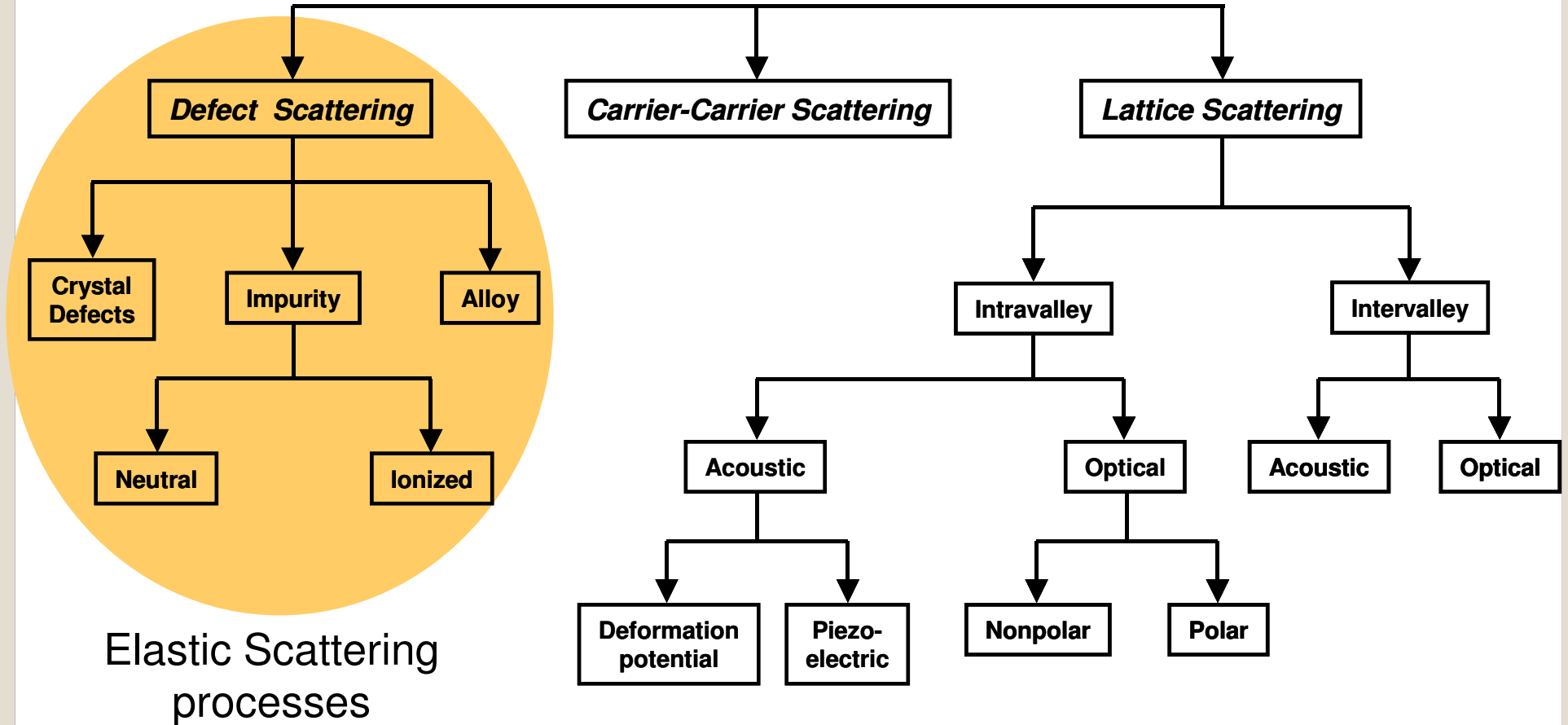


Coulomb Scattering

Dragica Vasileska
Professor
Arizona State University

What contributes to $\Gamma_{kk'}$?

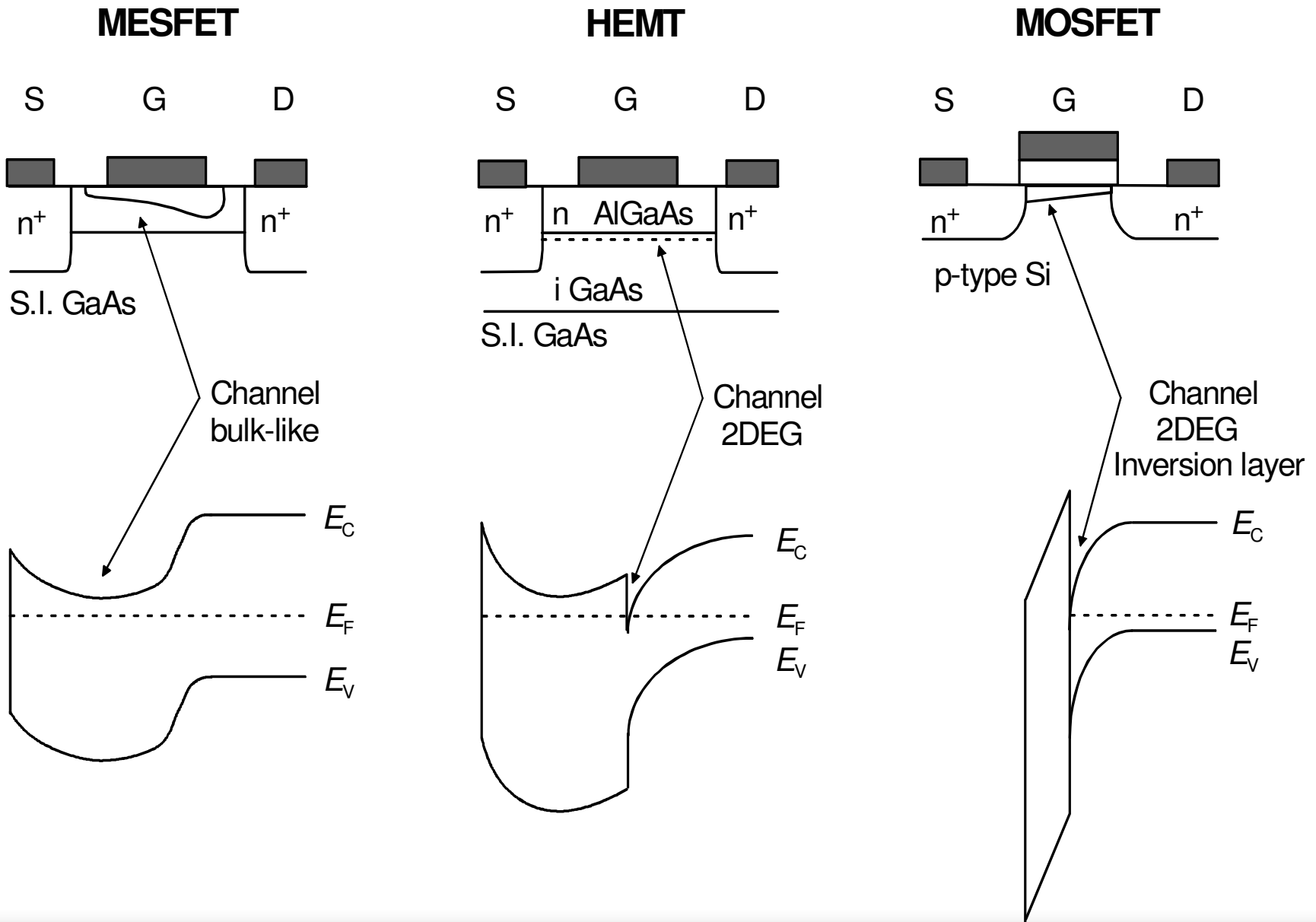
Scattering Mechanisms



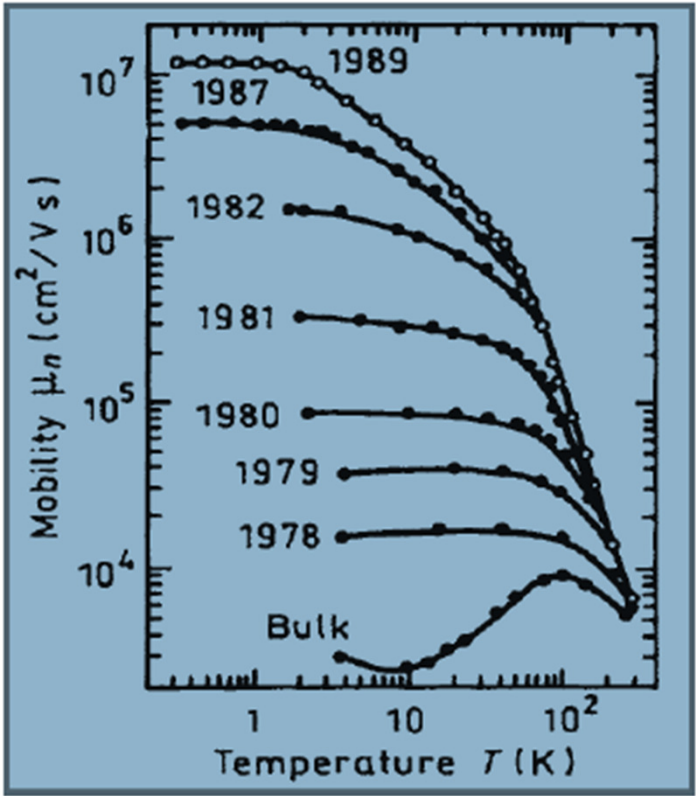
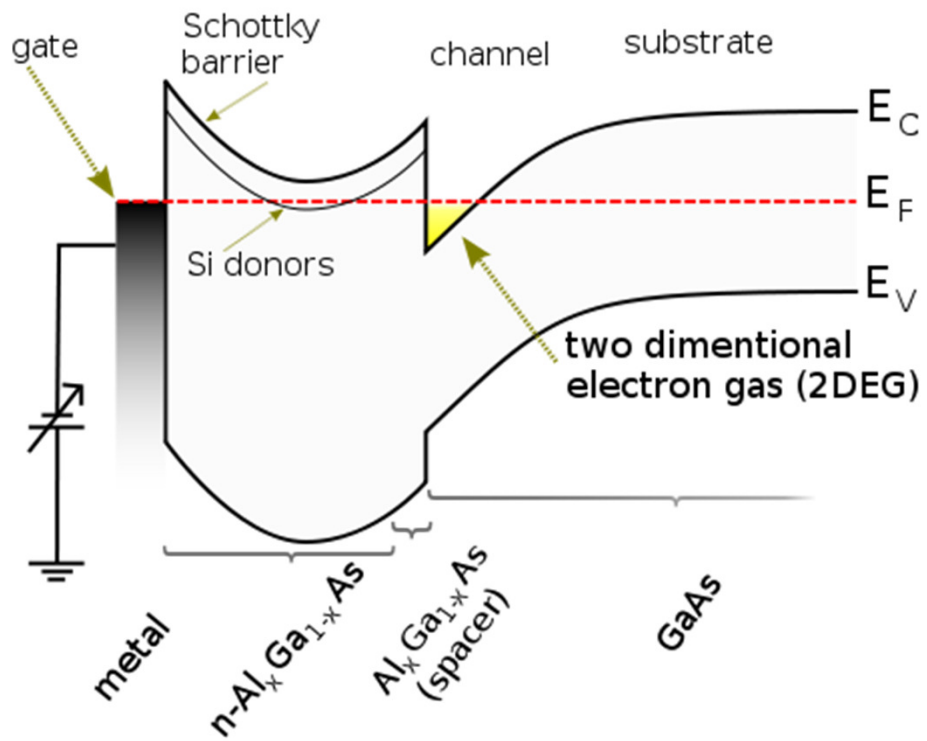
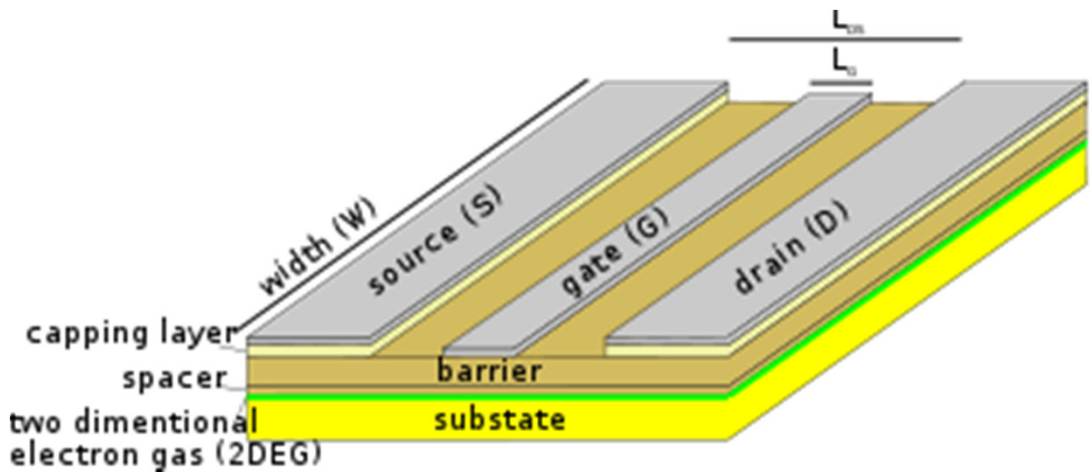
- Where is Coulomb Scattering Important:
 - Heavily doped bulk systems
 - Semiconductor devices
 - Nanoscale MOSFETs
 - MESFETs
 - PN Diodes
 - BJTs
 - Contact regions of FD SOI devices, Dual-gate transistors, FinFETS
 - HEMTs -> remote Coulomb scattering is important. Since remote Coulomb scattering is much weaker, we have very high mobilities in HEMT structures that are used in RF applications

Coulomb Scattering

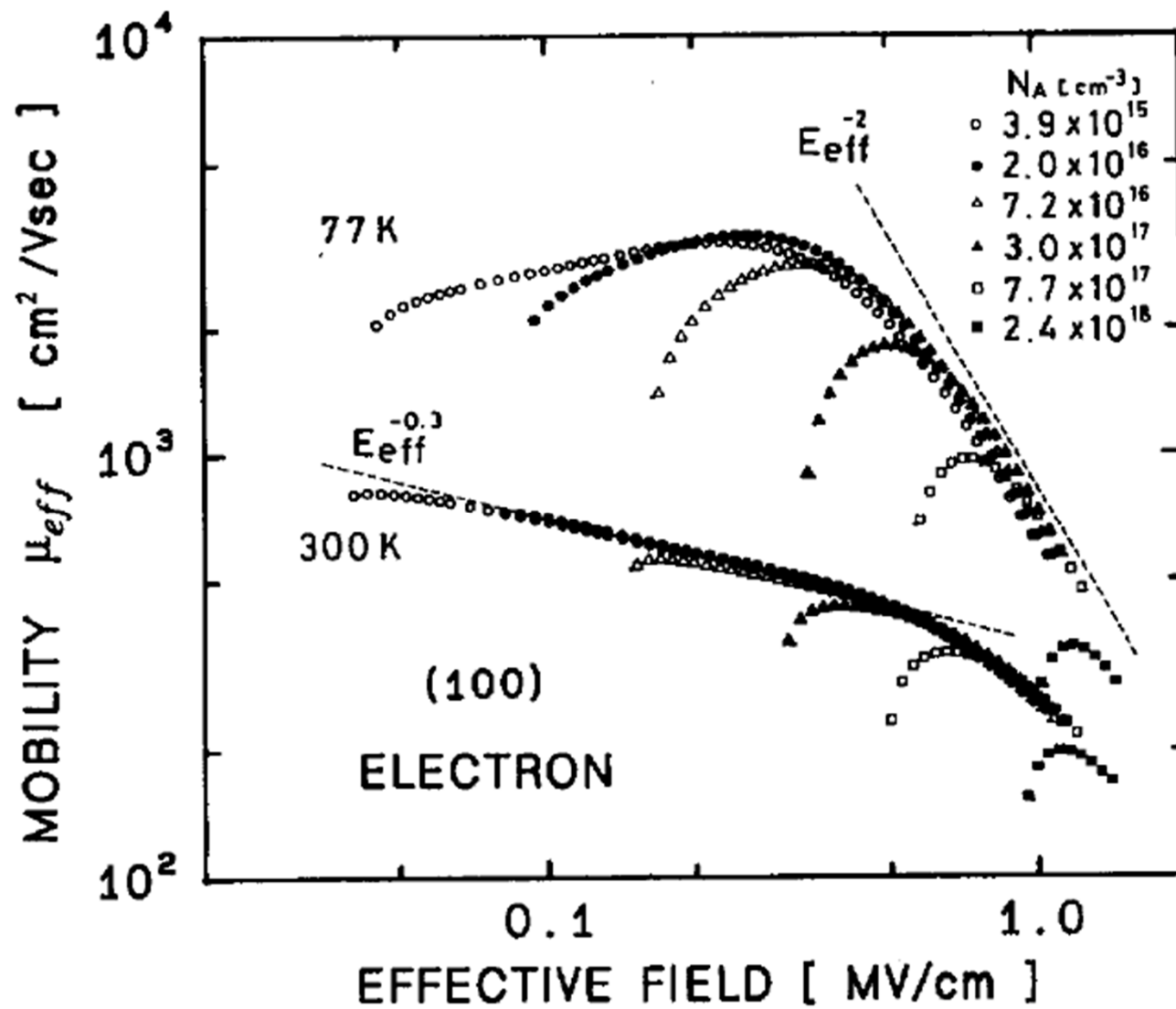
Location of the Channel in Different FET Types



HEMT



Si MOSFET



Ionized impurity scattering is due to:

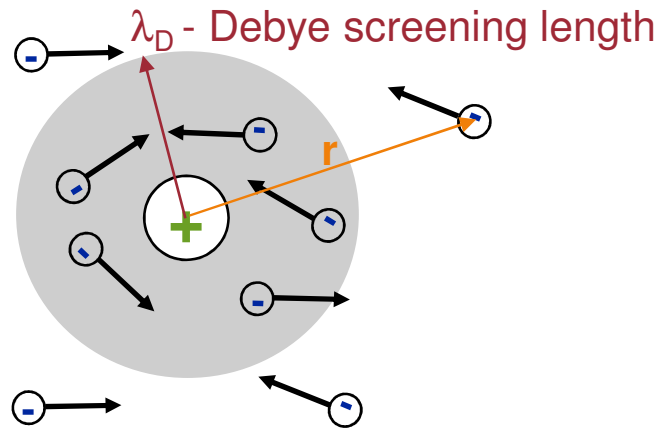
(Ionized donors/acceptors, substitutional impurities, charged surface states, etc.)

- 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?



$$\frac{1}{r} \xrightarrow{\text{screening cloud}} \frac{1}{r} e^{-r/\lambda_D}$$

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

- Screening is the damping of electric fields caused by the presence of mobile charge carriers.
- It is an important part of the behavior of charge-carrying fluids, such as ionized gases (classical plasmas) and conduction electrons in metals.
- In a fluid composed of electrically charged constituent particles, each pair of particles interact through the Coulomb force,

$$\mathbf{F} = \frac{q_1 q_2}{4\pi\epsilon_0 |\mathbf{r}|^2} \hat{\mathbf{r}}.$$

- In reality, these long-range effects are suppressed by the flow of the fluid particles in response to electric fields. This flow reduces the *effective* interaction between particles to a short-range "screened" Coulomb interaction.
- For example, consider a fluid composed of electrons. Each electron possesses an electric field which repels other electrons. As a result, it is surrounded by a region in which the density of electrons is lower than usual. This region can be treated as a positively-charged "screening hole". Viewed from a large distance, this screening hole has the effect of an overlaid positive charge which cancels the electric field produced by the electron. Only at short distances, inside the hole region, can the electron's field be detected.

- The first theoretical treatment of screening, due to [Debye](#) and [Hückel \(1923\)](#), dealt with a stationary point charge embedded in a fluid. This is known as electrostatic screening.
- Consider a fluid of electrons in a background of heavy, positively-charged ions. For simplicity, we ignore the motion and spatial distribution of the ions, approximating them as a uniform background charge. In [condensed matter physics](#), this model is referred to as [jellium](#).
- Let ρ denote the [number density](#) of electrons, and φ the [electric potential](#). At first, the electrons are evenly distributed so that there is zero net charge at every point. Therefore, φ is initially a constant as well.
- We now introduce a fixed point charge Q at the origin. The associated [charge density](#) is $Q\delta(r)$, where $\delta(r)$ is the [Dirac delta function](#). After the system has returned to equilibrium, let the change in the electron density and electric potential be $\Delta\rho(r)$ and $\Delta\varphi(r)$ respectively. The charge density and electric potential are related by the first of [Maxwell's equations](#), which gives

$$-\nabla^2[\Delta\varphi(r)] = \frac{1}{\epsilon_0}[Q\delta(r) - e\Delta\rho(r)].$$

- To proceed, we must find a second independent equation relating $\Delta\rho$ and $\Delta\varphi$. There are two possible approximations, under which the two quantities are proportional: the Debye-Hückel approximation, valid at high temperatures, and the Fermi-Thomas approximation, valid at low temperatures.

- In the Debye-Hückel approximation, we maintain the system in thermodynamic equilibrium, at a temperature T high enough that the fluid particles obey Maxwell-Boltzmann statistics. At each point in space, the density of electrons with energy j has the form

$$\rho_j(r) = \rho_j^{(0)}(r) \exp\left[\frac{e\phi(r)}{k_B T}\right]$$

where k_B is Boltzmann's constant. Perturbing in ϕ

$$e\Delta\rho \simeq \epsilon_0 k_0^2 \Delta\phi$$

where

$$k_0 \stackrel{\text{def}}{=} \sqrt{\frac{\rho e^2}{\epsilon_0 k_B T}}$$

Debye-Hückel approximation

- In the Fermi-Thomas approximation, we maintain the system at a constant chemical potential and at low temperatures. (The former condition corresponds, in a real experiment, to keeping the fluid in electrical contact at a fixed potential difference with ground.) The chemical potential μ is, by definition, the energy of adding an extra electron to the fluid. This energy may be decomposed into a kinetic energy T and the potential energy $-e\phi$. Since the chemical potential is kept constant,

$$\Delta\mu = \Delta T - e\Delta\phi = 0.$$

- If the temperature is extremely low, the behavior of the electrons comes close to the quantum mechanical model of a free electron gas. We thus approximate T by the kinetic energy of an additional electron in the free electron gas, which is simply the Fermi energy E_F . The Fermi energy is related to the density of electrons (including spin degeneracy) by

Fermi-Thomas approximation

$$\rho = 2 \frac{1}{(2\pi)^3} \frac{4}{3} \pi k_F^3, \quad E_F = \frac{\hbar^2 k_F^2}{2m}.$$

Perturbing to first order, we find that

$$\Delta\rho \simeq \frac{3\rho}{E_F} \Delta E_F.$$

Inserting this into the above equation for $\Delta\mu$ yields

$$e\Delta\rho \simeq \epsilon_0 k_0^2 \Delta\phi$$

where

$$k_0 \stackrel{\text{def}}{=} \sqrt{\frac{3e^2\rho}{\epsilon_0 E_F}} = \sqrt{\frac{me^2 k_f}{\epsilon_0 \pi^2 \hbar^2}}$$

is called the **Fermi-Thomas screening wave vector**.

- Our results from the Debye-Hückel or Fermi-Thomas approximation may now be inserted into the first Maxwell equation. The result is

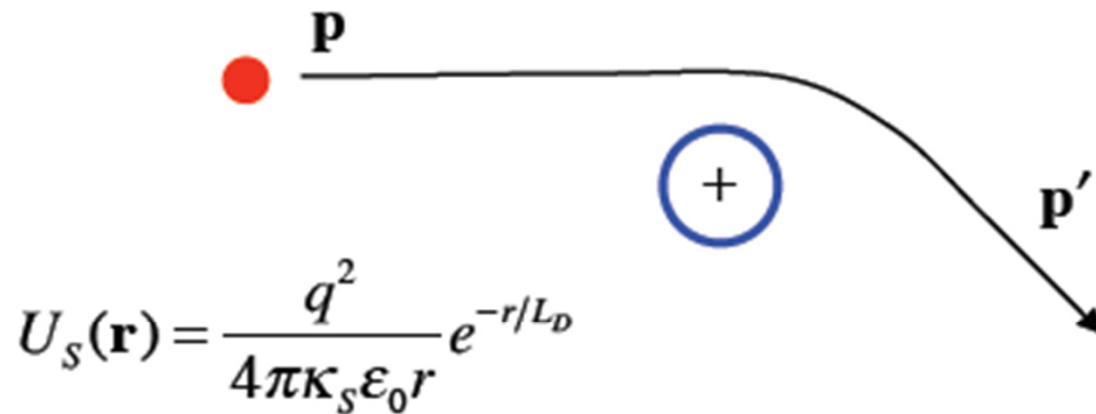
$$\left[\nabla^2 - k_0^2 \right] \phi(r) = -\frac{Q}{\epsilon_0} \delta(r)$$

which is known as the **screened Poisson equation**. The solution is

$$\phi(r) = \frac{Q}{4\pi\epsilon_0 r} e^{-k_0 r}$$

- which is called a screened Coulomb potential. It is a Coulomb potential multiplied by an exponential damping term, with the strength of the damping factor given by the magnitude of k_0 , the Debye or Fermi-Thomas wave vector. Note that this potential has the same form as the Yukawa potential.

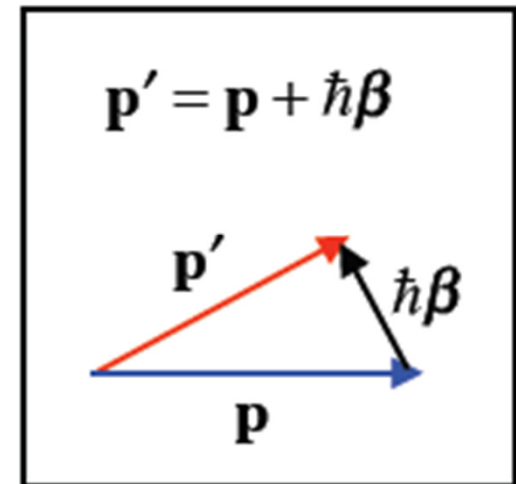
Screened Coulomb interactions



$$U_S(\mathbf{r}) = \frac{q^2}{4\pi\kappa_S\epsilon_0 r} e^{-r/L_D}$$

$$L_D = \sqrt{\frac{\kappa_S\epsilon_0 k_B T}{q^2 n_0}} \text{ Debye length}$$

$$\tilde{U}_S(\boldsymbol{\beta}) = \int_{-\infty}^{+\infty} U_S(\mathbf{r}) e^{-i\boldsymbol{\beta}\cdot\mathbf{r}} d\mathbf{r}$$



Brooks-Herring Approach

- 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

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

- 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 $n' \neq n$ [interband(valley)]. Therefore, for impurity scattering, the matrix element for scattering is approximately

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

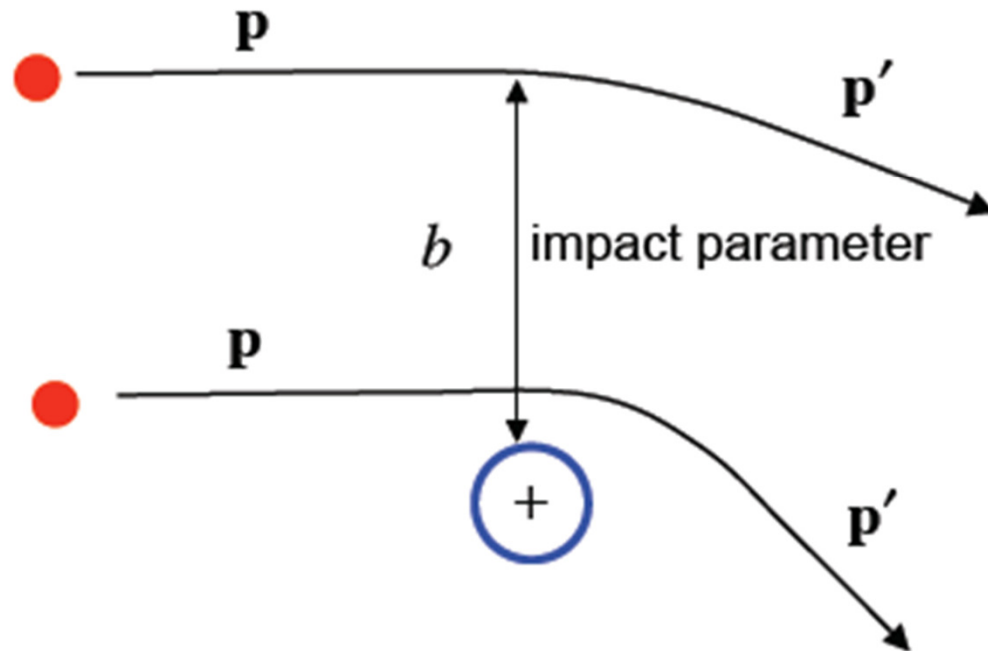
where the scattered wavevector is: $\mathbf{q} = \mathbf{k} - \mathbf{k}'$

- 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:

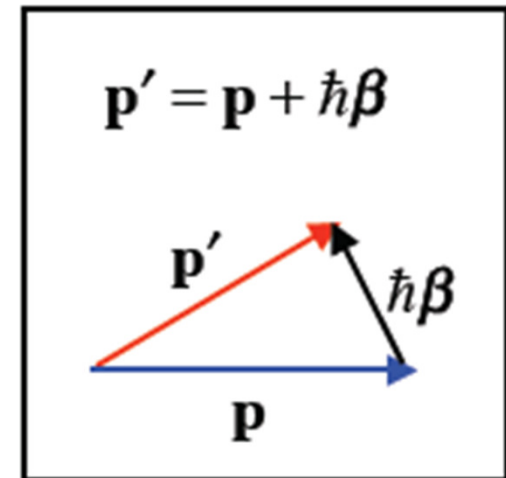
$$V_i^{kk'} \cong \frac{N_i Z^2 e^4}{V^2 (q^2 + \lambda^2) \epsilon_{sc}^2} = \frac{n_i Z^2 e^4}{V (q^2 + \lambda^2) \epsilon_{sc}^2}$$

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

small angle scattering



$$\tilde{U}_s(\boldsymbol{\beta}) = \frac{q^2}{\kappa_s \epsilon_0} \frac{1}{(\beta^2 + 1/L_D^2)}$$



From M. Lundstrom, private communication.

- 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:

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

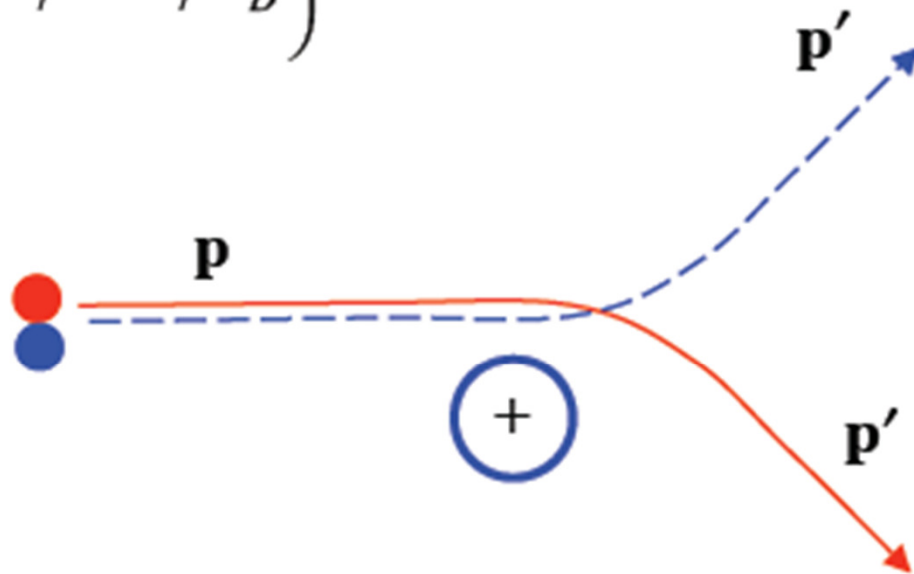
- Comments on the behavior of this scattering mechanism:
 - Increases linearly with impurity concentration
 - Decreases with increasing energy (k^2), favors lower T
 - Favors small angle scattering
 - Ionized Impurity-Dominates at low temperature, or room temperature in impure samples (highly doped regions)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

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

examine result

$$S(\mathbf{p}, \mathbf{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_s^2 \epsilon_0^2 \Omega} \frac{\delta(E' - E)}{\left(\frac{4p^2}{\hbar^2} \sin^2 \alpha/2 + 1/L_D^2 \right)^2}$$

- 1) $S(\mathbf{p}, \mathbf{p}') \sim N_I$
- 2) $S(\mathbf{p}, \mathbf{p}') \sim q^4$
- 3) $S(\mathbf{p}, \mathbf{p}') \sim 1/E^2$

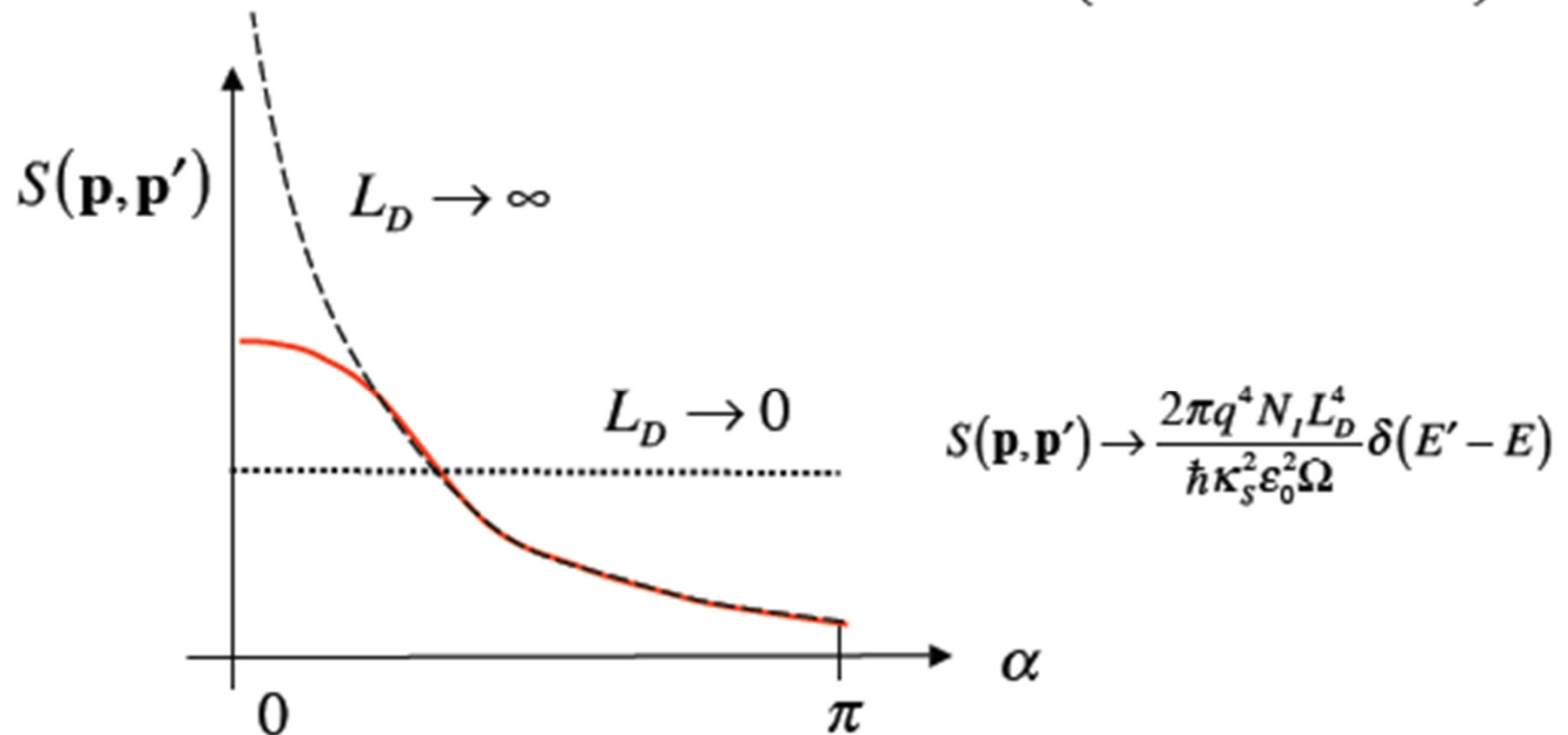


From M. Lundstrom, private communication.

examine result

4) α dependence

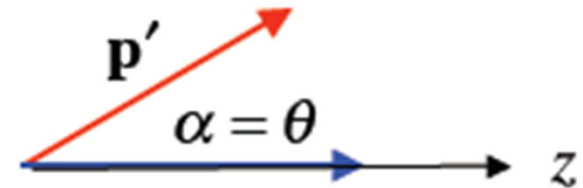
$$S(\mathbf{p}, \mathbf{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_s^2 \epsilon_0^2 \Omega} \frac{\delta(E' - E)}{\left(\frac{4p^2}{\hbar^2} \sin^2 \alpha / 2 + 1/L_D^2 \right)^2}$$



From M. Lundstrom, private communication.

momentum relaxation time

$$\frac{1}{\tau_m} = \sum_{\mathbf{p}'} S(\mathbf{p}, \mathbf{p}') (1 - \cos \alpha)$$



$$\tau_m(E) = \frac{16\sqrt{2m^*} \pi \kappa_s^2 \epsilon_0^2}{N_I q^4} \left[\ln(1 + \gamma^2) - \frac{\gamma^2}{1 + \gamma^2} \right] E^{3/2}$$

$$\gamma^2 = 8m^* EL_D^2 / \hbar^2$$

$$\tau_m(E) \sim E^{3/2}$$

$$\tau_m(E) = \tau_0 (E/k_B T)^{3/2} \quad s = 3/2$$

$$\tau_0 \sim T_L^{3/2}$$

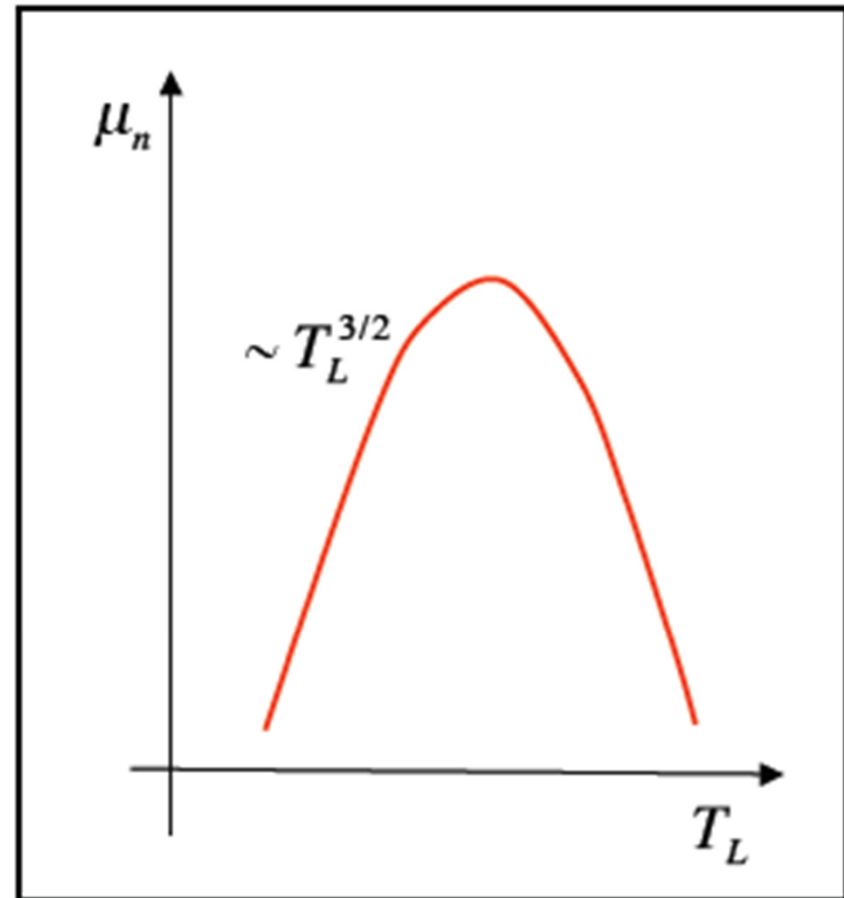
From M. Lundstrom, private communication.

Brooks-Herring mobility

$$\mu_n = \frac{q \langle \langle \tau_m \rangle \rangle}{m^*}$$

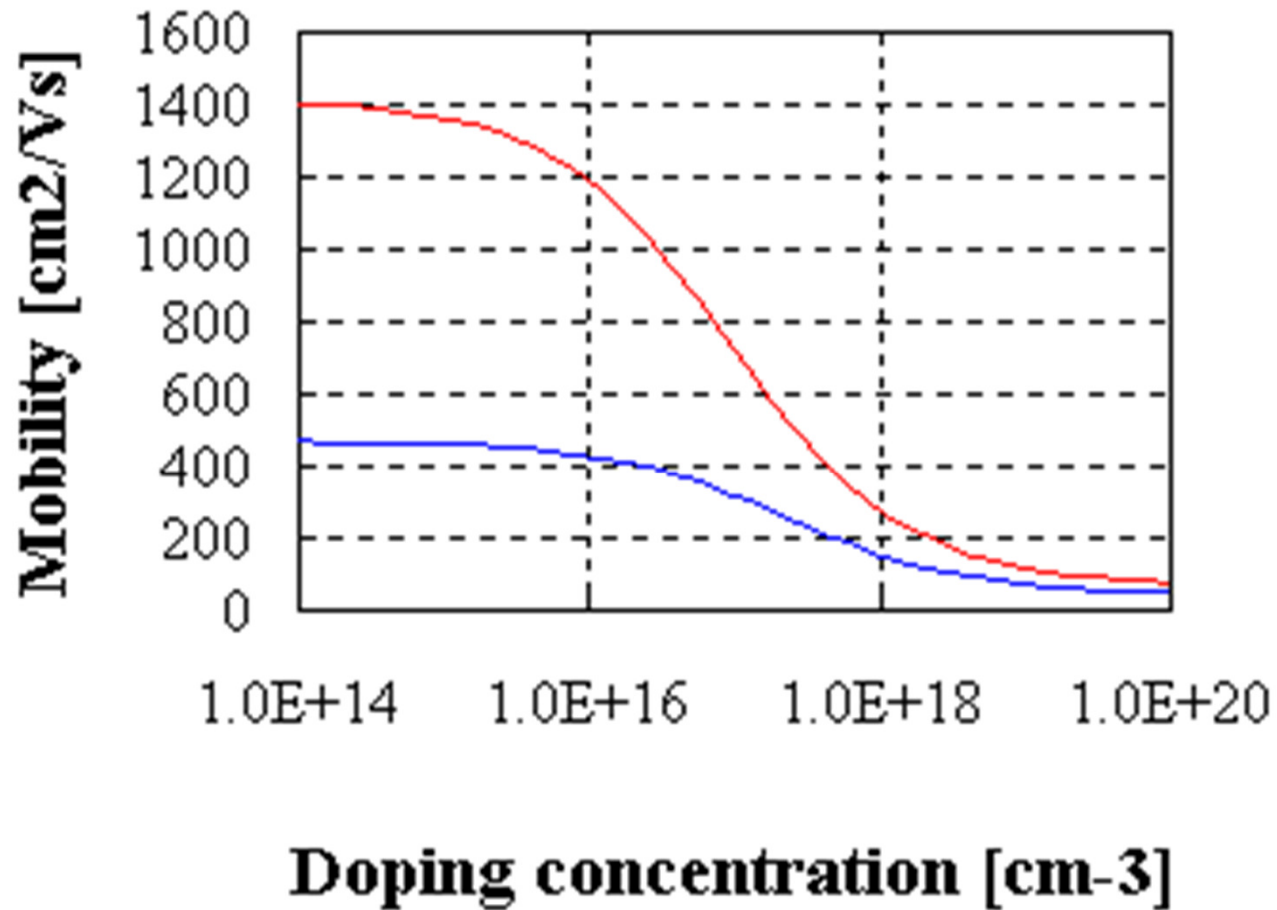
$$\langle \langle \tau_m \rangle \rangle = \tau_0 \frac{\Gamma(s + 5/2)}{\Gamma(5/2)} \quad s = 3/2$$

$$\mu_n = \frac{q\tau_0}{m^*} \frac{3\sqrt{\pi}}{4} \sim T_L^{3/2}$$



From M. Lundstrom, private communication.

Electron and hole mobility in bulk silicon at T=300K.



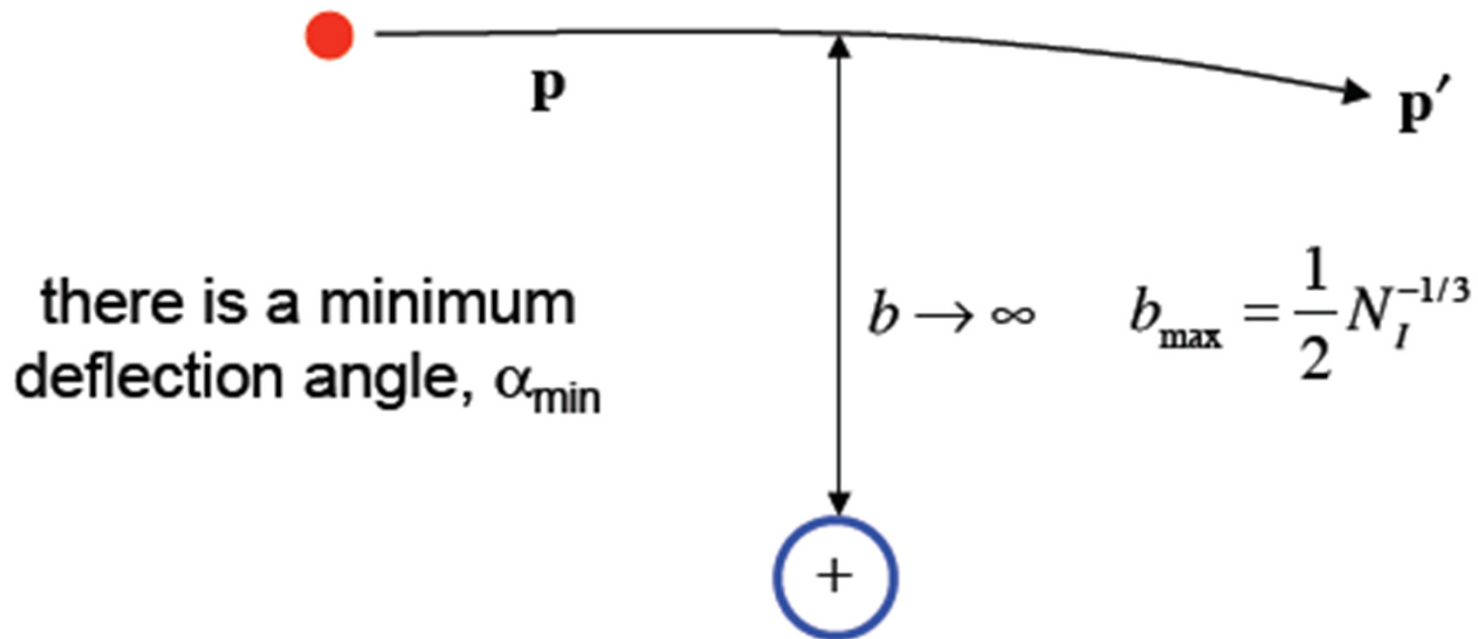
Doping Dependence of the Mobility

Conwell-Weiskopf approach

$$S(\mathbf{p}, \mathbf{p}') = \frac{2\pi q^4 N_I}{\hbar \kappa_s^2 \epsilon_0^2 \Omega} \frac{\delta(E' - E)}{\left(\frac{4p^2}{\hbar^2} \sin^2 \alpha/2 \right)^2}$$

unscreened Coulomb potential

$$S(\mathbf{p}, \mathbf{p}') \rightarrow \infty \text{ as } \alpha \rightarrow 0$$



From M. Lundstrom, private communication.

Conwell-Weiskopf approach

$$\tau_m(E) = \frac{16\pi\sqrt{2m^*}\kappa_s^2\epsilon_0^2}{N_I q^4} \left[\frac{1}{\ln(1 + \gamma_{CW}^2)} \right] E^{3/2}$$

$$\gamma^2 = b_{\max} / (q^2 / 8\pi\kappa_s\epsilon_0 E)$$

$$\tau_m(E) \sim E^{3/2}$$

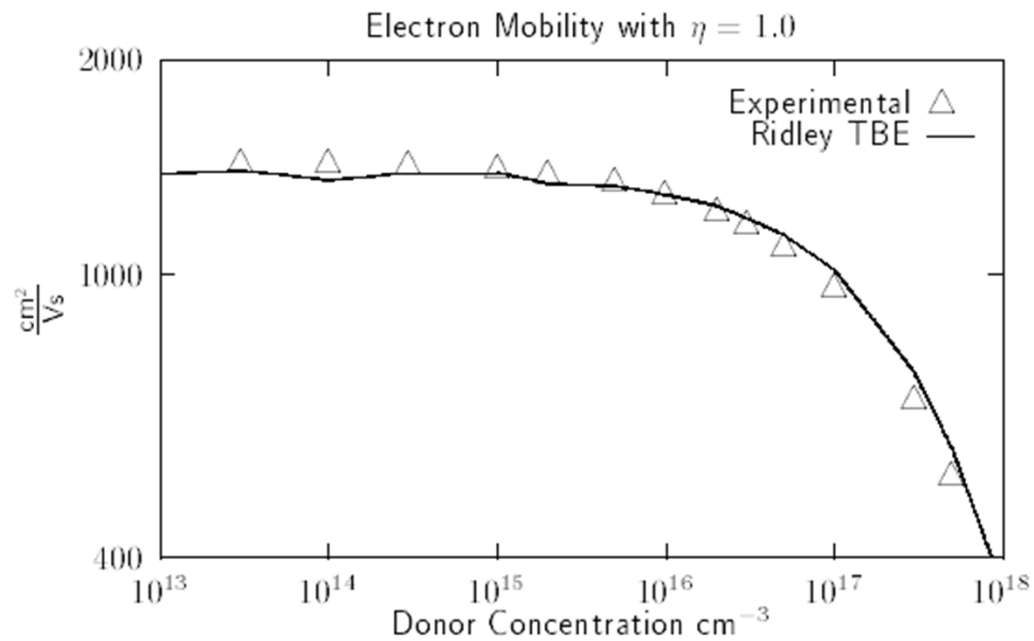
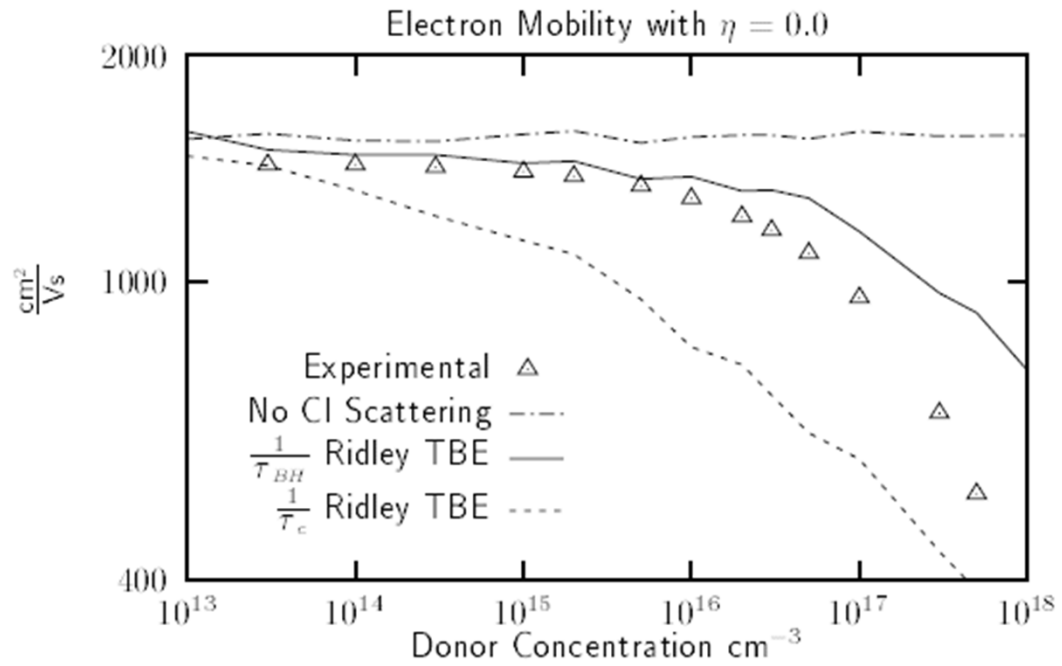
$$\mu_n \sim T_L^{3/2}$$

From M. Lundstrom, private communication.

Neutral Impurity 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 ($>1 \times 10^{19}/\text{cm}^3$).
- It is a dipole type of interaction and is weaker than direct Coulomb interaction

$$\frac{1}{\tau_{NI}} \approx \frac{20\kappa\hbar^3\eta N_N}{e^2 m_g m_c (1 + 2\alpha\epsilon)}$$



Mobility modeling can be separated in three parts:

- **Low-field mobility characterization** for bulk or inversion layers
- **High-field mobility characterization** to account for velocity saturation effect
- **Smooth interpolation** between the low-field and high-field regions

Mobility Modeling

Phonon scattering:

- Simple power-law dependence of the temperature
- Sah *et al.* model:
 - acoustic + optical and intervalley phonons combined via Mathiessen's rule

$$\mu_{n0} = \text{MUN} \left(\frac{T_L}{300} \right)^{-\text{TMUN}}$$

$$\mu_{p0} = \text{MUP} \left(\frac{T_L}{300} \right)^{-\text{TMUP}}$$

Table 3-27. User-Specifiable Parameters for the Constant Low-Field Mobility Model

Statement	Parameter	Default	Units
MOBILITY	MUN	1000	cm ² / (V·s)
MOBILITY	MUP	500	cm ² / (V·s)
MOBILITY	TMUN	1.5	
MOBILITY	TMUP	1.5	

Ionized impurity scattering:

- Conwell-Weiskopf model
- Brooks-Herring model

Low-Field Models for Bulk Materials

Combined phonon and ionized impurity scattering:

- Dorkel and Leturg model:
temperature-dependent phonon scattering +
ionized impurity scattering + carrier-carrier interactions

- Caughey and Thomas model:
temperature independent phonon scattering + ionized impurity scattering

$$\mu_{n0} = \text{MU1N, CAUG} \cdot \left(\frac{T_L}{300K}\right)^{\text{ALPHAN, CAUG}}$$

$$+ \frac{\text{MU2N, CAUG} \cdot \left(\frac{T_L}{300K}\right)^{\text{BETAN, CAUG}} - \text{MU1N, CAUG} \cdot \left(\frac{T_L}{300K}\right)^{\text{ALPHAN, CAUG}}}{1 + \left(\frac{T_L}{300K}\right)^{\text{GAMMAN, CAUG}} \cdot \left(\frac{N}{\text{NCRITN, CAUG}}\right)^{\text{DELTAN, CAUG}}}$$

$$\mu_{p0} = \text{MU1P, CAUG} \cdot \left(\frac{T_L}{300K}\right)^{\text{ALPHAP, CAUG}}$$

$$+ \frac{\text{MU2P, CAUG} \cdot \left(\frac{T_L}{300K}\right)^{\text{BETAP, CAUG}} - \text{MU1P, CAUG} \cdot \left(\frac{T_L}{300K}\right)^{\text{ALPHAP, CAUG}}}{1 + \left(\frac{T_L}{300K}\right)^{\text{GAMMAP, CAUG}} \cdot \left(\frac{N}{\text{NCRITP, CAUG}}\right)^{\text{DELTAP, CAUG}}}$$

Table 3-29. User-Specifiable Parameters for Equations 3-175 and 3-176

Statement	Parameter	Default	Units
MOBILITY	MU1N.CAUG	55.24	cm ² / (V · s)
MOBILITY	MU1P.CAUG	49.7	cm ² / (V · s)
MOBILITY	MU2N.CAUG	1429.23	cm ² / (V · s)
MOBILITY	MU2P.CAUG	479.37	cm ² / (V · s)
MOBILITY	ALPHAN.CAUG	0.0	arbitrary
MOBILITY	ALPHAP.CAUG	0.0	arbitrary
MOBILITY	BETAN. CAUG	-2.3	arbitrary
MOBILITY	BETAP. CAUG	-2.2	arbitrary
MOBILITY	GAMMAN.CAUG	-3.8	arbitrary

Table 3-29. User-Specifiable Parameters for Equations 3-175 and 3-176

Statement	Parameter	Default	Units
MOBILITY	GAMMAP.CAUG	-3.7	arbitrary
MOBILITY	DELTAN.CAUG	0.73	arbitrary
MOBILITY	DELTAP.CAUG	0.70	arbitrary
MOBILITY	NCRITN.CAUG	1.072×10 ¹⁷	cm ⁻³
MOBILITY	NCRITP.CAUG	1.606×10 ¹⁷	cm ⁻³

- Sharfetter-Gummel model:
phonon scattering + ionized impurity scattering (parameterized expression – does not use the Mathiessen's rule)

- Arora model:
similar to Caughey and Thomas, but with temperature dependent phonon scattering

$$\mu_{n0} = \text{MU1N} \cdot \text{ARORA} \left(\frac{T_L}{300} \right)^{\text{ALPHAN} \cdot \text{ARORA}} + \frac{\text{MU2N} \cdot \text{ARORA} \left(\frac{T_L}{300} \right)^{\text{BETAN} \cdot \text{ARORA}}}{1 + \frac{N}{\text{NCRITN} \cdot \text{ARORA} \cdot \left(\frac{T_L}{300} \right)^{\text{GAMMAN} \cdot \text{ARORA}}}}$$

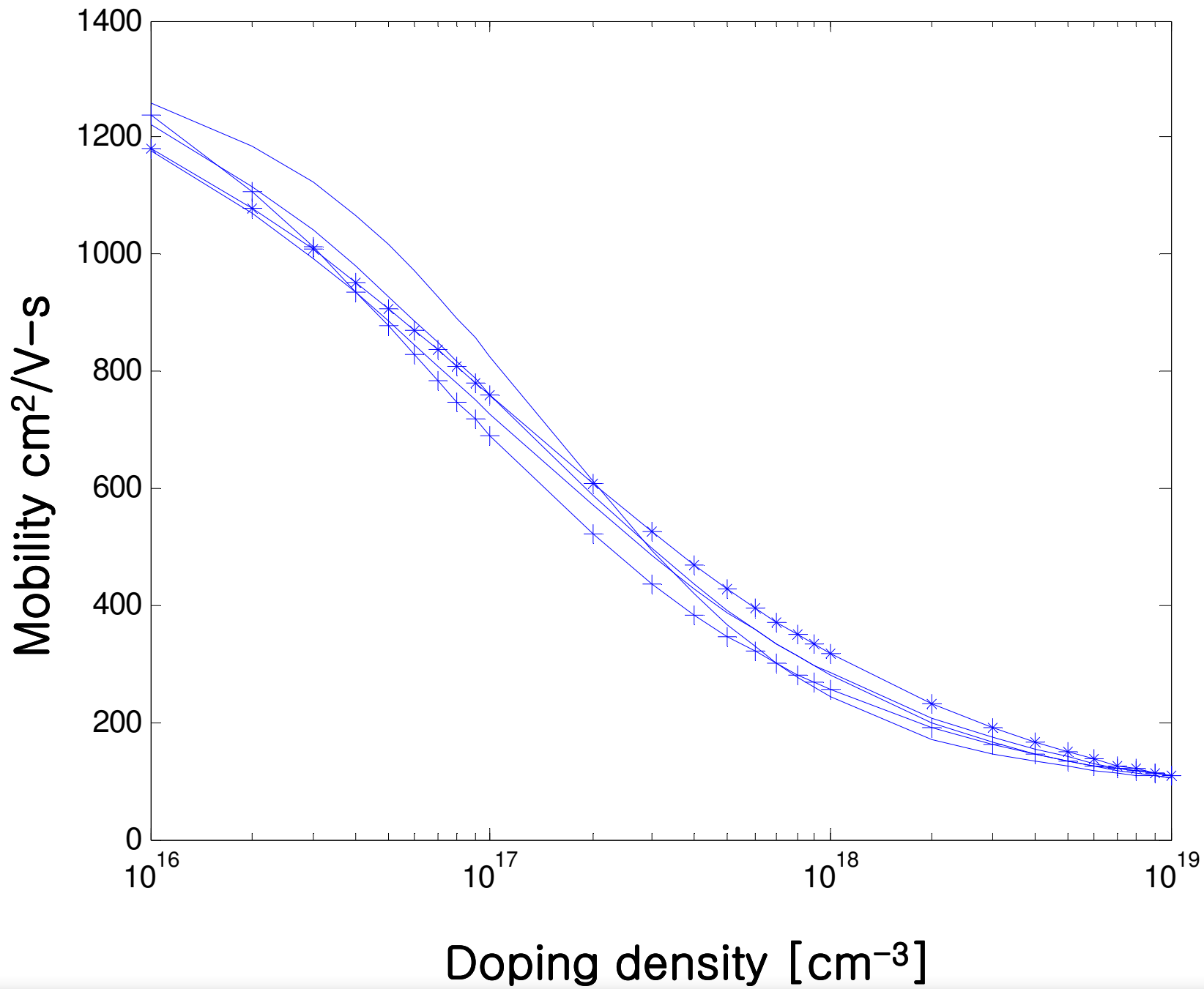
$$\mu_{p0} = \text{MU1P} \cdot \text{ARORA} \left(\frac{T_L}{300} \right)^{\text{ALPHAP} \cdot \text{ARORA}} + \frac{\text{MU2P} \cdot \text{ARORA} \left(\frac{T_L}{300} \right)^{\text{BETAP} \cdot \text{ARORA}}}{1 + \frac{N}{\text{NCRITP} \cdot \text{ARORA} \cdot \left(\frac{T_L}{300} \right)^{\text{GAMMAP} \cdot \text{ARORA}}}}$$

Table 3-30. User-Specifiable Parameters for Equations 3-177 and 3-178

Statement	Parameter	Default	Units
MOBILITY	MU1N.ARORA	88.0	cm ² / (V·s)
MOBILITY	MU1P.ARORA	54.3	cm ² / (V·s)
MOBILITY	MU2N.ARORA	1252.0	cm ² / (V·s)
MOBILITY	MU2P.ARORA	407.0	cm ² / (V·s)
MOBILITY	ALPHAN.ARORA	-0.57	
MOBILITY	ALPHAP.ARORA	-0.57	
MOBILITY	BETAN.ARORA	-2.33	

Table 3-30. User-Specifiable Parameters for Equations 3-177 and 3-178

Statement	Parameter	Default	Units
MOBILITY	BETAP.ARORA	-2.33	
MOBILITY	GAMMAN.ARORA	2.546	
MOBILITY	GAMMAP.ARORA	2.546	
MOBILITY	NCRITN.ARORA	1.432×10 ¹⁷	cm ⁻³
MOBILITY	NCRITP.ARORA	2.67×10 ¹⁷	cm ⁻³



Neutral impurity scattering:

- Li and Thorber model:

mobility component due to neutral impurity scattering is combined with the mobility due to lattice, ionized impurity and carrier-carrier scattering via the Mathiessen's rule

The field-dependent mobility model provides smooth transition between low-field and high-field behavior

$$\mu(E) = \frac{\mu_0}{\left[1 + \left(\frac{\mu_0 E}{v_{sat}}\right)^\beta\right]^{1/\beta}} \quad \begin{array}{l} \beta = 1 \text{ for electrons} \\ \beta = 2 \text{ for holes} \end{array}$$

v_{sat} is modeled as a temperature-dependent quantity:

$$v_{sat}(T) = \frac{2.4 \times 10^7}{1 + 0.8 \exp\left(\frac{T_L}{600}\right)} \text{ cm/s}$$

Field-Dependent Mobility