(D) PIEZOELECTRIC SCATTERING - INTRAVALLEY

- As mentioned in the previous section, in polar materials, the vibrations of the oppositely charged atoms give rise to long-range macroscopic electric fields in addition to deformation potentials. The interaction of the electrons with these fields produces additional component for scattering.

→ First-order polarization occurs in connection with the contrary motion of the two atoms in the primitive unit cell that is characteristic of the longitudinally polarized optical mode (Electron - longitudinal polar optical phonon scattering)

→ Second-order polarization occurs in connection with acoustic strain and is associated with the piezoelectric effect. This scattering mechanism is discussed here.

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

$$\boxed{\vec{P} = e_{pz}\,\nabla\cdot\vec{u}} \quad (1)$$

where e_{pz} is the piezoelectric constant, which in a more rigorous treatment represents tensor quantity. To find the interaction of an electron with this polarization, we note that if there is no free charge, the divergence of the electric displacement vanishes, i.e.

$$\nabla\cdot\vec{D} = \varepsilon_\infty \nabla\cdot\vec{E} + \nabla\cdot\vec{P} = 0$$

The electrostatic potential for this electric field is $\vec{E} = -\nabla\varphi$, i.e.

$$\varepsilon_\infty \nabla\cdot(-\nabla\varphi) + \nabla\cdot\vec{P} = 0$$

or:

$$\boxed{\varepsilon_\infty \nabla^2\varphi = \nabla\cdot\vec{P}} \quad (2) \qquad \Rightarrow \varepsilon_\infty \nabla^2\varphi = \nabla\cdot(e_{pz}\cdot\nabla u)$$

- Expressing the displacement in terms of normal coordinates, i.e.

$$\vec{u} = \sum_{q\nu} \sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\left[\hat{a}_{q\nu}\, e^{i\vec{q}\cdot\vec{r}} + \hat{a}_{q\nu}^{+}\, e^{-i\vec{q}\cdot\vec{r}}\right]$$

gives:

$$\nabla\vec{u} = \sum_{q,\nu} \sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\; i\vec{q}\left[\hat{a}_{q\nu}\, e^{i\vec{q}\cdot\vec{r}} + \hat{a}_{q\nu}^{+}\, e^{-i\vec{q}\cdot\vec{r}}\right]$$

or:

$$\nabla\cdot\nabla\vec{u} = \sum_{q,\nu} \sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\;(-q^2)\left[\hat{a}_{q\nu}\, e^{i\vec{q}\cdot\vec{r}} + \hat{a}_{q\nu}^{+}\, e^{-i\vec{q}\cdot\vec{r}}\right]$$

Now, representing $\varphi(\vec{r})$ in terms of its Fourier components:

$$\varphi(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{q}\left[\Phi_q\, e^{i\vec{q}\cdot\vec{r}} + \Phi_q^{+}\, e^{-i\vec{q}\cdot\vec{r}}\right]$$

gives:

$$\nabla^2\varphi = \frac{1}{\sqrt{N}}\sum_q (-q^2)\left[\Phi_q e^{i\vec{q}\cdot\vec{r}} + \Phi_q^+ e^{-i\vec{q}\cdot\vec{r}}\right]$$

Substituting these results into (2) leads to:

$$\sum_q \frac{1}{\sqrt{N}}\varepsilon_\infty(-q^2)\left[\Phi_q e^{i\vec{q}\cdot\vec{r}} + \Phi_q^+ e^{-i\vec{q}\cdot\vec{r}}\right] =$$

$$= \sum_{q\nu}\sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\,(-e_{pz}q^2)\left[\hat{a}_{q\nu} e^{i\vec{q}\cdot\vec{r}} + \hat{a}_{q\nu}^+ e^{-i\vec{q}\cdot\vec{r}}\right]$$

which gives:

$$\frac{1}{\sqrt{N}}\Phi_q = \frac{e_{pz}}{\varepsilon_\infty}\sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\,\hat{a}_{q\nu}$$

$$\frac{1}{\sqrt{N}}\Phi_q^+ = \frac{e_{pz}}{\varepsilon_\infty}\sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\,\hat{a}_{q\nu}^+$$

i.e.

$$\varphi(\vec{r}) = \frac{e_{pz}}{\varepsilon_\infty}\sum_{q\nu}\sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\left[\hat{a}_{q\nu} e^{i\vec{q}\cdot\vec{r}} + \hat{a}_{q\nu}^+ e^{-i\vec{q}\cdot\vec{r}}\right]$$

- Therefore, the interaction potential is given by:

$$H_{ep}(\vec{r}) = -e\,\varphi(\vec{r}) = -\frac{e\,e_{pz}}{\varepsilon_\infty}\sum_{q\nu}\sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\left[\hat{a}_{q\nu} e^{i\vec{q}\cdot\vec{r}} + \hat{a}_{q\nu}^+ e^{-i\vec{q}\cdot\vec{r}}\right]$$

The electronic part of the electron-phonon interaction for piezoelectric scattering is then given by:

$$\boxed{H_{q\nu}(\vec{r}) = -\frac{e\,e_{pz}}{\varepsilon_\infty}} \quad (3)\ ,$$

which leads to the following expression for the matrix element squared for this scattering mechanism:

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

(top-sign ⇒ absorption, bottom-sign ⇒ emission)

- Important comments: Piezoelectric scattering predominantly occurs at low temperatures and very pure (dislocation-free) semiconductors. Small effective mass also favors piezoelectric scattering. In polar semiconductors with purities available at present, ionized impurity scattering will probably dominate. Hence, there are only few applications for piezoelectric scattering.

→ The piezoelectric constant is obtained from piezoelectric measurements and is on the order of 10^{-5} A·s/cm^2.

- Momentum relaxation rate for piezoelectric scattering:

In the elastic and equipartition approximation, we have:

→ $E_K' \approx E_K$ for both absorption and emission processes

→ $N_q = \frac{1}{e^{\hbar\omega_q/k_BT}-1} \approx \frac{1}{1+\frac{\hbar\omega_q}{k_BT}-1} \approx \frac{k_BT}{\hbar q v_s} = \frac{k_BT}{\hbar\omega_q} \gg 1$

Therefore, $N_q \approx N_q+1$

(except at low temperatures, this is satisfied)

With these approximations, and assuming high energy electrons ($q_{min}=0$, $q_{max}=2k$), we get:

$$\frac{1}{\tau_m(k)} = \frac{m^* \cancel{V}}{4\pi\hbar^3k^3}\int_0^{2k} q^3 \, \underbrace{\cancel{2}}_{\text{absorption + emission}} \frac{\hbar}{\cancel{2}\rho \cancel{V}\omega_q v}\left(\frac{e e_{pz}}{\varepsilon_\infty}\right)^2 \frac{k_BT}{\hbar\omega_q}\,dq$$

$$= \frac{m^*(e e_{pz}/\varepsilon_\infty)^2 k_BT}{4\pi\hbar^3k^3\rho v_s^2}\underbrace{\int_0^{2k} q^3\frac{1}{q^2}\,dq}_{\int_0^{2k} q\,dq = \frac{1}{2}q^2\Big|_0^{2k} = \frac{1}{2}(2k)^2 = 2k^2}$$

$$= \frac{m^*(e e_{pz}/\varepsilon_\infty)^2 k_BT}{\cancel{4}_2\pi\hbar^3 k^{\cancel{3}}\rho v_s^2}\cdot \cancel{2}\cancel{k^2} = \boxed{\left(\frac{e e_{pz}}{\varepsilon_\infty}\right)^2\frac{m^* k_BT}{2\pi\hbar^3\rho v_s^2}\cdot\frac{1}{k} = \frac{1}{\tau_m(k)}}$$

For parabolic bands $k=\sqrt{2m^*E/\hbar^2}$, which means that

$$\boxed{\tau_m(E) = \tau_0 E^{1/2}}$$

- Scattering rate: one needs to include screening, in which case:

$$|M(k,q)|^2 = \cancel{2}\frac{\cancel{\hbar}}{\cancel{2}\rho V\omega_q v}\frac{k_BT}{\cancel{\hbar}\omega_q v}\left(\frac{e e_{pz}}{\varepsilon_\infty}\right)^2\delta(\vec{k}-\vec{k}'\pm\vec{q}) = \frac{k_BT}{\rho V v_s^2}\left(\frac{e e_{pz}}{\varepsilon_\infty}\right)^2\frac{1}{q^2}\delta(\;)$$

with screening:

$$|M(\vec{k},\vec{q})|^2 \to \frac{k_BT}{\rho V v_s^2}\left(\frac{e e_{pz}}{\varepsilon_\infty}\right)^2\frac{1}{q^2+q_D^2}\delta(\;)$$; where $q_D = 1/\lambda_D$ (λ_D = Debye l.)

The scattering rate is then:

$$\frac{1}{\tau(k)} = \frac{m^*\cancel{V}}{2\pi\hbar^3k}\int_0^{2k}\frac{k_BT}{\rho\cancel{V}}\left(\frac{e e_{pz}}{v_s\varepsilon_\infty}\right)^2\frac{q\,dq}{q^2+q_D^2} = \frac{m^*k_BT}{2\pi\hbar^3k\rho}\left(\frac{e e_{pz}}{v_s\varepsilon_\infty}\right)^2\frac{1}{2}\ln(q^2+q_D^2)\Big|_0^{2K}$$

$$\boxed{\frac{1}{\tau(k)} = \frac{m^*k_BT}{4\pi\hbar^3k\rho}\left(\frac{e e_{pz}}{v_s\varepsilon_\infty}\right)^2\ln\left(1+4\frac{k^2}{q_D^2}\right)} \Rightarrow \boxed{\tau(E) \cong \tau_0 E^{-1/2}}$$ large screening