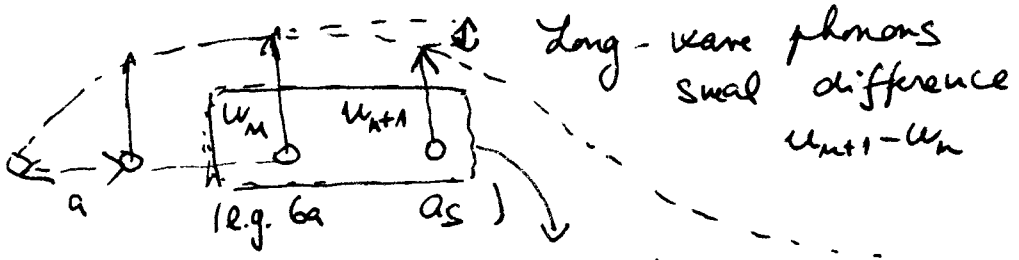
Scattering on acoustical phonons (non-poler)

Acoustic phonons – atoms in the elementary cell oscillate in phase

non-poler means, that the bond between atoms is covalent

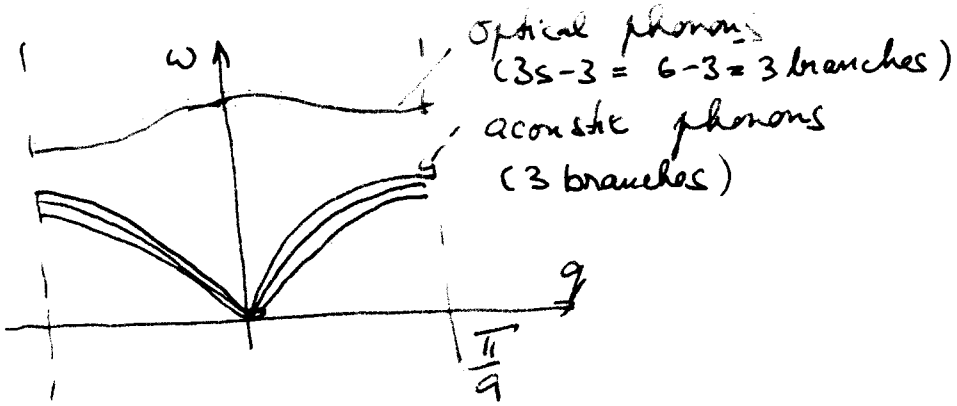


$s = 2$. elementary cell

2 atoms in the elementary cell

Let us suppose, that there are two different atoms in the elementary cell – either physically different (Ga, As) or the same, but with different bond strength to the neighbors ($s = 2$)

If these atoms oscillate in one direction (in phase) we call the phonons acoustic



In case of long wavelengths λ (small q) the difference of u_n and u_{n+1} is small

$$\vec{u}_{n\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\vec{q}\,j} \left\{ \vec{e}_{lj}(\vec{q})\, b_j(\vec{q})\, e^{i\vec{q}\vec{a}_n} + \vec{e}_{lj}^{\,*}(\vec{q})\, b_j^{+}(q)\, e^{-i\vec{q}\vec{a}_n} \right\}$$

$b_j(\vec{q})$ ... amplitude

$\vec{e}_{lj}(\vec{q})$ .. polarization vector
determines the direction of oscillation of the l-th atom participating in a monochromatic wave with wave vector $\vec{q}$ of the j-th branch, i.e. with frequency $\omega_j(\vec{q})$

Electrons scatter on acoustic phonons, because during propagation of the acoustic wave comes to deformation of elementary cell resulting in a change of lattice constant as already mentioned, in the long-wavelength case the difference of shift vectors of neighboring atoms $\vec{u}_n$, $\vec{u}_{n+1}$ small. Therefore the interaction energy (perturbation Hamiltonian $\mathcal{H}'$) is a function of the first derivative of the shift vector $\vec{u}_n$. We can write for $\mathcal{H}'$

$$\mathcal{H}'_{AF} = E_1 \cdot \operatorname{div} \vec{u}_{LA}(\vec{r})$$

E_1 ... deformation potential of the conduction band (material parameter)

$\Rightarrow \quad \mathcal{H}'_{AF} \sim i\vec{q}\vec{e}$

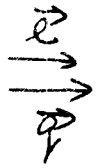
$\Rightarrow \quad$ if $\vec{q} \perp \vec{e}$, $\mathcal{H}'_{AF} = 0$

$\vec{e}$ ... transversal directions of atom shift

$\vec{q}$ ... direction of propagation of the acoustic wave

$\Rightarrow$ Transversal phonons do not interact with electrons, because the corresponding matrix element $M(\vec{k},\vec{k}') = \frac{2\pi}{\hbar} \langle \psi^* | \mathcal{H}' | \psi \rangle = 0$

$\Downarrow$ only longitudal (non polar) long-wave acoustic phonons interact with electrons.



We will show only long-wavelenth phonons (acoustic) participate in scattering of electrons. We use the laws of conservation of energy and momentum.

$$\mathcal{E}(\vec{k}') = \mathcal{E}(\vec{k}) \pm \hbar\omega_q$$

$$\frac{\hbar^2 k'^2}{2m_e^*} = \frac{\hbar^2 k^2}{2m_e^*} \pm \hbar\omega_q$$

$$\vec{k}' - \vec{k} \pm \vec{q}$$

$$k'^2 = k^2 \pm 2\vec{k}\cdot\vec{q} + \vec{q}^{\,2}$$

$$k'^2 = k^2 \pm 2kq\cos\theta + q^2$$

$k' \neq k$ nonelastic scattering

$$\frac{\hbar^2 k^2}{2m_e^*} \pm \frac{\hbar^2}{2m_e^*} 2kq\cos\theta + \frac{\hbar^2 q^2}{2m_e^*} = \frac{\hbar^2 k^2}{2m_e^*} \pm \hbar\omega_q$$

$$q^2 = \mp 2kq\cos\theta \pm \frac{2m_e^*}{\hbar}\omega(\vec{q})$$

$$q = \mp 2k\cos\theta + \frac{2m_e^*}{\hbar q}\omega(\vec{q})$$

$$q = 2k\left(\mp\cos\theta \pm \frac{m^*}{\hbar k q}\omega(\vec{q})\right)$$

$$m_e^* v = \hbar k$$

$$q = 2k\left(\mp\cos\theta \pm \frac{\omega(\vec{q})}{vq}\right)$$

For acoustic phonons $\omega(q) \sim v_s q$

v_s ... velocity of sound

$$\Rightarrow \quad q = 2k\left(\mp\cos\theta \pm \frac{v_s}{v}\right)$$

$$q_{max} = 2k\left(1 \pm \frac{v_s}{v}\right)$$

$v_s \sim 10^3$ m/s (at 300K)

$v \sim 10^5$ m/s

$$\Rightarrow \quad \frac{v_s}{v} << 1 \quad \Rightarrow \quad q_{max} \approx 2k$$

$$\frac{q_{max}}{\frac{\pi}{a}} \approx \frac{2m_e^* \cdot v}{\hbar \cdot \frac{\pi}{a}} \approx \frac{1}{4}$$

Only long-wavelength Acoustic phonons (approx. from 1/4 th of the Brillouin zone) can participate in interactions with electrons.

Matrix element for scattering on non-polar longitudinal acoustic phonons

$$|M_{LA}(\vec{q},\vec{k}')|^2 = E_1^2 \Delta T \cdot \frac{1}{\rho v_s^2 V}$$

E_1 ... deformation potential
ρ .. density of matter

Calculation of relaxation time for scattering on longitudinal acoustic phonons

$$\frac{1}{\tau_{LA}} = \frac{\pi V}{2\hbar} g(\varepsilon) \int_0^{\pi} |M_{LA}|^2 (1-\cos\theta)\sin\theta \, d\theta =$$

$$= \frac{\pi V}{2\hbar} \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} \varepsilon^{1/2} \cdot \frac{E_{1c}^2 \Delta T}{\rho v_s^2 V} \int_0^{\pi} (1-\cos\theta)\sin\theta \, d\theta$$

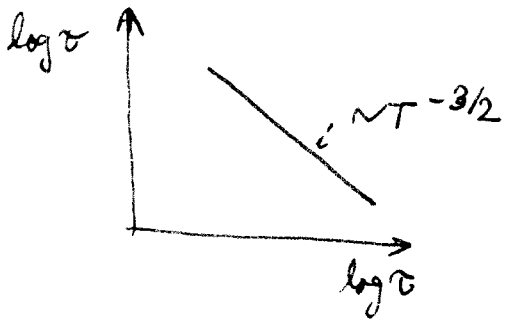
$$\int_0^{\pi} (1-\cos\theta)\sin\theta \, d\theta = -\int_1^{-1} (1+x)\,dx = \int_{-1}^{+1} (1-x)\,dx =$$

$$= [x]_{-1}^{+1} - \left[\frac{x^2}{2}\right]_{-1}^{+1} = 2$$

$$\Rightarrow \frac{1}{\tau_{LA}} \sim \varepsilon^{1/2} \Delta T \qquad \varepsilon \sim \Delta T$$

$$\Rightarrow \frac{1}{\tau_{LA}} \sim (\Delta T)^{3/2} \qquad \tau_{LA} \sim T^{-3/2}$$

$$\log \tau_{LA} = -\frac{3}{2} \log T$$



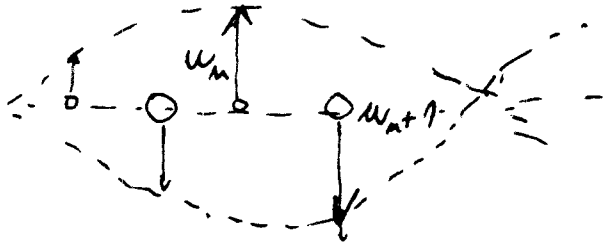
Scattering on polar acoustic phonons (piezoacoustic scattering)

In crystals without a center of symmetry with a partially ionic bond there is together with the deformation Hamiltonian H_{AF} also a perturbation Hamiltonian connected with electric dipole of the oscillation.

The temperature dependence of the relaxation time is $\tau_{PAF} = \tau_{PZ} \sim T^{-1/2}$

Scattering on non-polar optical phonons

Optical phonons – the atoms in the elementary cell oscillate in counterphase



$\frac{1}{\tau_{LO}^{NP}} \sim T^{-3/2}$

In case of a covalent bond the main scattering mechanism is lattice deformation (change of the lattice constant)

The interaction (perturbation) Hamiltonian is

$$H'^{NP}_{LO} = \frac{\Pi}{a} \cdot D_0 \cdot u \quad ; \quad u \text{ .. atomic shift}$$

D_0 .. deformation potential for optical phonons

Scattering by polar optical phonons

Atoms in the elementary cell vibrate in counterphase. If the atomic bond is ionic or partially ionic, the vibration results in oscillations of an electromagnetic dipole. The corresponding polarization can be written as

$$\vec{P}(\vec{r}) = \left(\frac{NM\omega^2(\vec{q})}{V\varepsilon_0\varepsilon_r}\right)^{1/2}(\vec{u}_1 - \vec{u}_2) = \vec{u}_1 \text{ (or } \vec{u}_2\text{)}$$

$$= \left(\frac{NM\omega^2(\vec{q})}{V\varepsilon_0\varepsilon_r}\right)^{1/2} \sum_{\vec{q},j=n,o} (\vec{e}_1(\vec{q}) - \vec{e}_2(\vec{q}))(b_j(\vec{q})e^{i\vec{q}\cdot\vec{r}} + b_j^*(\vec{q})e^{-i\vec{q}\cdot\vec{r}})$$

optical branches

$M = M_1 + M_2$

(in the long-wave approximation)

Introducing $\vec{e}_j = \vec{e}_{1j} - \vec{e}_{2j}$

$$\Rightarrow \quad \vec{P}(\vec{r}) \sim \vec{e}_j(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}$$

We know from Maxwell equations

$$\vec{D} = \varepsilon_0\vec{E} + \vec{P} \qquad \left(\operatorname{div}\vec{D} = \operatorname{div}\vec{P} = \frac{\rho}{\varepsilon_0} = \operatorname{div}\vec{E}\right)$$

$\operatorname{div}\vec{D} = \rho_{ext}$ density of free charge can be neglected in most cases ($\rho_{ext} = 0$)

$$\Rightarrow \quad \operatorname{div}\vec{E} = -\frac{\operatorname{div}\vec{P}}{\varepsilon_0} = \frac{\rho}{\varepsilon_0}$$

$$\Delta\varphi = -\frac{\rho}{\varepsilon_0} = -\frac{(\rho_f + \rho')}{\varepsilon_0} \doteq -\frac{\rho'}{\varepsilon_0}$$

Poisson equation

$$\Rightarrow \Delta\varphi = \frac{\operatorname{div}\vec{P}}{\varepsilon_0}$$

$$\operatorname{div}\vec{P} \sim i\vec{q}\cdot\vec{e}_j(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}$$

$$\Delta\varphi \sim i(\vec{q}\cdot\vec{e}_j(\vec{q}))e^{i\vec{q}\cdot\vec{r}} \qquad / \int d\vec{r}$$

$$\nabla_r\varphi \sim \frac{i\vec{q}\cdot\vec{e}_j(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}}{iq} \qquad / \int d\vec{r}$$

$$\varphi \sim \frac{i\vec{q}\cdot\vec{e}_j(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}}{(i\cdot i)q^2}$$

$$\Rightarrow \mathcal{H}' = -e\varphi \sim \vec{q}\cdot\vec{e}_j(\vec{q})$$

$$\vec{q}\cdot\vec{e}_j(\vec{q}) = 0 \quad \text{if} \quad \vec{q} \perp \vec{e}_j(\vec{q})$$

$\Rightarrow$ only longitudinal phonons participate in interactions

When finally the relaxation time is calculated, we obtain

$$\tau_{LO}^{(P)} \sim T^{-1/2}$$ (at high temperatures when the scattering is nearly elastic and we can use the relaxation time approx.)

Summary of scattering for phonons at a high-temperature limit (when this type of scattering usually dominates)

Non-polar acoustic phonons	$\tau_{LA} \sim T^{-3/2}$
Polar acoustic phonons	$\tau_{PZ} \sim T^{-1/2}$
Non-polar optical phonons	$\tau_{LO}^{(np)} \sim T^{-3/2}$
Polar optical phonons	$\tau_{LO}^{(p)} \sim T^{-1/2}$

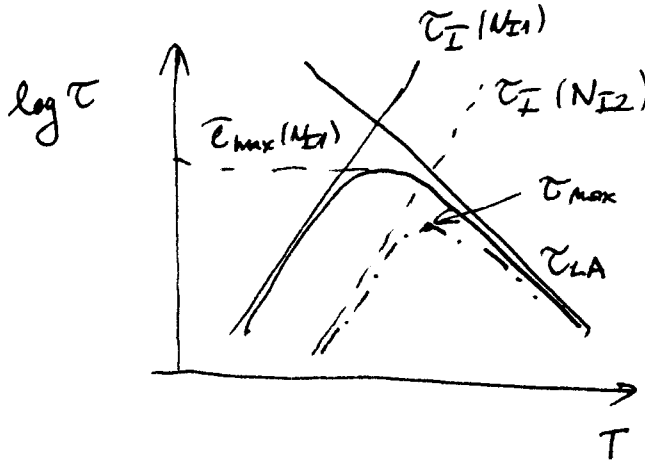
Scattering on ionized impurities

$$\frac{1}{\tau_I} \sim \varepsilon^{-3/2} \quad (\sim T^{-3/2})$$

$$\tau_I \sim T^{3/2}$$

Combined scattering on ionized impurities and phonons (presented for acoustic phonons)

$$\frac{1}{\tau} = \frac{1}{\tau_I} + \frac{1}{\tau_{LA}}$$



We can see that relaxation time τ has a maximum for a given concentration of ionized impurities N_I. If this concentration is higher (the maximum τ is smaller and shifted to higher temperatures.

The whole diagram can be drawn also for the physical quantity "mobility",

$$\mu = \frac{e}{m_e^*} \cdot \tau .$$