

# MASSACHUSETTS INSTITUTE OF TECHNOLOGY

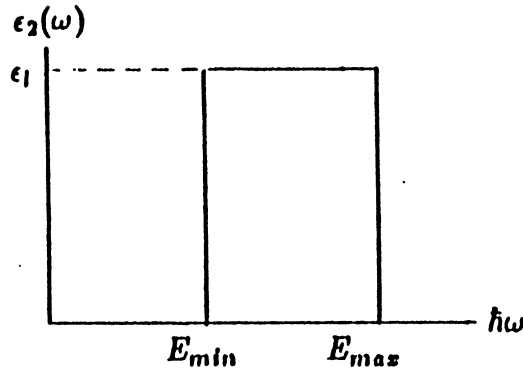
Physics of Solids II — 6.732

PROBLEM SET # 6

Issued: October 24, 2001

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  $\omega$ . Take  $\epsilon_1 = 1$  for  $\omega = \infty$  and express your answer in terms of  $E_{max}$ ,  $E_{min}$ , and  $\epsilon_l$ .
- 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.

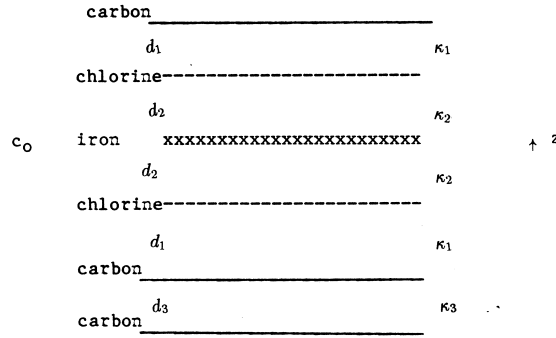
- Reflectivity measurements show that the LO and TO phonon ( $\omega_{LO}$  and  $\omega_{TO}$ ) features for NaCl occur at  $38 \mu\text{m}$  and  $61 \mu\text{m}$ , respectively.
  - From this information, estimate the force constant  $\kappa$  for the TO phonon mode assuming only nearest neighbor interactions.
  - From the measured  $\omega_{LO}$  and  $\omega_{TO}$  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  $\omega_{TO1}$  and  $\omega_{TO2}$ . 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–FeCl<sub>3</sub> layered compound (chemical formula C<sub>24</sub>FeCl<sub>3</sub>) with a unit cell consisting of 5

distinct layers as indicated in the diagram.



with the force constants  $\kappa_1$ ,  $\kappa_2$ , and  $\kappa_3$  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:  $^{70}\text{Ge}$ ,  $^{74}\text{Ge}$ , and  $^{76}\text{Ge}$ . Compare your results with those in Fig. 6.9 in class notes.