

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

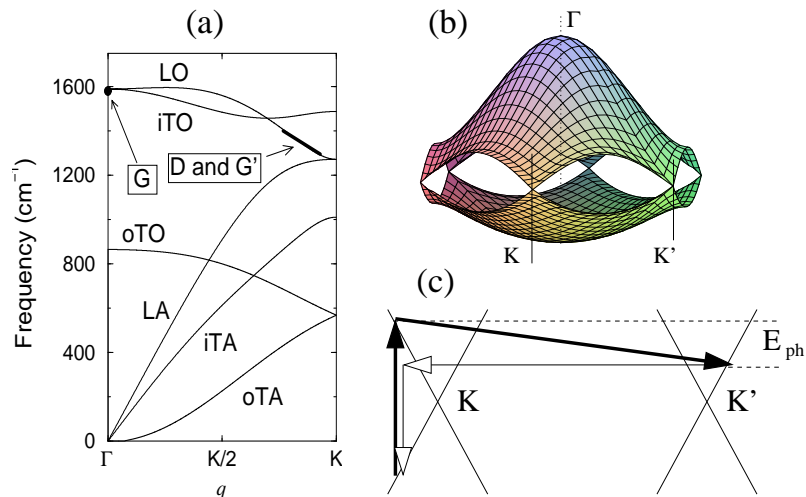
Physics of Solids II —6.732

PROBLEM SET # 7

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1. The Raman spectra of Graphite exhibits three main features: (i) the G -band feature ($\omega_G = 1580 \text{ cm}^{-1}$) that comes from the Γ point degenerate longitudinal optical (LO) and the in plane transverse optical (iTO) modes, (ii) the disorder-induced D -band ($\omega_D = 1200 - 1400 \text{ cm}^{-1}$) that comes from the LO phonon branch close to the K point, and (iii) its overtone, the G' -band ($\omega_{G'} \sim 2\omega_D = 2400 - 2800 \text{ cm}^{-1}$), which is a Raman process that involves two D -band phonons. The phonon diagram is shown in Fig. 1(a).
 - (a) Explain why the G -band and G' -band appear in the Raman spectra of a perfect graphite crystal (HOPG - highly oriented pyrolytic graphite) while the D -band is observed only in defective graphitic materials.
 - (b) The G -band scattering is a first-order Raman process, while the D -band and G' -band scattering are second-order Raman processes. For the D -band, one of the scattering processes is elastic due to interaction of the electron/hole with a lattice defect. Draw one Feynman diagram for the G , D and G' scattering processes (3 diagrams in all).
 - (c) (Optional) Graphite is a semi-metal since the valence and conduction band meet at the K point [see Fig. 1(b)]. Therefore, a resonance Raman effect is observed for electrons and phonons close to the K point. The reason why the second-order D and G' bands have enough Raman cross section to be visible in the Raman spectra with an intensity comparable to the first-order G -band is the resonance nature of their scattering processes, that involve two resonance processes, where not only the incident or scattered photons are associated with real electronic transitions, but also one of the intermediate scattering states, mediated by phonons (or by the defect in the case of the D -band), induces also an electronic transition between two real electronic states. One of these effects is illustrated in Fig. 1(c). This process is called a double resonance process. Based on the various possible double resonance processes and on the phonon dispersion shown in Fig. 1(a), explain why the D -band for defective graphite materials is composed of three peaks, where the intermediate frequency peak has twice the intensity of the lowest and highest frequency peaks (consider only Stokes scattering processes). Draw the Feynman diagrams for the possible Stokes processes of the D -band spectra.



2. (a) How can the ratio of the Stokes to anti-Stokes intensities in the Raman scattering spectra of optical phonons be used to determine the lattice temperature of a 3D solid?
- (b) How do these arguments in (a) have to be modified for a one-dimensional system, such as a carbon nanotube?

3. Find the non-linear (electric field E dependent) reflectivity $[R(E) - R(0)]$ and the absorption coefficient $[\alpha(E) - \alpha(0)]$ for the case where the complex dielectric function $\epsilon_1 + i\epsilon_2$ shows a dependence on field intensity of the form

$$\epsilon_1 + i\epsilon_2 = \epsilon_1^0 + i\epsilon_2^0 + (\epsilon_1^{NL} + i\epsilon_2^{NL})E$$

where ϵ_1^0 and ϵ_2^0 are the linear terms and the superscript 'NL' denotes the non-linear terms in the dielectric function.

4. (a) Suppose that it takes 1 hour to do a critical experiment for your thesis and that your experiment requires an atomically clean surface (i.e., less than 0.1 monolayer of contaminant coverage). Assuming your sample to be a semiconductor and oxygen to be the contaminant (sticking coefficient = 1), find the maximum allowable pressure (in torr) required for your experimental chamber in order to carry out your critical experiment. Consider the case of:
- room temperature operation.
 - operation at 77 K.
- (b) Photoemission results show that the Fermi level for pure potassium is 2.0 eV above the conduction band minimum. For a particular compound of potassium this Fermi level is at 1.25 eV. Assuming a nearly free electron model for the alkali metal s -band, find the fraction of the alkali metal s -band that is occupied in the compound, assuming 1 electron/atom for the pure alkali metal. Neglect any changes in m^* in forming the compound.
- (c) Auger electron spectroscopy measurements on a particular copper-nickel sample indicates a composition of 70% copper and 30% nickel from an analysis of the relative heights of the Auger peaks. The same sample when subjected to an electron microprobe analysis (beam penetration $\sim 1\mu\text{m}$) indicates a 50%-50% composition. From these two measurements what can you conclude about the composition of this sample?
- (d) Find the tunneling current flowing in the tip of a scanning tunneling microscope when the tungsten tip is 2\AA from a n^+ doped Ge surface ($\rho = 1\Omega\text{cm}$). A voltage of 5V is applied to the tip, and the backside of the Ge sample ($1\mu\text{m}$ thick) is grounded. The work function for Ge is 4.8eV and the work function for W is 4.6eV.