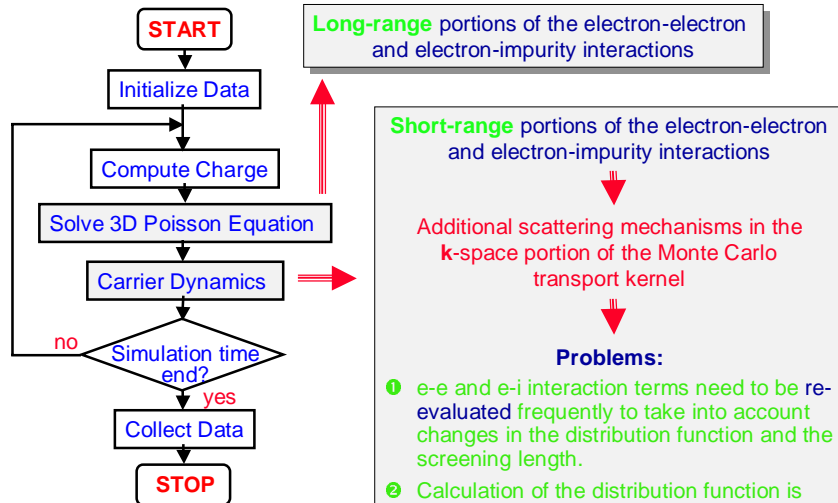
Output characteristics



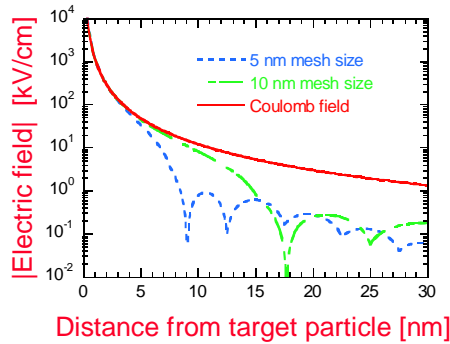
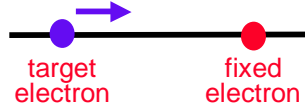
The differences between the Monte Carlo and the Silvaco simulations are due to the following reasons:

- Different transport models used (non-stationary transport is taking place in this device structure).
- Surface-roughness and Coulomb scattering are not included in the theoretical model used in the 2D-MCPS.

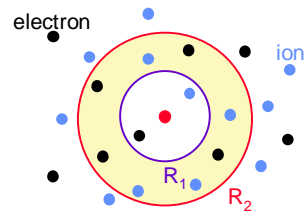
4.4 Short-Range Coulomb Force Treatment in particle-based simulations



(A) Description of our approach:



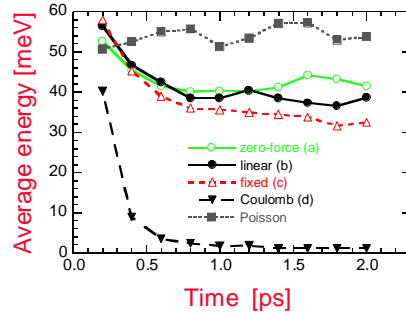
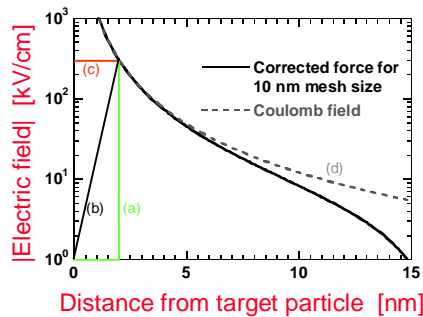
- ♥ Double-counting of the Coulomb force is eliminated
- ♥ Limitation: must use uniform mesh spacing
- ♥ The generated look-up table gives us information about the proper cut-off range



R_2 must be greater than $2 \times$ the mesh spacing

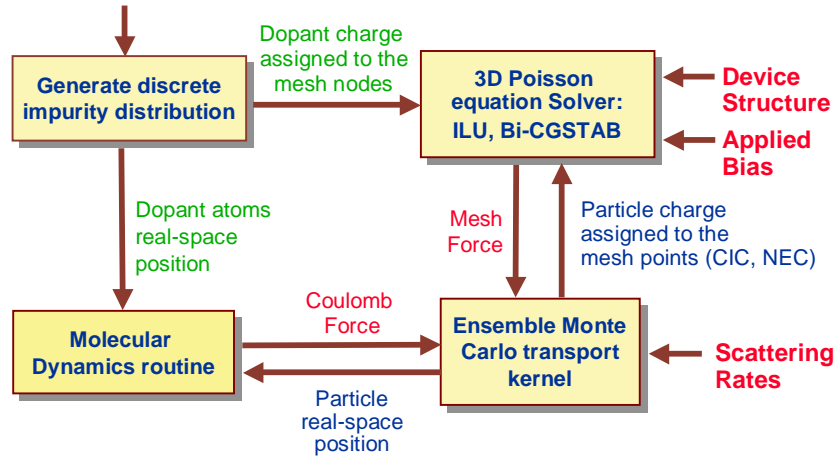
(B) Correction-Force Modifications

- ♥ The use of the simple Coulomb interaction in the source and drain regions leads to electron trapping which, in turn, prevents the filling of the channel with electrons.
- ♥ The carrier trapping can be eliminated through the use of modified short-range Coulomb correction force.



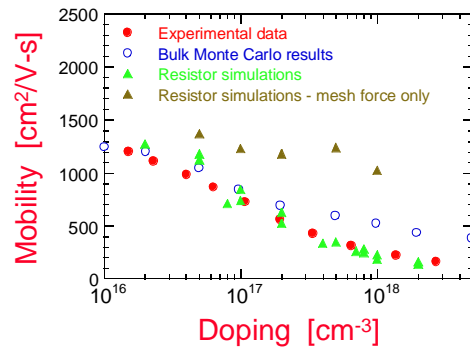
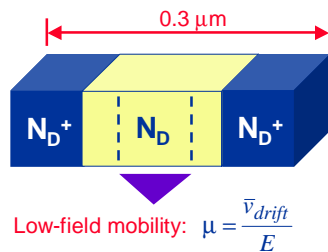
(C) Description of the 3D Device Simulator

Nominal Doping Density



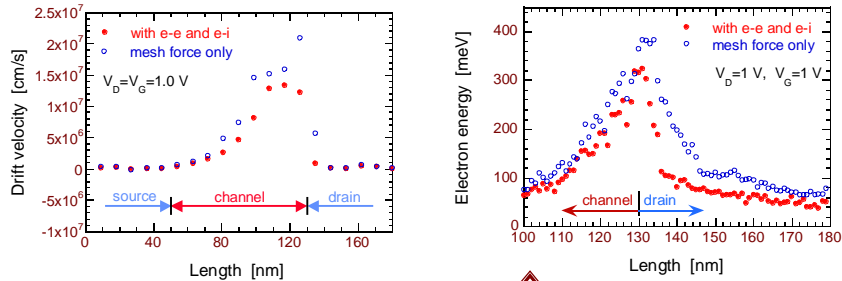
(D) Low Field Electron Mobility - Resistor Simulations

- ♥ Doping of the N^+ - regions:
 $N_D^+ = 10^{19} \text{ cm}^{-3}$.
- ♥ Mesh: uniform mesh spacing in all directions equal to 10 nm.
- ♥ Cases considered:
 - Mesh force only
 - Mesh force + short-range $e-e$ and $e-i$ interaction terms

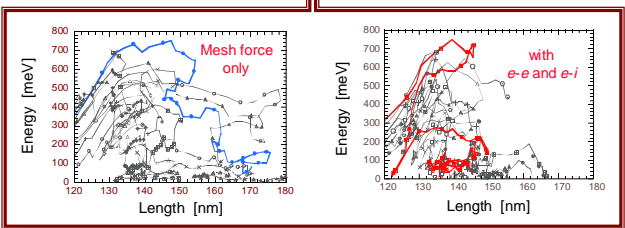


- ♥ The **mesh force only** does not give the correct doping dependence of the low-field electron mobility.
- ♥ The inclusion of the **short-range interaction terms** gives simulation low-field mobility data in agreement with experimental values.

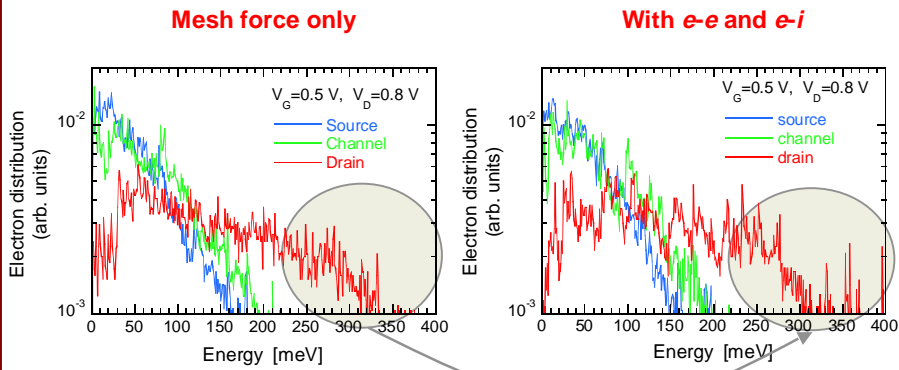
(E) MOSFETs - Role of the *E-E* and *E-I*



Individual electron trajectories over time



The form of the distribution function:



Short-range *e - e* and *e - i* interactions push some of the electrons towards higher energies.

Degradation of the Device Output Characteristics:

- ♥ The short range $e-e$ and $e-i$ interactions have significant influence on the device output characteristics.
- ♥ There is almost a factor of two decrease in current when these two interaction terms are considered.

