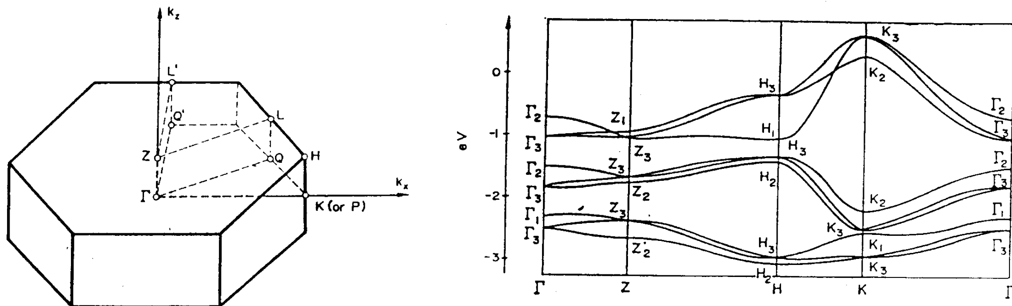
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics of Solids II —6.732

PROBLEM SET # 2

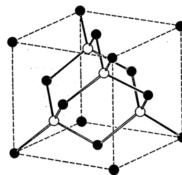
Issued: September 17, 2001 Due: September 24, 2001

1. [1] Consider the band structure diagram given below for tellurium which crystallizes in a hexagonal structure with three Te atoms/unit cell. The atomic configuration for tellurium is $5s^2 5p^4$. (Note: in the diagram the authors use Z rather than A in the hexagonal Brillouin zone.)
   (a) Sketch the approximate position of the Fermi Level E_F on the band diagram and give your reasons for this placement of E_F.
   (b) Indicate which energy bands on the diagram correspond to s, p and d bands. If the energy bands with these atomic origins are not shown, are they at higher or lower energy than those shown in the diagram?
   (c) From the diagram, where will carrier pockets form by thermal excitation? Identify electrons or holes carrier pockets. How many carrier pockets of each type are there?
   (d) From the band diagram, what is the shape of the constant energy surfaces for electrons and for holes? Along which directions will electrons (holes) have light effective masses and along which directions will the masses be heavy?
   (e) Is tellurium transparent to visible light ($\lambda = 5000$Å)? Explain! Is the optical absorption strong or weak at the threshold for optical transitions (e.g., in comparison to GaAs)? Explain!



2. Consider the two-dimensional simple triangular lattice for a free electron metal with two electrons/atom.
   (a) Assuming a lattice constant of a, find the areas of the electron and hole pockets that are formed in the second and first Brillouin zones, respectively.
   (b) Find the shapes of the electron and hole Fermi surfaces in the reduced zone, obtained through translation by a reciprocal lattice vector.

3. Consider the direct band gap semiconductor GaAs (at room temperature $E_g = 1.43$ eV) with 10^{16} hydrogenic donor impurities/cm^3.



[1]For those students who had difficulty with problem #3 on Problem Set #1, please work on problem #1 of this problem set. For the other students, this problem is optional.

(a) Write an expression for the temperature dependence of the Fermi level. Take $E_g = 1.40$ eV for the direct band gap, $m_e^* = 0.07m_0$ for the conduction band mass and $m_{hh} = 0.68m_0$, $m_{lh} = 0.12m_0$ for the heavy and light holes bands and ignore the effect of the split–off band Δ =0.33 eV below the top of the valence band associated with the spin–orbit interaction. The static dielectric constant for GaAs is 15.

(b) Find the value of the Fermi energy at 300K and at 30K.

(c) What are the electron and hole carrier concentrations at room temperature (300 K)? at 30 K?

(d) Estimate the hole concentration in the split–off band ($m_{soh}^* = 0.20m_0$). This calculation should justify the neglect of the split–off band in the calculation (a).

(e) Why must the spin orbit interaction be included when considering acceptor doping in GaAs?

(f) At what doping concentration would you expect a substitutional impurity in GaAs to start forming an impurity band for the electron? How does an impurity band differ from an isolated impurity level?

(g) The bandgap for the indirect gap semiconductor AlAs (with the same crystal structure and nearly identical lattice constants as the direct gap semiconductor GaAs) is 2.13 eV. Why is it not correct to use Vegard's law to find the bandgap for $Ga_{0.9}Al_{0.1}As$? Hint: Vegard's law is an interpolation formula for property X given by

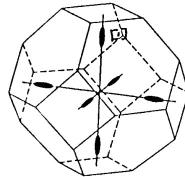
$$X(x) = X(0) + x[X(1) - X(0)]$$

where x is the concentration of Al in the alloy $Ga_{1-x}Al_xAs$.

4. Silicon crystallizes in the diamond structure. The lowest conduction band is at a Δ–point of the F.C.C. Brillouin zone 0.85 of the distance from Γ to X along a (100) direction, and its equivalent directions. Six (6) ellipsoidal constant energy surfaces (ellipsoids of revolution) are formed, following the dispersion relation:

$$E(\vec{k}) = \frac{\hbar^2 k_\ell^2}{2m_\ell} + \frac{\hbar^2(k_{t1}^2 + k_{t2}^2)}{2m_t}$$

where m_ℓ is the longitudinal effective mass component along the ΓX direction and m_t is the transverse effective mass component perpendicular to this direction. For $(m_\ell/m_0) = 0.98$ and $(m_t/m_0) = 0.19$, find the contribution to the electrical conductivity from a single carrier pocket (labeled [1] in the figure) for the following cases:



(a) The electric field $\vec{E} \parallel (001)$

(b) The electric field $\vec{E} \parallel (111)$
Assume that each carrier pocket contains 10^{18} electrons/cm^3 and $\tau = 10^{-14}$ sec is the relaxation time. The figure shows the ellipsoidal energy surfaces of silicon corresponding to conduction band carrier pockets along the six $\langle 100 \rangle$ directions.

(c) Find the contribution to the electrical conductivity from all 6 electron pockets for $\vec{E} \parallel (001)$ and $\vec{E} \parallel (111)$ [see (a) and (b)]. It can generally be shown that for cubic materials, σ is independent of the direction of the applied electric field. Assume that the $E(\vec{k})$ relation applies to all six constant energy surfaces.