Scattering Mechanisms

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Description of the Various Scattering Mechanisms

1 Elastic Scattering Mechanisms

(A) Ionized Impurities scattering

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

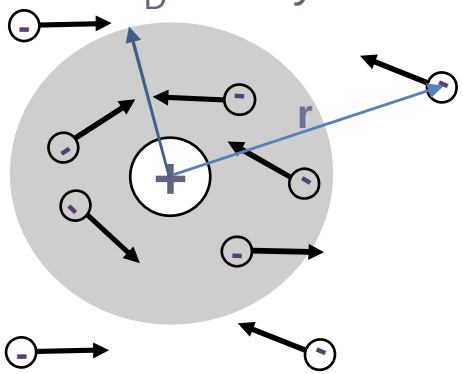
- The potential due to a single ionized impurity with net charge *Ze* is:

$$V_i^0(\mathrm{r}) = -\frac{Ze^2}{4\pi\varepsilon r} \quad \textit{mks units}$$

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

What is Screening?

λ_D - Debye screening length



Example:

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

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

Dielectric Function

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

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

In the above expression, **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 $\varepsilon(\mathbf{q},\omega)$ 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

$$\varepsilon(\mathrm{q},\omega) = 1 - \lim_{s\to\infty} \frac{e^2}{\varepsilon_{sc} q^2} \sum_{\mathrm{k}} \frac{f_0\left(E_{\mathrm{k+q}}\right) - f_0\left(E_{\mathrm{k}}\right)}{E_{\mathrm{k+q}} - E_k + \hbar\omega + i\delta}$$

Thomas-Fermi Approximation

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

$$\lim_{\omega,q\to 0} \varepsilon(q,\omega) \approx 1 + \frac{\lambda^2}{q^2}$$

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

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

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:

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

Overlap Integral

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

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

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

$$= \sum_{\mathrm{G}} V^{-1} \int d\mathrm{r} e^{-i\mathrm{k}'\cdot\mathrm{r}} V_i(\mathrm{r}) e^{i\mathrm{k}\cdot\mathrm{r}} e^{-i\mathrm{G}\cdot\mathrm{r}} U_{nn'kk'}(\mathrm{G})$$
$$= \sum_{\mathrm{G}} V^{-1} \int d\mathrm{r} e^{-i\mathrm{k}'\cdot\mathrm{r}} V_i(\mathrm{r}) e^{i\mathrm{k}\cdot\mathrm{r}} e^{-i\mathrm{G}\cdot\mathrm{r}} \int_{\Omega} d\mathrm{r}' u^*_{n',k'}(\mathrm{r}') u_{n,k}(\mathrm{r}') e^{i\mathrm{G}\cdot\mathrm{r}'}$$

- For impurity scattering, the matrix element has a 1/q type dependence which usually means **G**≠0 terms are small

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

Coulomb Scattering Potential

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

$$\left|\left\langle \mathrm{k}'\left|V_i(\mathrm{r})\right|\mathrm{k}\right\rangle\right|^2 = \left|V_i(\mathrm{q})\right|^2 \cong \frac{Z^2e^4}{V^2\left(q^2+\lambda^2\right)\varepsilon_{sc}^2};\ V = volume$$

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

- 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:

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

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

Coulomb Scattering Rate

- The total scattering rate from **k** to **k′** is given from Fermi's golden rule as:

$$\Gamma^{i}_{kk'} = \frac{2\pi n_i Z^2 e^4}{V\hbar\left(q^2+\lambda^2\right)^2\varepsilon_{sc}^2}\delta\left(E_{k'}-E_{k}\right)$$

  If θ is the angle between **k** and **k′**, then:

$$q = \left|k-k'\right| = k^2 + k'^2 - 2kk'\cos\theta = 2k^2\left(1-\cos\theta\right)$$

- 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 **k′** gives the total scattering rate Γ_k :

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

Other Elastic Processes

(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 (>1x10^{19}/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 quaternay compounds, particularly at low temperature.
- The total scattering rate out of state **k** for this scattering mechanism is of the form:

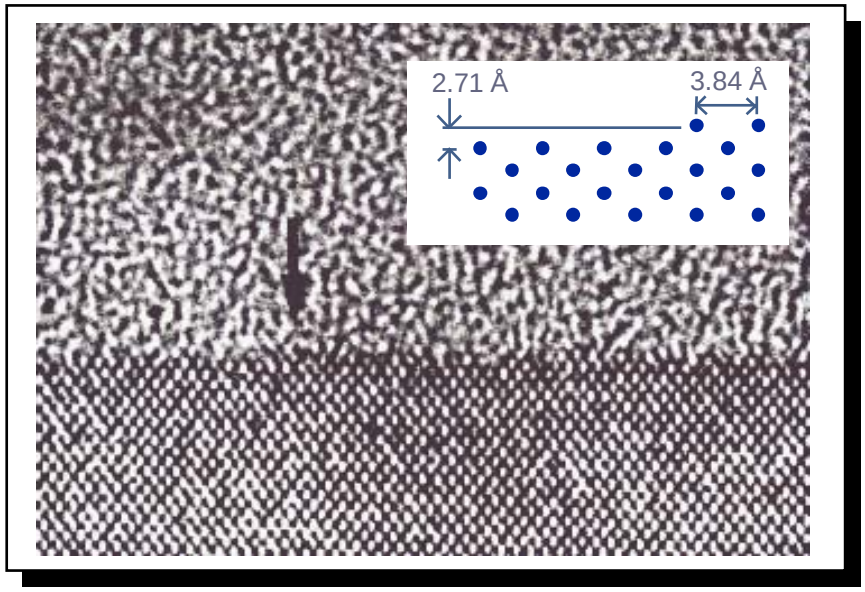
$$\Gamma_k^{alloy} = \frac{(\delta E)^2}{2\pi\hbar}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E^{1/2}$$

Surface Roughness

(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 SiO_2
(Goodnick et al., Phys. Rev. B 32, pp. 8171, 1985)



Modeling surface-roughness scattering potential:

$$H'(\mathbf{r},z) = V_o\theta[-z+\Delta(\mathbf{r})] - V_o\theta[-z]$$

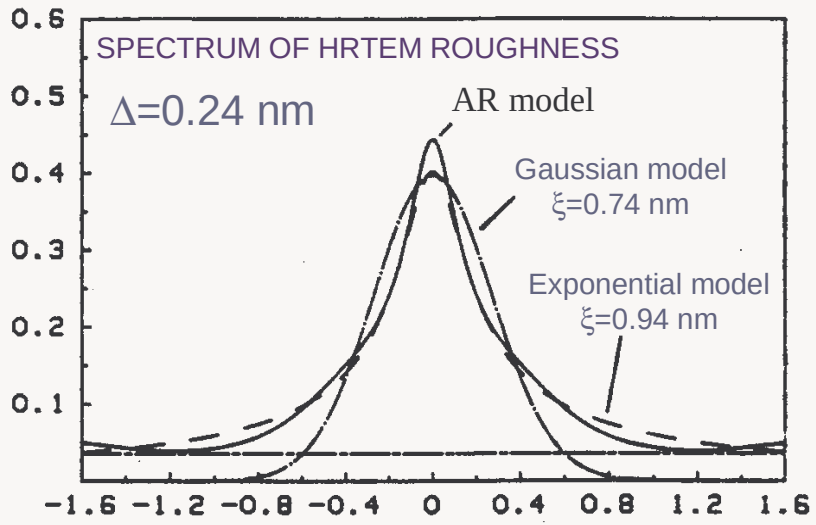
$$\approx V_o\delta(z)\Delta(\mathbf{r})$$

random function that describes the deviation from an atomically flat interface

Surface-Roughness Continued

- 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:** $S_E(q) = \frac{\pi\Delta^2\zeta^2}{\left(1+q^2\zeta^2/2\right)^{3/2}}$

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

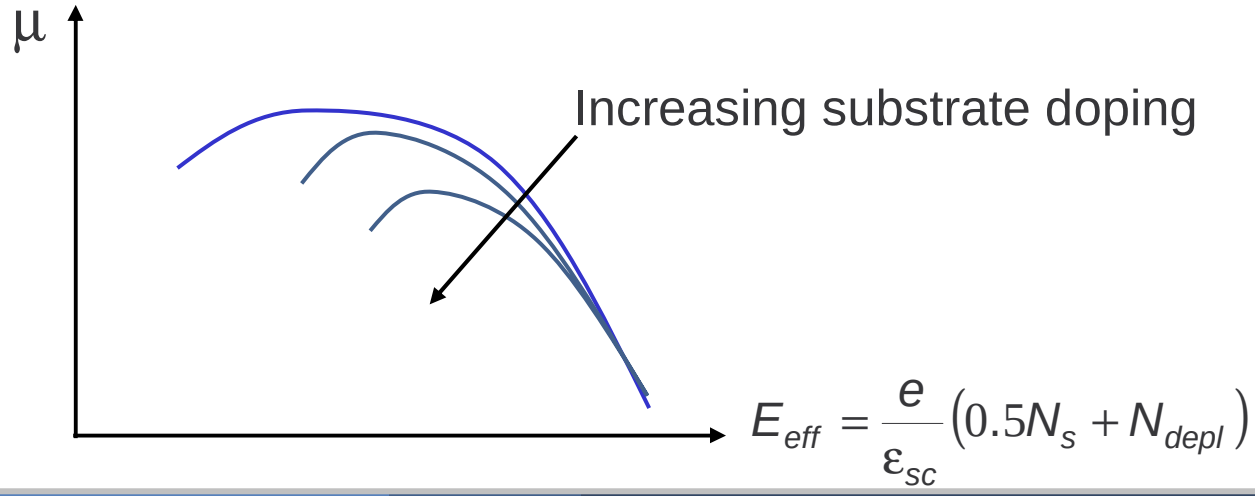
Universal Mobility Behavior

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

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

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

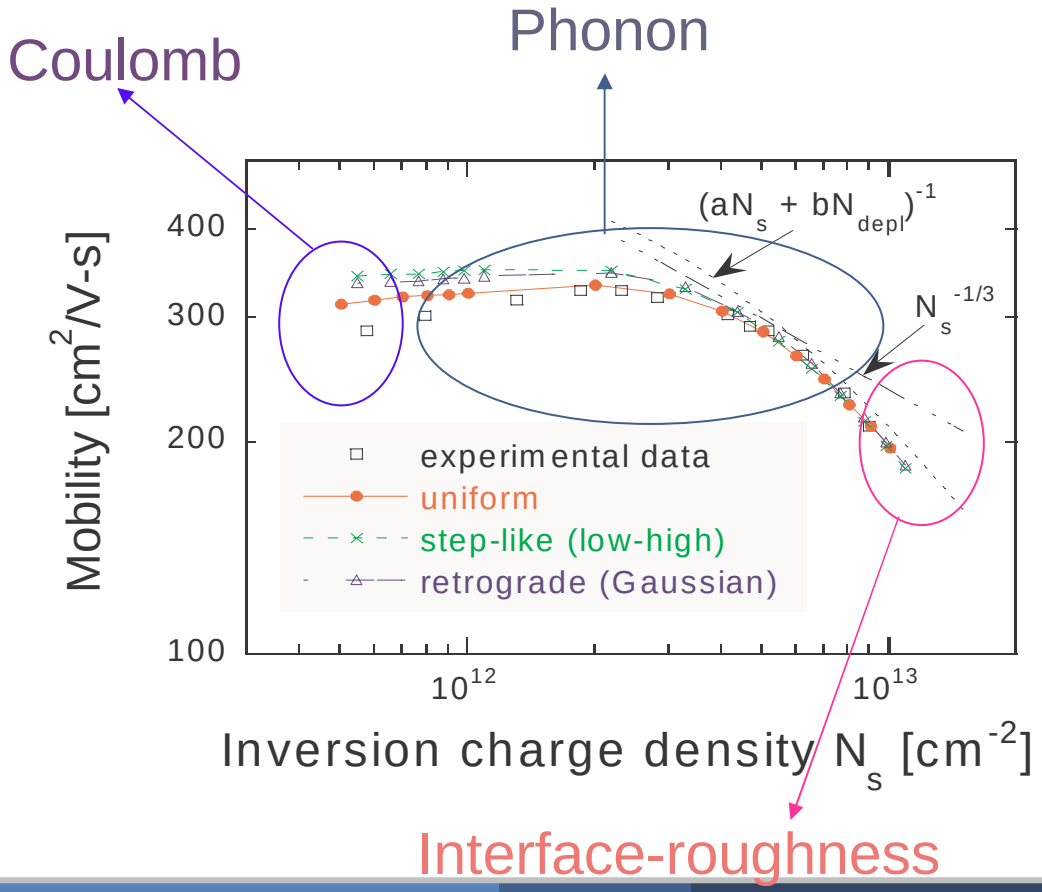
- It is interesting to note that this scattering mechanism leads to what is known as the *universal mobility behavior*, used in mobility models described earlier.



Simulation Experiments

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).



Inelastic Scattering Mechanisms

2.2 Inelastic Scattering Mechanisms

2.2.1 Some general considerations

- The Electron Lattice Hamiltonian is of the following form:

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

$$H_e = Electron\ Hamiltonian; H_l = lattice\ Hamiltonian$$

$$H_{ep} = Electron - Phonon\ coupling$$

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

- For the lattice Hamiltonian we have:

$$H_l\phi_l = E_l\phi_l \quad \phi_l \Rightarrow \left| n_{\mathrm{q}1} n_{\mathrm{q}2} n_{\mathrm{q}3} \ldots \right\rangle$$

$$E_l = \sum_{\xi,\mathrm{q}} \hbar\omega_{\mathrm{q}}^{\xi}\left(n_{\mathrm{q}}^{\xi} + \tfrac{1}{2}\right)$$

Second quantized representation, where $n_{\mathbf{q}}$ is the number of *phonons* with wave-vector **q**, mode ξ.

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 $\omega^{\xi}_{\boldsymbol{q}}$

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

q labels the wavevector corresponding to traveling wave solutions for individual components,

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

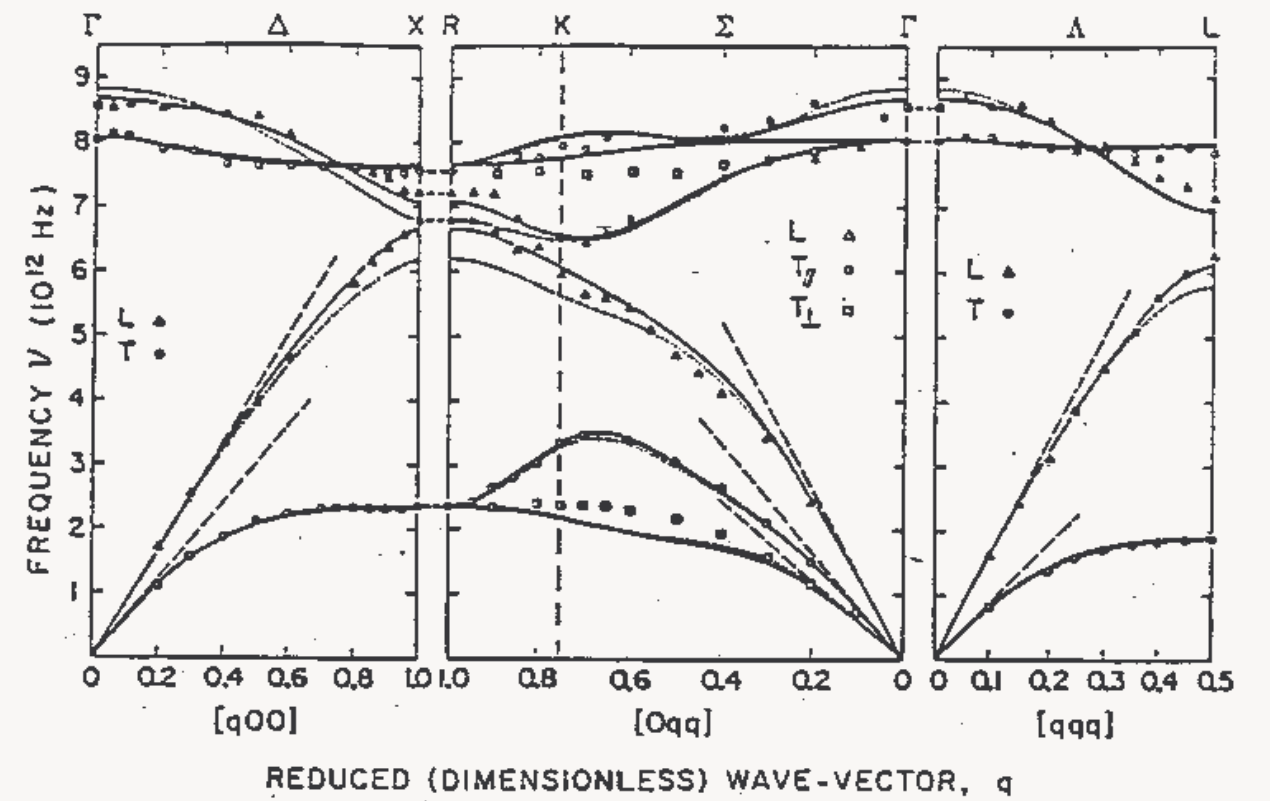
$$v_q^{\xi} = \partial\omega_q^{\xi} / \partial q$$

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

Phonons Dispersion Curves

(1) For acoustic modes, $\lim_{q\to 0} v_q^{\xi} = \partial\omega_q^{\xi} / \partial q = u^{\xi}$, 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.

Electron-Phonon Interaction

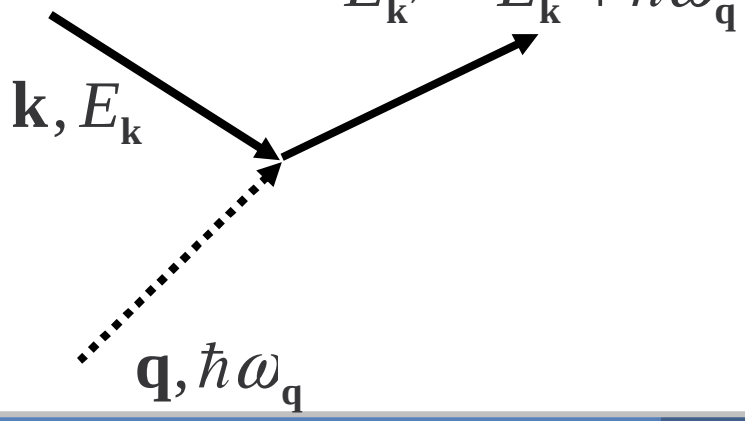
- The Electron-Phonon Interaction is categorized as to mode (acoustic or optical), polarization (transverse or longitudinal), and mechanism (deformation potential, polar, piezoelectric).

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

Absorption:

$$\mathbf{k}' = \mathbf{k} + \mathbf{q}$$

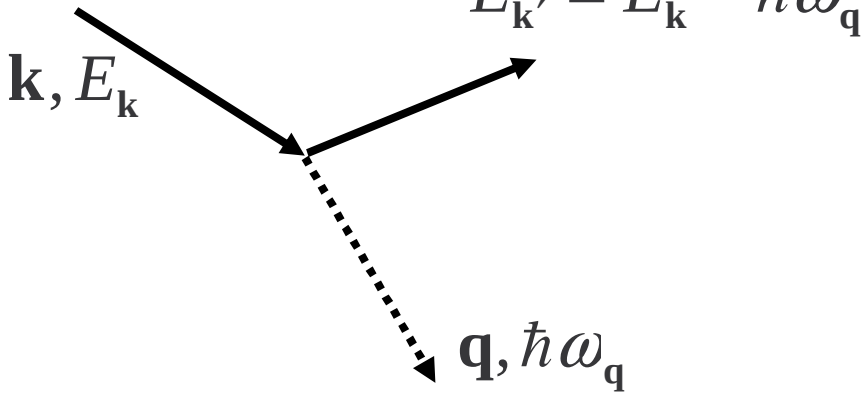
$$E_{\mathbf{k}'} = E_{\mathbf{k}} + \hbar\omega_{\mathbf{q}}$$



Emission:

$$\mathbf{k}' = \mathbf{k} - \mathbf{q}$$

$$E_{\mathbf{k}'} = E_{\mathbf{k}} - \hbar\omega_{\mathbf{q}}$$



Deformation Potential Scattering

- 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 **r** resulting from a lattice mode of wavevector **q**

(A) Acoustic deformation potential scattering

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

$$E(\mathrm{k}) = E^0(\mathrm{k}) + E_1\Delta + \vartheta(e^2)$$

Acoustic Phonons

where:

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

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

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

and **u** is the displacement operator of the lattice

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

$$\vec{\mathrm{e}}_{\mathrm{q},\xi} = \textit{polarization vector}$$

- Taking the divergence gives factor of **e·q** of the form:

$$\vec{\mathrm{e}}_{\mathrm{q},\xi} \cdot \mathrm{q} = q \quad \textit{for longitudinal modes}$$

$$\vec{\mathrm{e}}_{\mathrm{q},\xi} \cdot \mathrm{q} = 0 \quad \textit{for transverse modes}$$

Therefore, only longitudinal modes contribute.

Scattering Matrix Element

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

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

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

Scattering Matrix Element:

Assuming $\omega_q = u_l q$, then:

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

- At sufficient high temperature, (equipartition approximation):

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

Scattering Rate

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

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

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

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

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

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

$$\omega_q \to 0 \; as \; q \to 0$$

Assumptions Used

- Integrating gives (assuming a parabolic band model)

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

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:

  a) spherical parabolic bands
  b) equipartition (not valid at low temperatires)
  c) quasi-elastic process (non-dissipative)
  d) deformation potential Ansatz

Optical Deformation Potential Scattering

(B) Optical deformation potential scattering

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

- Assume no dispersion:

$$\omega_q \rightarrow \omega_0 \; as \; q \rightarrow 0$$

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)

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

The matrix element for spherical bands is given by

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

which is independent of **q** .

Scattering Rate

- The total scattering rate is obtained by integrating over all **k'** for both absorption and emission

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

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

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

Intervalley Scattering

(C) Intervalley scattering

- May occur between equivalent or nonequivalent sets of valleys

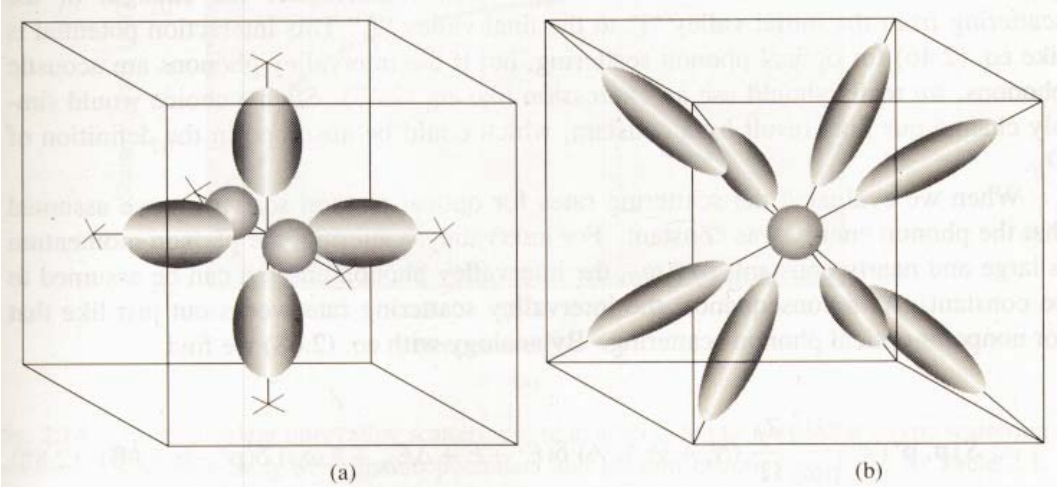


Fig. 2.12 Constant energy surfaces for (a) silicon and (b) gallium arsenide.

- 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

Intervalley Scattering …

- Since $\Delta\mathbf{k}$ is large compared to $\mathbf{k}$, assume $\omega_q \rightarrow \omega_{\Delta q}$ 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

$$\omega_q \rightarrow \omega_{ij}$$

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

$$\Gamma_k^{iv} = \sum_j \frac{m_{d_j}^{3/2} D_{ij}^{\ 2}}{\sqrt{2}\pi\rho\hbar^3\omega_{ij}} \left\{ \begin{array}{l} n_{\omega_{ij}} \left(E - \Delta E_{ij} + \hbar\omega_{ij}\right)^{1/2} + \\ \left[n_{\omega_{ij}} + 1\right]\left(E - \Delta E_{ij} - \hbar\omega_{ij}\right)^{1/2} \Theta\left(E - \Delta E_{ij} - \hbar\omega_0\right) \end{array} \right\}$$

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	=>	polar optical phonon scattering (very strong scattering mechanism for compound semiconductors such as GaAs)
acoustic phonons	=>	piezoelectric scattering (important at low temperatures in very pure semiconductors)

POP Scattering

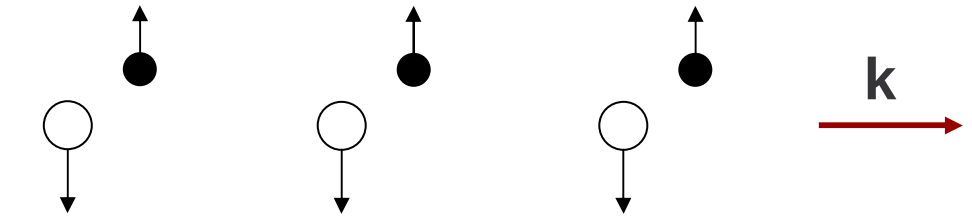
(A) Polar Optical Phonon Scattering (POP)

Scattering Potential:

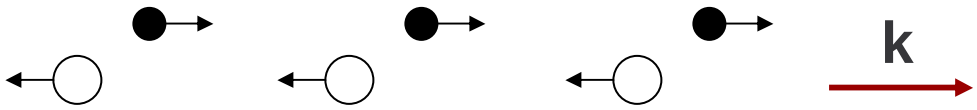
Microscopic model is difficult. A simpler approach is to consider the contribution of this dipole to the polarization of the crystal and its effect on the high- and low-frequency dielectric constants.

- Consider a diatomic lattice in the long-wavelength limit (**k**≈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 **P**.

Transverse mode:



Longitudinal mode:



POP Scattering …

- Associated with this polarization are macroscopic electric field **E** and electric displacement **D**, related by:

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

↑

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

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

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

↓ ↓

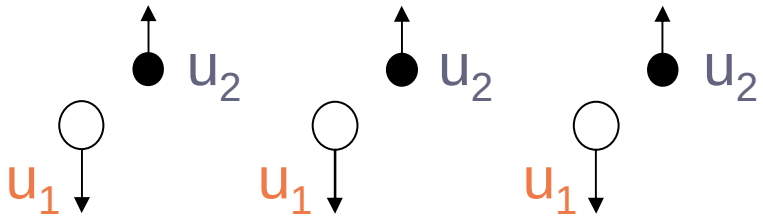
$\mathbf{k}\perp\mathbf{D}$ or $\mathbf{D}=0$ $\mathbf{k}\parallel\mathbf{E}$ or $\mathbf{E}=0$

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

POP Scattering …

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

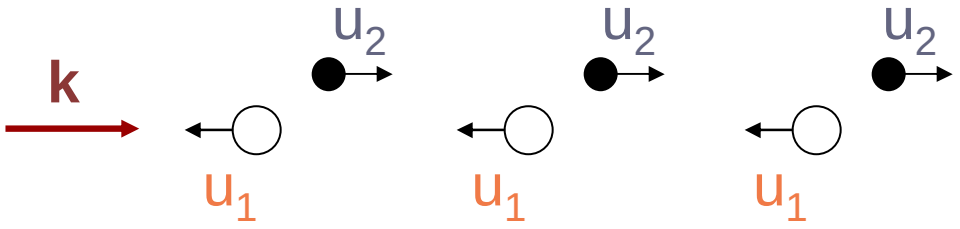
Transverse mode:



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

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

Longitudinal mode:



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

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

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

Polarization Constant

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

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

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

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

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

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

Scattering Rate

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

$$\nabla\cdot\mathbf{D} = i\mathbf{k}\cdot\mathbf{D} = \nabla\cdot\left(\varepsilon_\infty\mathbf{E}_{ind}+\mathbf{P}\right)=0 \Rightarrow \mathbf{D}=0 \text{ and } \mathbf{E}_{ind}=-\frac{\mathbf{P}}{\varepsilon_\infty}$$

- Consider only one Fourier component:

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

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

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

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

Scattering Rate …

Scattering Rate Calculation:

- Matrix element squared for this interaction:

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

- Transition rate per unit time from state **k** to state **k'**:

$$\Gamma_{k,k'} = \frac{2\pi}{\hbar}\left|V_{k,k'}\right|^2 \delta(\varepsilon_{\mathbf{k'}} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{L0})$$

$$= \frac{\pi e^2}{V\gamma\omega_{LO}}\frac{1}{q^2}\left(N_0 + \tfrac{1}{2} \mp \tfrac{1}{2}\right)\delta(\mathbf{k'}-\mathbf{k} \mp \mathbf{q})\delta(\varepsilon_{\mathbf{k'}} - \varepsilon_{\mathbf{k}} \mp \hbar\omega_{L0})$$

- Total scattering rate per unit time out of state **k**:

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

Final Values

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

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

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

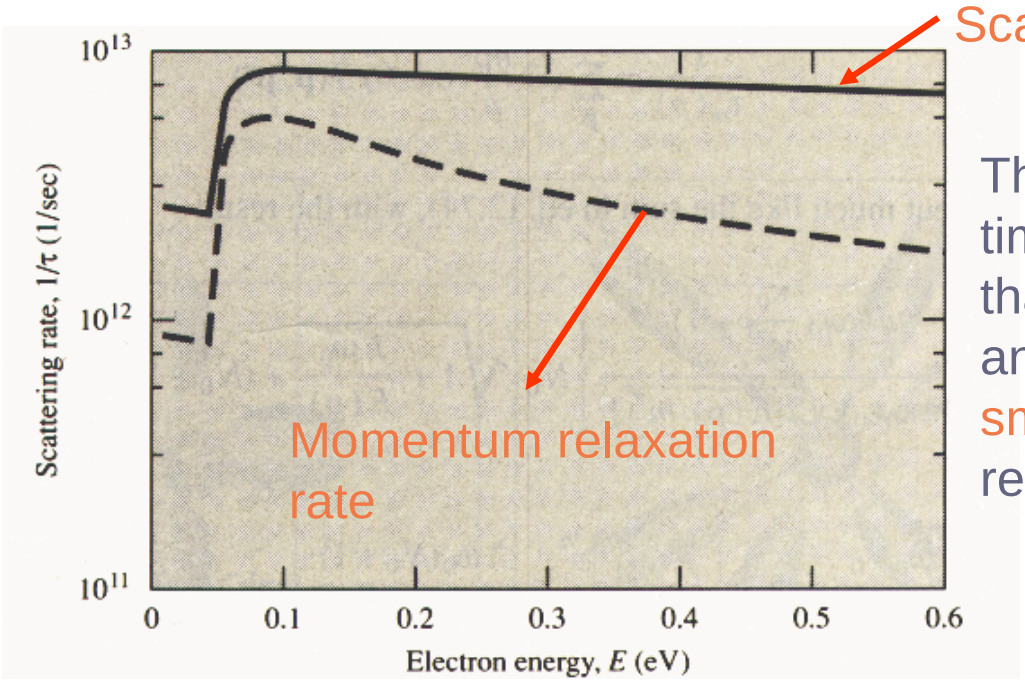
- Final expression for Γ_k

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

Graphical Representation

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)



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.

Piezoelectric Scattering

(B) Piezoelectric scattering

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

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

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

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

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

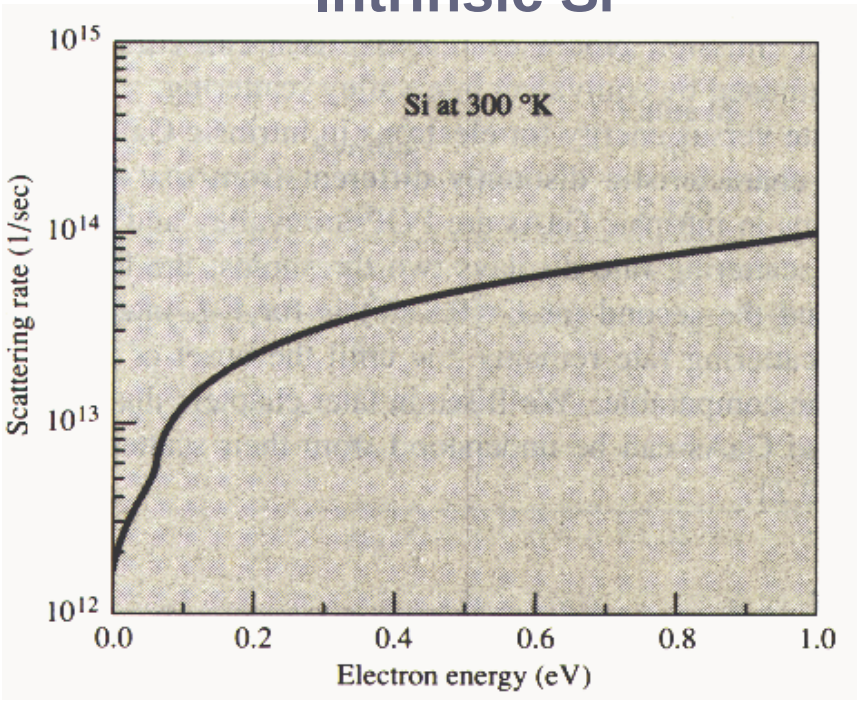
$$\Gamma_k = \frac{m^* k_B T}{4\pi\hbar^3 k \rho} \left(\frac{e e_{pz}}{\varepsilon_\infty v_s}\right)^2 \ln\left(1 + 4\frac{k^2}{q_D^2}\right)$$

where q_D is the screening wavevector.

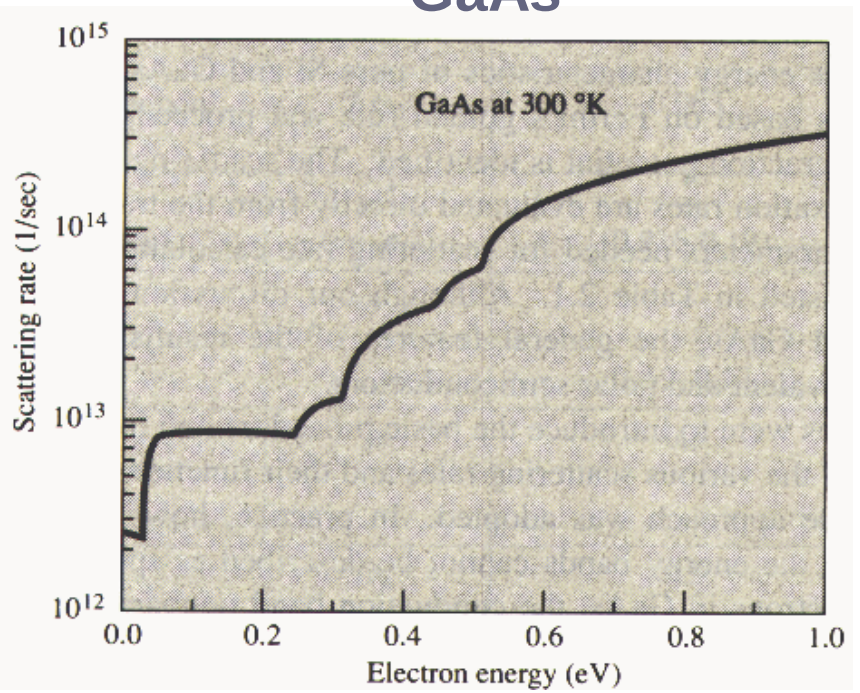
Total Scattering Rates

Total Electron Scattering Rate Versus Energy:

Intrinsic Si



GaAs



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