

THEREFORE, WE CAN WRITE

$$\frac{\Omega_{LO}^2}{\Omega_{TO}^2} = \frac{\epsilon_{ST}}{\epsilon_{\infty}}$$

THIS RELATION IS KNOWN AS LYDDANE-SACHS-TELLER (LST) RELATIONSHIP. ITS VALIDITY CAN BE CHECKED BY COMPARING THE VALUES OF Ω_{LO}/Ω_{TO} FROM RAMAN OR NEUTRON SCATTERING EXPERIMENTS WITH THOSE CALCULATED USING THE EQ. ABOVE AND THE KNOWN DIELECTRIC FUNCTIONS.

MAT.	Ω_{LO}/Ω_{TO}	$(\epsilon_{ST}/\epsilon_{\infty})^{1/2}$
Si	1	1
Ge	1.07	1.08
AlAs	1.12	1.11
Bu	1.24	1.26
ZnSe	1.19	1.19
HgO	1.81	1.83
AgF	1.88	1.88

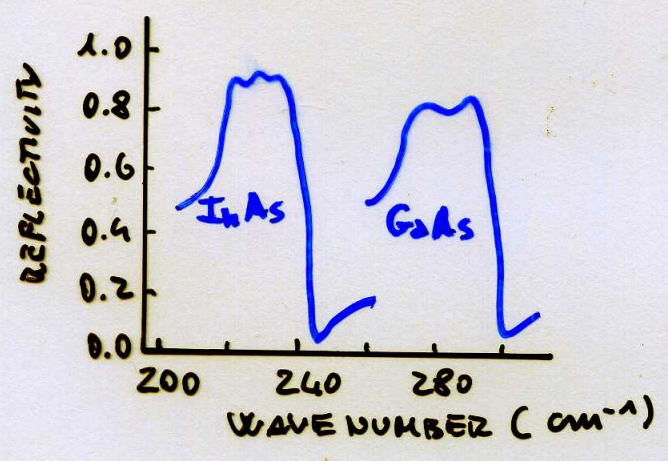
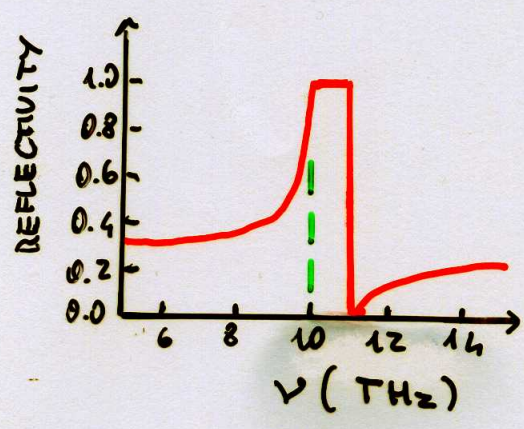
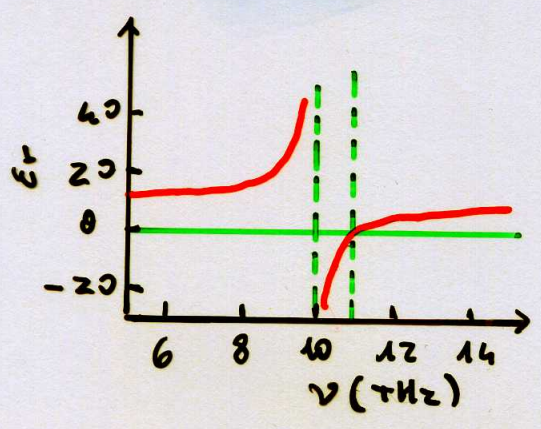
IMPORTANT IS TO NOTE ALSO THAT FOR NON-POLAR CRYSTALS THE T.O. AND L.O. MODES ARE DEGENERATE. THIS IS A CONSEQUENCE OF THE ABSENCE OF IR RESONANCES, THEREFORE $\epsilon_{ST} = \epsilon_{\infty}$. THIS IS THE CASE OF Si, Ge, C (DIAMOND).

WE CAN NOW CALCULATE THE IR OPTICAL CONSTANTS. FOR SIMPLICITY WE CONSIDER MATERIAL WHERE $\kappa \rightarrow 0$ AND THE DIELECTRIC FUNCTION HAS THE FOLLOWING DEPENDENCE

$$\epsilon_r(\nu) = \epsilon_{\infty} + (\epsilon_{ST} - \epsilon_{\infty}) \frac{\nu_{TO}^2}{(\nu_{TO}^2 - \nu^2)}$$

THE EFFECT OF THE κ WILL BE DISCUSSED WHEN COMPARING

THE CALCULATED VALUES WITH THE EXPERIMENT. IF WE CALCULATE $\epsilon_r(\nu)$ FOR $\nu_{TO} = 10 \text{ THz}$, $\nu_{LO} = 11 \text{ THz}$, $\epsilon_{st} = 12.1$ AND $\epsilon_{\infty} = 10$ (THE PHONON FREQUENCIES HAVE BEEN CHOSEN TO SATISFY THE LST CONDITIONS), WE OBTAIN:



AT LOW FREQUENCIES $\epsilon_r \approx \epsilon_{st}$.
 BY INCREASING ν , $\epsilon(\nu)$ INCREASES
 AND AT ν_{TO} IT DIVERGES. BETWEEN
 ν_{TO} AND ν_{LO} ϵ_r IS NEGATIVE (AT
 $\nu = \nu_{LO}$, $\epsilon_r = 0$. FOR $\nu > \nu_{LO}$, ϵ_r
 INCREASES AND FOR HIGH ν $\epsilon_r \rightarrow \epsilon_{\infty}$

THE MOST IMPORTANT PROPERTY OF A POLAR SOLID IN THE IR IS THE REFLECTIVITY. THIS CAN BE CALCULATED FROM THE DIELECTRIC FUNCTION USING THE FRESNEL'S ERS.

$$R = \left| \frac{\tilde{n} - 1}{\tilde{n} + 1} \right|^2 = \left| \frac{\sqrt{\epsilon_r} - 1}{\sqrt{\epsilon_r} + 1} \right|^2$$

THE RESULTS ARE SHOWN IN THE UPPER FIG. AT LOW ν THE REFLECTIVITY IS

$$R \approx \left| \frac{\sqrt{\epsilon_{st}} - 1}{\sqrt{\epsilon_{st}} + 1} \right|^2$$

FOR INCREASING $\nu \rightarrow \nu_{TO}$ $R \rightarrow 1$; $R \approx 1$ FOR $\nu_{TO} < \nu < \nu_{LO}$ ($\sqrt{\epsilon}$ IS IMAGINARY); $R \rightarrow 0$ FOR $\nu \rightarrow \nu_{LO}$ AND FOR $\nu \gg \nu_{LO}$ $R \rightarrow$ ITS ASYMPTOTE OF $(\sqrt{\epsilon_{\infty}} - 1)^2 / (\sqrt{\epsilon_{\infty}} + 1)^2$.

THE REGION WHERE $\nu < \nu < \nu_{L0}$ AND $R \rightarrow 1$ IS KNOWN AS "RESTSTRAHLEN" REGION OR RESIDUAL RAY AND IN THIS SPECTRAL RANGE THE LIGHT DOES NOT PROPAGATE IN THE MEDIUM.

IN SOLIDS, AS FOR MOLECULES, WHEN A PHOTON IS ABSORBED AT A FREQUENCY OF A QUANTIZED VIBRATION (ω IN SOLIDS) THE SYSTEM GETS EXCITED AND A STRONG ABSORPTION LINE IS OBSERVED. OF COURSE ABSORPTION OR REFLECTION ARE RELATED TO THE DIELECTRIC FUNCTION THROUGH THE FRESNELL RELATIONS SO THESE TWO MEASUREMENTS CAN BE REGARDED EQUIVALENT TO THE END OF THE MEASURE OF $\epsilon_r(\nu)$. HOWEVER, IN SOLIDS IS OFTEN PREFERRED MEASURING THE REFLECTIVITY UNLESS THE CRYSTAL IS THINNER ENOUGH MAKING THE MEASUREMENTS IN TRANSMISSION FEASIBLE. THE ABSORPTION COEFFICIENT EXPECTED AT THE RESONANCE WITH THE ω PHOON CAN BE CALCULATED FROM THE IMAGINARY PART OF THE DIELECTRIC FUNCTION. AT $\omega = \omega_{T0}$ WE HAVE

$$\epsilon_r(\omega_{T0}) = \epsilon_{\infty} + i(\epsilon_{ST} - \epsilon_{\infty}) \frac{\omega_{T0}}{\gamma}$$

NOW REMEMBERING THE FOLLOWING EQUATIONS:

$n = \sqrt{\epsilon_r}$ WHERE $\tilde{\epsilon}_r$ CAN BE COMPLEX: $\tilde{\epsilon}_r = \epsilon_1 + i\epsilon_2 \Rightarrow \tilde{n} = n + ik$

$\tilde{n} = n + ik \Rightarrow \epsilon_1 = n^2 - k^2, \epsilon_2 = 2nk$ AND

$$n = \frac{1}{\sqrt{2}} \left(\epsilon_1 + (\epsilon_1^2 + \epsilon_2^2)^{1/2} \right)^{1/2}$$

$$k = \frac{1}{\sqrt{2}} \left(-\epsilon_1 + (\epsilon_1^2 + \epsilon_2^2)^{1/2} \right)^{1/2}$$

AND FOR k SMALL $n = \sqrt{\epsilon_1} \quad k = \frac{\epsilon_2}{2n}$

WE OBTAIN $\alpha = \frac{4\pi k}{\lambda}$

[THIS LAST EQUATION IS OBTAINED FROM THE PROPAGATING FIELD EQUATION IN AN ABSORBING MEDIUM. $\bar{E}(z,t) = \bar{E}_0 e^{i(\tilde{k}kz - \omega t)}$
 $= \bar{E}_0 e^{i(\tilde{n}\frac{2\pi}{\lambda}z - \omega t)} = \bar{E}_0 e^{i(\tilde{n}\omega z/c - \omega t)}$
 $= \bar{E}_0 e^{i(\omega z/c - \omega t)} e^{-k\omega z/c}$. THIS LAST TERM REPRESENTS

THE EXPONENTIAL DECAY DUE TO THE ABSORPTION. SINCE THE INTENSITY IS PROPORTIONAL TO THE SQUARE OF THE FIELD $I \propto \bar{E} \cdot \bar{E}^*$ AND THE TRANSMITTED INTENSITY IS $I = I_0 e^{-\alpha z}$
 $\alpha = \frac{2k\omega}{c} = \frac{4\pi k}{\lambda}$. NOTE THAT THE UNITS OF α IS A L^{-1} I.E. m^{-1}]

AS AN EXAMPLE LET'S CALCULATE THE UPPER AND LOWER LIMIT OF THE RESTSTRAHLEN BAND, THE REFLECTIVITY AT $50 \mu m$ AND THE ABSORPTION COEFFICIENT KNOWING THAT :

$\epsilon_{ST} = 5.9$, $\epsilon_{\infty} = 2.25$ $\gamma_{PHONON} = 10^{-12} s^{-1}$ AND $\nu_{TO} = 4.9 THz$.

- 1 WE CAN CALCULATE ν_{LO} FROM THE LST RELATION

$$\nu_{LO} = \left(\frac{\epsilon_{ST}}{\epsilon_{\infty}} \right)^{1/2} \times \nu_{TO} = \left(\frac{5.9}{2.25} \right)^{1/2} \times 4.9 THz = 7.9 THz$$

THEREFORE THE RESTSTRAHLEN RANGE $\nu_{TO} < \nu < \nu_{LO}$ IS $4.9 - 7.9 THz$

2 - AT $50 \mu m$ WE ARE IN THE MIDDLE OF THE RESTSTRAHLEN BAND AND THE REFLECTIVITY IS VERY HIGH. WE MUST CALCULATE FIRST

$$\epsilon_r = 2.25 + 3.65 \frac{(4.9)^2}{(4.9)^2 - 6^2 - i(1)(6)/2\pi} = -5.0 + i 0.57$$

$$n = \frac{1}{\sqrt{2}} \left(-5.0 + [(-5.0)^2 + (0.57)^2]^{1/2} \right)^{1/2} = 0.13$$

$$k = \frac{1}{\sqrt{2}} \left(+5.0 + [(-5.0)^2 + (0.57)^2]^{1/2} \right)^{1/2} = 2.2$$

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} = \frac{(-0.87)^2 + (2.2)^2}{(1.13)^2 + (2.2)^2} = 0.91$$

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$$\alpha = \frac{4\pi k}{\lambda} = \frac{4\pi \times 2.2}{50 \times 10^{-6}} = 5.5 \times 10^5 \text{ m}^{-1}$$

POLARITONS

AFTER HAVING DISCUSSED THE DISPERSION CURVE OF THE PHOTONS AND THE TO PHONONS IN GENERAL TERMS, WE CAN CONSIDER NOW SOME DETAILS. AS WE WILL SEE THE TWO DISPERSION CURVES DO NOT ACTUALLY CROSS EACH OTHER, THIS IS A CONSEQUENCE OF THE STRONG COUPLING BETWEEN THE TO PHONONS AND THE PHOTON WHEN THEIR FREQUENCY AND WAVE VECTOR MATCH. THIS LEADS TO THE CHARACTERISTIC ANTICROSSING BEHAVIOR WHICH IS OBSERVED IN MANY COUPLED SYSTEMS. THE COUPLED PHONON-PHOTON WAVES ARE CALLED POLARITONS. THE DISPERSION OF THE POLARITONS CAN BE DEDUCED FROM THE RELATIONSHIP

$$\omega = vq = \frac{c}{\sqrt{\epsilon_r}} q$$

WHERE WE MADE USE OF THE RELATION $v = \frac{1}{\sqrt{\epsilon_r \mu_r}} c$

USING $\mu_r = 1$. THE RESONANT RESPONSE OF THE POLAR SOLID IS CONTAINED IMPLICITLY IN THE FREQUENCY DEPENDENCE OF ϵ_r .

