

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

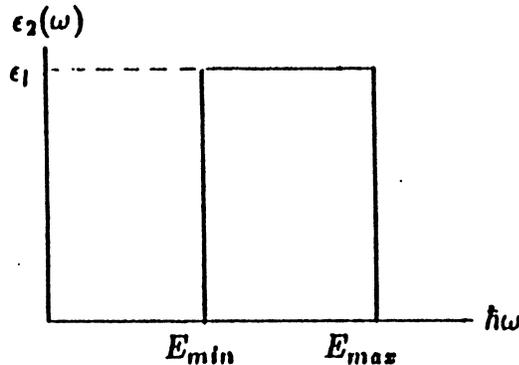
Physics of Solids II — 6.732

PROBLEM SET # 6

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Due: November 2, 2001

1. Suppose that we model the interband transitions in Ge as a step function $\epsilon_2(\omega) = \epsilon_l$ for $E_{min} < \hbar\omega < E_{max}$ (see diagram) and $\epsilon_2(\omega) = 0$ otherwise.



- Use the Kramers–Kronig relation to find an expression for $\epsilon_1(\omega)$ for all ω . Take $\epsilon_1 = 1$ for $\omega = \infty$ and express your answer in terms of E_{max} , E_{min} , and ϵ_l .
- For what photon energies does $\epsilon_1(\omega)$ exhibit structure? Is your answer physically reasonable and why?
- Obtain an explicit expression for $\epsilon_1(0)$ at zero frequency, and use this result to explain why narrow gap semiconductors tend to have large dielectric constants at $\omega = 0$.
- Use the Kramers–Kronig relations to show the sum rule

$$\frac{ne^2}{m} = \frac{1}{2\pi^2} \int_0^\infty \epsilon_2(\omega) \omega d\omega$$

where n is the total carrier density in the semiconductor.

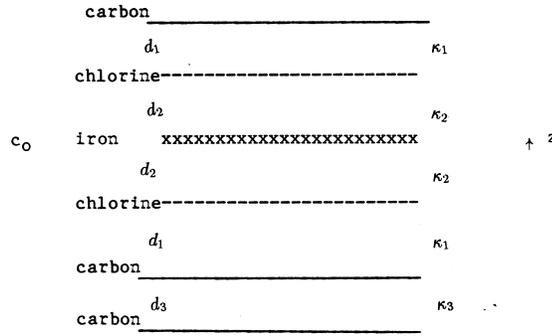
- Reflectivity measurements show that the LO and TO phonon (ω_{LO} and ω_{TO}) features for NaCl occur at $38 \mu\text{m}$ and $61 \mu\text{m}$, respectively.
 - From this information, estimate the force constant κ for the TO phonon mode assuming only nearest neighbor interactions.
 - From the measured ω_{LO} and ω_{TO} splitting find the magnitude of the lattice polarization contribution to the dielectric constant for crystalline NaCl.
 - Is $(\omega_{LO} - \omega_{TO})$ for NaCl expected to be temperature dependent? Why?
 - Suppose that we have a material where there are 3 atoms per unit cell so that there are two different transverse optical frequencies ω_{TO1} and ω_{TO2} . Assume further that for this material, the dielectric function has a frequency dependence

$$\epsilon(\omega) = A + \frac{B_1}{\omega^2 - \omega_{TO1}^2} + \frac{B_2}{\omega^2 - \omega_{TO2}^2}$$

Generalize the Lyddane–Sachs–Teller relation to apply to this material.

- Consider a stage 2 graphite–FeCl₃ layered compound (chemical formula C₂₄FeCl₃) with a unit cell consisting of 5

distinct layers as indicated in the diagram.



with the force constants κ_1 , κ_2 , and κ_3 coupling the carbon-chlorine layers, the chlorine-iron layers and the carbon-carbon layers, respectively. The masses M_C , M_{Cl} , and M_{Fe} denote the mass densities in the carbon, chlorine, and iron layers, respectively. Assume that d_1 , d_2 , and d_3 give the interlayer separation between carbon-chlorine layers, chlorine-iron layers and carbon-carbon layers, respectively. In solving this problem consider the number of layers, number of atoms per unit cell, and masses for each type of layer.

- What are the mode frequencies for phonons propagating perpendicular to the layer planes (z -direction)?
- Which modes are excited by incident electromagnetic radiation at their respective mode frequencies?
- Which modes are Raman-active?
- With which experimental technique could you measure the entire phonon branch $\omega(q_z)$, for all q_z ?

4. Temperature dependence and isotopic shift of bandgaps:

- Show that the temperature (T) dependence of an interband gap energy E_g can be written as

$$E_g(T) - E_g(0) = A \left(\frac{2}{\exp[\hbar\Omega/(k_B T)] - 1} + 1 \right),$$

where A is a temperature-independent constant, k_B is the Boltzmann constant, and $\hbar\Omega$ represents an average phonon energy. Hint: the term inside the parenthesis in the above equation represents the ensemble-averaged square of the phonon displacement.

- Show that $\Delta E_g(T) = E_g(T) - E_g(0)$ becomes linear in T in the limit of $k_B T \gg \hbar\Omega$.
- For small T , $\Delta E_g(T)$ can also be written as

$$\Delta E_g(T) = \left(\frac{\partial E_g}{\partial V} \right)_T \left(\frac{dV}{dT} \right)_P \Delta T + \left(\frac{\partial E_g}{\partial T} \right)_V \Delta T$$

where the first term describes the change in E_g caused by thermal expansion. Its sign can be positive or negative. The second term is the result of electron-phonon interaction. Its sign is usually negative. Estimate the contribution of these effects to $E_g(0)$ by extrapolating $E_g(T)$ to $T = 0$ using its linear dependence at large T . The resultant energy is known as the *renormalization* of the bandgap at $T = 0$ by electron-phonon interaction. Determine this energy for the E_0 gap of Ge from Fig. 6.7 in class notes.

- The result in part (c) can be used to estimate the dependence of bandgap on isotopic mass. Since the bonding between atoms is not affected by the isotopic mass, the average phonon energy $\hbar\Omega$ in solids with two identical atoms per unit cell, like Ge, can be assumed to depend on atomic mass M as $M^{-1/2}$. Calculate the difference in the E_0 bandgap energies between the following isotopes: ^{70}Ge , ^{74}Ge , and ^{76}Ge . Compare your results with those in Fig. 6.9 in class notes.