

Electron-phonon scattering (Finish Lundstrom Chapter 2)

Deformation potentials

The mechanism of electron-phonon coupling is treated as a perturbation of the band energies due to the lattice vibration.

Equilibrium atomic positions: $R_1^\circ, R_2^\circ, R_3^\circ, \dots$

Lattice vibrations cause perturbations about equilibrium: $R^\circ + \delta R$. Energy bands shift locally due to perturbation. In a linear approximation:

$$\delta E_c = D_c \frac{\delta R}{a}$$

$$\delta E_v = D_v \frac{\delta R}{a}$$

D_c, D_v are constants known as deformation potentials.

Lattice vibration waves lead to sinusoidal variations δE . These mix Bloch waves for the electrons which leads to scattering. We will use δE as a perturbation and then apply Fermi's Golden Rule to get the scattering rates.

Energy and momentum conservation

We consider inelastic scattering where an electron makes a transition from momentum p to $p\zeta$ involving emission or absorption of a phonon q :

Energy conservation:

+ sign phonon absorption

- sign phonon emission

Assuming spherical, parabolic bands, and intra-valley scattering (i.e. both initial and final electron states are within the same parabolic band):

(1)

Momentum conservation tells us that:

$$\vec{p}' = \vec{p} \pm \hbar \vec{q}$$

take

$$\hbar^2 p'^2 = \hbar^2 p^2 \pm 2\hbar p q \cos\theta + \hbar^2 q^2$$

$$= p^2 + \hbar^2 q^2 \pm 2\hbar p q \cos\theta \quad (2)$$

compare (1) & (2) to obtain:

$$\pm 2m^* \hbar \omega = \hbar^2 q^2 \pm 2\hbar p q \cos\theta$$

simplifying:

$$\hbar q = 2p \left[\mp \cos\theta \pm \frac{\omega}{qv_e} \right] \quad (3)$$

where $v_e = \frac{p}{m^*}$.

(3) sets min, max values for phonon wave vectors via $-1 \leq \cos\theta \leq 1$

Intravalley acoustic phonon scattering.

$$\omega = qv_s \quad v_s: \text{ sound velocity}$$

$$\hbar q = 2p \left[\mp \cos\theta \pm \frac{v_s}{v_e} \right]$$

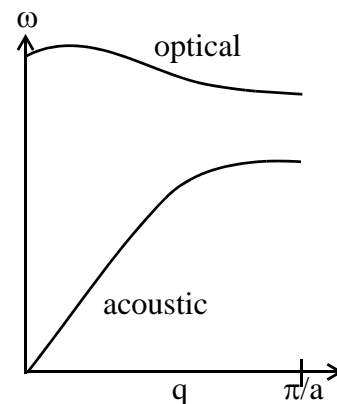
$$q_{\max}: \theta = \pi \quad \text{absorption}$$

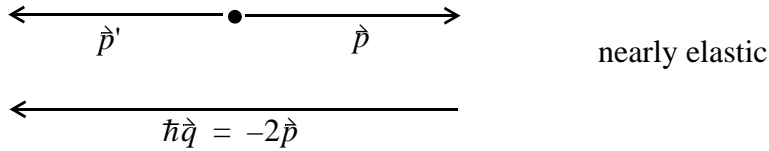
$$\theta = 0 \quad \text{emission}$$

$$\omega = qv_s = \frac{2p}{\hbar} \left[\mp \cos\theta \pm \frac{v_s}{v_e} \right] v_s$$

Typically, $v_s \sim 10^5$ cm/sec and $v_e \sim 10^7$ cm/sec (300K). So,

$$\frac{v_s}{v_e} \ll 1$$





$$\text{magnitude of } q_{\max} = \frac{2m^*v_e}{\hbar}$$

For $m^* \sim 0.5m_0$, with $v_e \sim 10^7$ cm/sec, we find



where a is taken as 5 \AA . Thus, for intravalley acoustic phonon scattering, the participating phonons are near zone center.

Energy transfer

$\Delta E_{\max} = \hbar\omega_{\max} = \hbar q_{\max} v_s \cong 10^{-3} \text{ eV}$, which is small, so we find that intravalley acoustic phonon scattering is nearly elastic

Intravalley optical phonon scattering

Optic phonon energies ω_o are in the range of 30 - 50meV, so optic phonon scattering is definitely inelastic. Once again applying the conservation law (3):



$$-\hbar q^2 \mp 2pq \cos \theta \pm 2p \frac{\omega_o}{v_e} = 0$$

Solving for q :

$$q = \frac{\pm 2p \cos \theta - \sqrt{4p^2 \cos^2 \theta \pm 8\hbar\omega_o m^*}}{-2\hbar}$$

(only the - sqrt term is physical, since q is a magnitude, hence must be positive.
So:

$$\begin{aligned}\hbar q &= p \left[\mp \cos \theta + \sqrt{\cos^2 \theta \pm \hbar \omega_o \left(\frac{2m^*}{p^2} \right)} \right] \\ &= p \left[\mp \cos \theta + \sqrt{\cos^2 \theta \pm \hbar \omega_o / E} \right]\end{aligned}$$



for room temp $E \sim (\hbar \omega_o)/2$

$\hbar q_{\max} \cong 2.7p$, which again involves phonons near zone center since the electron energy is usually thermal, hence the electron momentum is small.

Scattering rates

Fermi golden rule:

$$S(\vec{p}, \vec{p}') = \frac{2\pi}{\hbar} |H_{pp'}|^2 \delta(E(p') - E(p) \mp \hbar \omega_q) \quad \begin{array}{|c|} \hline - \text{abs} \\ + \text{emiss} \\ \hline \end{array}$$

For deformation potential scattering

In the case of optic phonons, $\delta a \propto u$, since the atoms are moving in opposite directions.

On the other hand, for acoustic phonons, $\delta a \propto \frac{\partial u}{\partial x}$, since, for acoustic phonons, the atoms are moving in nominally the same direction. So we have:



D_A - acoustic deformation potential

$\delta E_o = D_o u$ D_o - optic deformation potential

Acoustic

Since



$$|H_{p'p}|^2 = (D_A q A_q)^2 \delta(\vec{p}' - \vec{p} - \hbar \vec{G} \pm \hbar \vec{q})$$

Where the parameter A_q is derived from the quantum mechanics of phonons. Recall the phonon operator:

$$\delta R = \sum_q \left(\frac{\hbar}{2M\omega_q} \right)^{1/2} \hat{e}_q [a_q e^{i\vec{q} \cdot \vec{r}} + a_{-q}^\dagger e^{-i\vec{q} \cdot \vec{r}}]$$

For phonon absorption:

$$A_q^2 = \frac{\hbar}{2M\omega_q} |\langle N_q + 1 | a_q^\dagger | N_q \rangle|^2 = \frac{(N_q + 1)\hbar}{2M\omega_q}$$

where N_q = phonon occupation for mode q . For phonon emission we get:

$$A_q^2 = \frac{\hbar}{2M\omega_q} |\langle N_q + 1 | a_q^\dagger | N_q \rangle|^2 = \frac{(N_q + 1)\hbar}{2M\omega_q}$$

At room temperature, N_q is typically $\gg 1$, so $N_q \cong N_q + 1 \cong \frac{kT}{\hbar\omega}$. We can therefore add the emission and absorption processes. If we neglect $G \neq 0$ processes, which are generally weaker, we obtain the acoustic phonon scattering rate:

$$S(p', p) = \frac{2\pi D_A^2 kT}{\hbar M \omega^2} q^2 \delta(\vec{p}' - \vec{p} \mp \hbar\vec{q}) \delta(E' - E \mp \hbar\omega)$$

After integration over all allowed p' , and use of $\omega = qv_s$ (see text for full details), we obtain:

$$S(p) = \frac{1}{\tau} = \frac{\pi V_{cell} D_A^2 kT}{\hbar M v_s^2} D(E)$$

density of electron states

$$=$$

where $\rho = \frac{M}{\text{unit V}}$ is the mass density. Again a power law in E:

$$=$$

for acoustic phonon scattering.

Optic deformation potential scattering

In this case, the perturbation of the band energy goes as $\delta E_o = D_o u$. Since the process is so inherently “inelastic,” we can’t combine absorption and emission. The matrix element is similar to the acoustic phonon case. For phonon absorption:



For phonon emission:

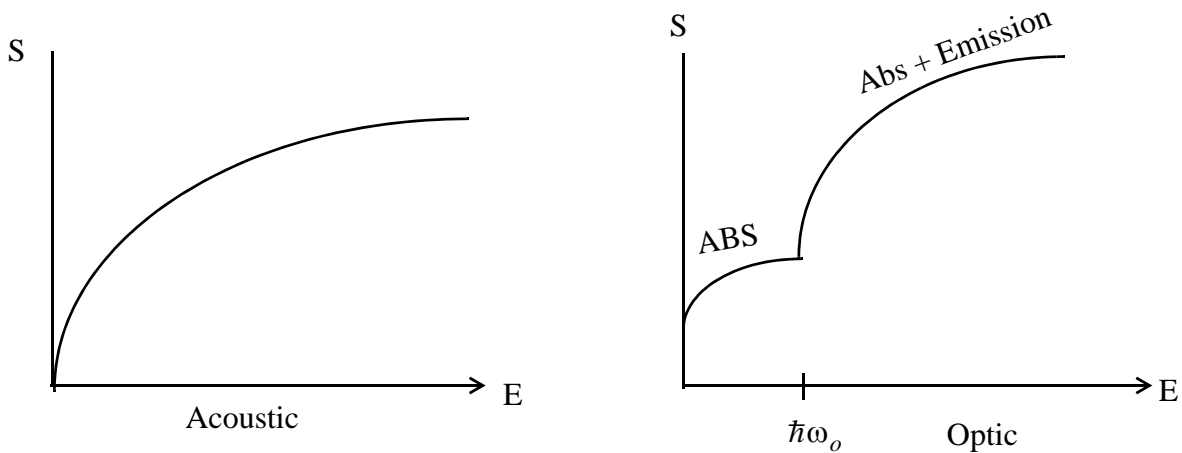
$$|H_{pp'}|^2 = \frac{\hbar D_o^2}{2M\omega_o} (N_q + 1) \delta(\hbar\vec{p}' - p + \hbar\vec{q}_o)$$

The scattering rate is a sum of emission and absorption scattering:

$$S(p) = \frac{D_o^2 (2m^*)^{3/2}}{2\pi\rho\hbar^3\omega_o} \left[N_q (E + \hbar\omega_o)^{1/2} + (N_q + 1) (E - \hbar\omega_o)^{1/2} \underbrace{u_o(E - \hbar\omega_o)} \right]$$

Heaviside or unit-step function

Phonon Scattering Rates



Polar optic phonon scattering

This is the process that usually dominates in compound semiconductors. In this case, since we are considering optic phonons, the induced dipole is directly proportional to the phonon amplitude:

$$p = e^* Q u$$

where e^* is the effective charge on the dipole. A simple analysis leads to an expression for the perturbation energy:

$$V_c \frac{1}{V_c} \int \frac{1}{V_c} \left(\frac{1}{\epsilon_\infty - \epsilon(o)} \right) \left[N_q \sinh^{-1} \left(\frac{E}{\hbar \omega_o} \right)^{1/2} + (N_q + 1) \sinh^{-1} \left(\frac{E}{\hbar \omega_o} - 1 \right)^{1/2} \right]$$

Here, V_c is the unit cell volume. The resulting scattering rate for the unscreened case is (see text):

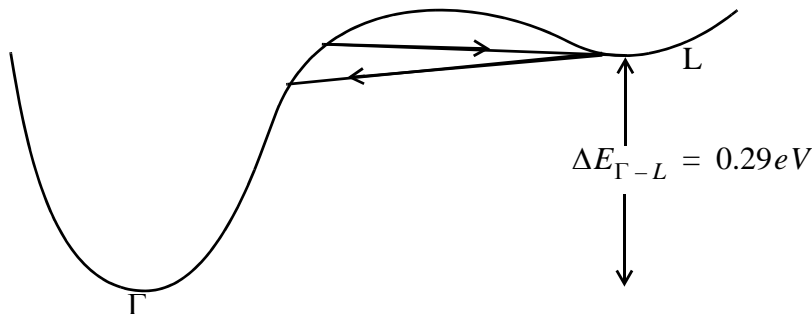
$$S(p) = \frac{e^2 \omega_o}{2\pi \hbar \sqrt{2E/m^*}} \left(\frac{1}{\epsilon_\infty - \epsilon(o)} \right) \left[N_q \sinh^{-1} \left(\frac{E}{\hbar \omega_o} \right)^{1/2} + (N_q + 1) \sinh^{-1} \left(\frac{E}{\hbar \omega_o} - 1 \right)^{1/2} \right]$$

The screened result for this case is a complex expression (see Ferry if interested).

Intervalley scattering

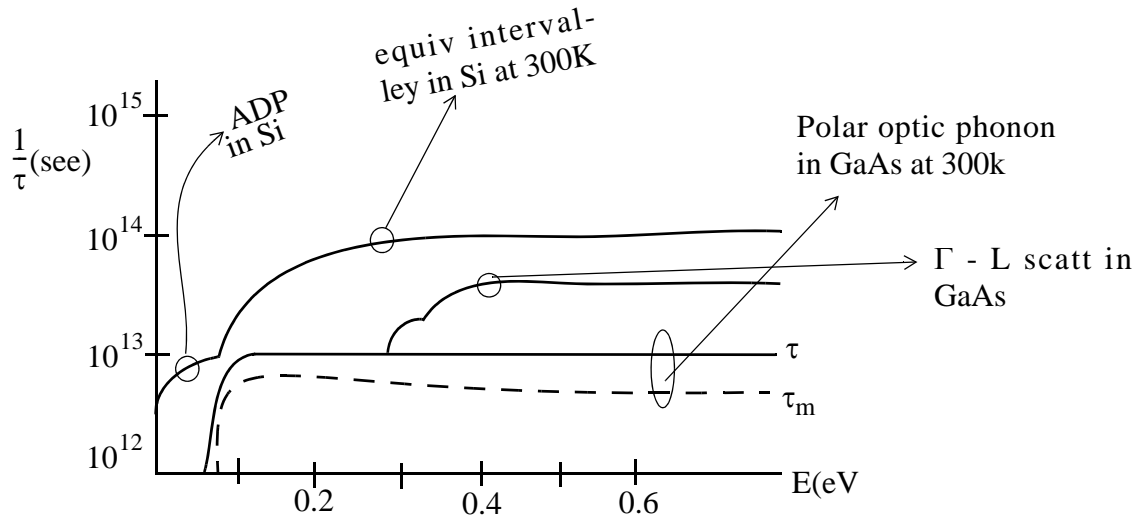
In Si, zone edge phonons (optical or high energy acoustic) can move carriers from one equivalent valley to another. Optical deformation potential scattering rate applies, modified by Z_f , the number of equivalent final valleys, and using D_{if} , which is defined as the intervalley deformation potential.

In GaAs



only very high energy carriers in Γ valley can scatter to L valley. This only occurs in high fields, or certain laser excitation expts.

Summary - Scattering in intrinsic Si, GaAs (Lundstrom 2.11)



- ADP scattering dominates for $E < \hbar\omega_{op}$ for both Si, GaAs
- Si has equivalent intervalley scattering for low energies involving optic phonons.
- In GaAs, no intervalley scattering for $E < 0.29\text{eV}$. Low field behavior in GaAs dominated by POP scattering. This is weaker and \sim const with energy.