

CHAPTER – 3

ELECTRICAL

AND

OPTICAL PROPERTIES

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ELECTRICAL AND OPTICAL PROPERTIES

A semiconductor is often defined as having an electrical conductivity intermediate between that of an insulator and a metal. The properties of semiconductors which are generally termed as their electrical properties include (1) Electrical conductivity, (2) The Hall coefficient which determines the carrier density and type (3) Hall mobility of the charge carriers under the influence of transverse electric field and magnetic field (4) Magnetoresistivity whereby semiconductors change their resistance when subjected to magnetic field (5) The thermoelectric power in which a temperature difference maintained between the ends of the specimen gives rise to an EMF across the two ends. Among these, the electrical conductivity is the most basic and commonly measured property. The electrical conductivity of the vacuum deposited and heat treated thin films can give important information regarding the defect structure and density of defects present in the as-grown thin films and can throw light on the changes that take place during annealing process in the film. It is also possible to study the influence of deposition parameters on the defect density and structure of thin films by the conductivity measurement.

Bi_2Te_3 is a p-type semi conductor. At room temperature, the thermoelectric

power perpendicular to the C - axis is $218 \mu\text{V/K}$ [1]. Its electrical resistivity is about $1.6 \times 10^{-5} \text{ ohm-m}$ [1]. At room temperature, the Hall coefficient and carrier concentration are $0.42 \times 10^{-6} \text{ m}^3/\text{A.sec.}$ and $1.75 \times 10^{25} \text{ m}^{-3}$, respectively [1,2] Electrical conductivity and thermoelectric power of its thin films increase with thickness and attain constant values of $0.3 \times 10^5 \text{ ohm}^{-1} \text{ m}^{-1}$ and $200 \mu\text{V/K}$, respectively, for thickness above $\sim 2000 \text{ \AA}$ [3]. The thickness dependence has been explained in terms of size effect. The absolute values of TCR and activation energy are $40 \times 10^{-4} \text{ }^\circ\text{C}^{-1}$ and 0.0287 eV , respectively [3]. Anisotropy of carrier density and its composition dependence in $\text{Bi}_{2-x} \text{In}_x \text{Te}_3$ has been studied by Kutasov et al [4]. Horak et al [5] and V.A Kutasov et al have reported a study of thermoelectric and galvanomagnetic properties of $n\text{-Bi}_2\text{Te}_{3-x-y}\text{Se}_x\text{S}_y$ solid solution for $0.12 \leq x \leq 0.36$ and $0.12 \leq y \leq 0.21$ within $80 - 300 \text{ K}$ temperature region and L.N. Phong has reported low temperature cooling for IR detectors [6-7].

According to quantum theory, electrical conduction in metals is due to electrons, while electrical resistivity results from the scattering of these electrons by the lattice. Because of their wave nature, electrons can pass through a perfect lattice without any attenuation. Actually no lattice is perfect. Electrons always undergo some scattering as they travel through a solid; the average distance that they travel between successive collisions being called the mean free path (mfp) [8]. Bloch showed that the mfp of an electron travelling through a perfect rigid

lattice is infinite. In other words the electron can move without resistance in a perfect lattice. But lattice imperfections present in real samples give rise to electrical resistivity. Impurity atoms, vacancies, dislocations, grain boundaries and stacking faults are static defects while the dynamic imperfections are due to thermal motion of the atoms in the lattice. The vibrational modes of atoms are quantized and are called phonons. The number of phonons in a given lattice increases with temperature causing increasing electron-phonon collisions with increasing temperature and hence the resistivity increases according to the relation

$$\rho_o = \rho_{ph}(T) + \rho_i \quad \dots\dots 1$$

where ρ_o = total resistivity, ρ_{ph} = temperature dependent resistivity due to phonons and ρ_i = resistivity due to impurities.

Normally the dimensions of bulk conductors are of several orders of magnitude larger than the mfp of conduction electrons. Hence the number of surface collisions are very small compared to the total number of collisions taking place in the bulk. However, the surface collisions cannot be neglected if one or more dimensions of the conductor approaches to or are less than the mfp, as in the case of thin films. Polycrystalline films are made up of small single crystals in contact with one another. Except for the size, the crystallites in polycrystalline films should be similar to larger single crystals. However, the additional

scattering due to grain boundaries will reduced the effective carrier mobility compared to the bulk value and hence the measurements of electronic properties of films should yield results which represent the average of contributions of the crystallites and the grain boundaries as well as the average of anisotropies of the randomly oriented grains. As the size of the grains becomes smaller, the role of the grain boundaries becomes more important and the material begins to resemble an amorphous solid. Thus, an estimate of the maximum possible contribution to the resistivity from the grain boundaries may be arrived at by considering the resistivities of liquid metals. In the case of films, electrical resistivity depends on the growth stages the films undergo while being deposited and the films may be granular or island-like porous (network) or continuous. Each stage has its characteristic electrical properties.

Thermoelectric Power :

The thermoelectric power is obtained as [9].

$$\alpha (T)= \Delta V(T)/\Delta T \quad \text{.....2}$$

where ΔT is temperature gradient and $\Delta V(T)$ the thermo E.M.F. at absolute temperature, T.

The thermoelectric power α depends strongly on the carrier concentration n and the electrical conductivity σ ; α and σ are related by

$$\alpha = A - B \log \sigma$$

α varies with n from a few tenths of a μV per $^{\circ}C$ to 1000-1500 μV per $^{\circ}C$ in certain semiconductors; α also depends on the scattering mechanism and on the effective mass m^* .

Hall Effect Measurement :

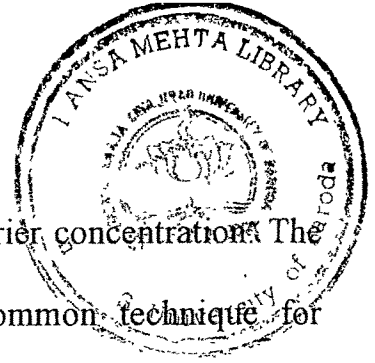
For determining the carrier concentration normally the Hall effect is used. When a conductor is placed in a magnetic field perpendicular to the direction of current flow, a field E_y is developed across the specimen in the direction perpendicular to both the current, J_x , and the magnetic field, H_z . The field, called the “Hall field”, is given by

$$E_y = \frac{J_x H_z}{ne} \quad \dots\dots 3$$

where J_x is the current density and n is the number of carriers per unit volume. Thus the Hall field is proportional to the product of the current density and the magnetic flux density. The proportionality constant, R_H , known as the Hall coefficient is given by

$$R_H = \frac{E_y}{J_x H_z} = \frac{1}{ne} \quad \dots\dots 4$$

The product of Hall field and width of the film (i.e. dimension normal to the field) is known as the Hall voltage. A measurement of the Hall voltage for a



known current and magnetic field yields the value of carrier concentration. The measurement of the sign of the Hall voltage is a common technique for determining whether the sample is p-type or n-type.

The carrier density (p) in the extrinsic region has been calculated using the relation [10].

$$P = \frac{3\pi}{8 R_H e} \quad \dots 4$$

where, R_H is the room temperature Hall coefficient and e is the electronic charge. The mobility, μ , of the charge carriers was determined from the relation [11].

$$\mu = 1/\rho p e \quad \dots 5$$

where, ρ = room temperature resistivity.

OPTICAL BAND GAP

The theoretical and experimental investigations of the optical behavior of solids deal primarily with optical reflection, transmission and absorption properties, and their relation to the optical constants both of the bulk and thin film forms. As a result of these studies, complex multilayer optical device systems with remarkable reflection, antireflection, interference and polarization properties have emerged for both laboratory and industrial applications. The absorption studies have led to a variety of interesting thin film optical phenomena which

have thrown considerable light on the electronic structure of solids.

The optical measurement constitutes the most important means of determining the band structure of semiconductors. For absorption studies, photons of selective energy are used. Optical properties of a thin film generally differ from those of the bulk. The differences are usually attributed to the microstructure of the films.

Principally there are several methods to determine the optical constants, such as Abbe's method, spectroscopic methods, polarimetric method and critical angle method [12-15]. The spectroscopic method is probably the most widely used one for optical measurements. The most direct and the simplest method for determining the band structure is to measure the absorption spectrum.

There have been a few reports on the optical study on Bi_2Te_3 in bulk and thin film forms [16-18]. Black et al [16] have studied the optical absorption of Bi_2Te_3 crystals grown by Bridgman method. Morsy et al [18] have reported optical properties of thermally deposited Bi_2Te_3 thin films in the wave length range of 2.5 to $10\mu\text{m}$ and have used transmittance and reflectance spectra to obtain band gap which was found to be about 0.21 eV.

It is apparent that a photon with energy $h\nu \geq E_g$ can be absorbed in a semiconductor, where E_g is the band gap of the semiconductor. Since the valence band contains many electrons and the conduction band has many empty states

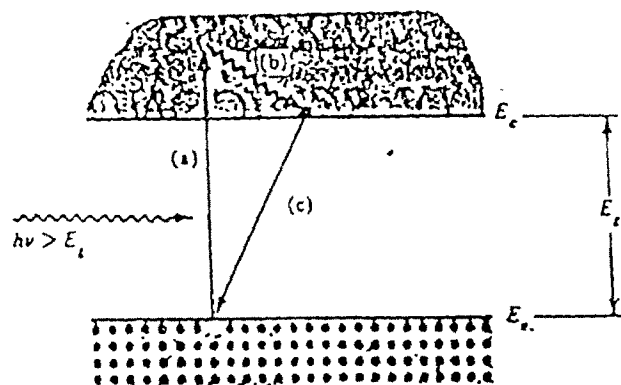


Figure - 1. Optical absorption of a photon with $h\nu > E_g$: (a) an EHP is created during photon absorption; (b) the excited electron gives up energy to the lattice by scattering events; (c) the electron recombines with a hole in the valence band.

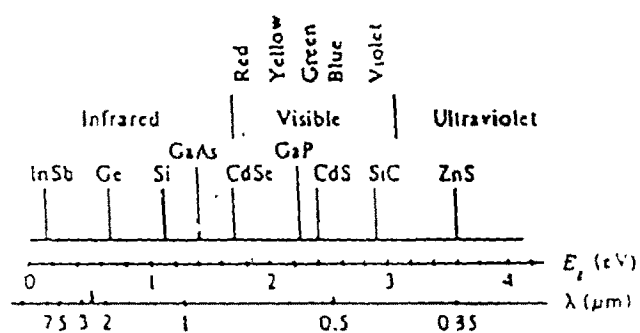


Figure - 2. Band gaps of some common semiconductors relative to the optical spectrum.

If a beam of photons with $h\nu > E_g$ falls on a semiconductor, there will be some predictable amount of absorption determined by the properties of the material. The ratio of transmitted to incident light intensity depends on the photon wave length and the thickness of the sample

The intensity of light transmitted through the sample of thickness t , is given by

$$I = I_0 e^{-\alpha t} \quad 1$$

where α is the absorption coefficient, I_0 is the incident photon beam intensity and I is the transmitted intensity

Near the absorption edge, the absorption coefficient is expressed as [20]

$$\alpha \sim (h\nu - E_g)^\gamma \quad \dots 2$$

where $h\nu$ is the photon energy, E_g is the optical gap, γ is a constant which is equal to $1/2$ and $3/2$ for allowed direct transition and forbidden direct transition, respectively [with $K(\min) = K(\max)$ as in transitions (a) and (b) shown in Figure – 3] It equals 2 for indirect transition [transition (c)], where phonons must be incorporated. In addition, γ equals $1/2$ for allowed indirect transitions to exciton states where an exciton is a bound electron - hole pair with energy levels in the band gap and moving through the crystal lattice as a unit.

The possible transitions are thus

- 1 Band to band.

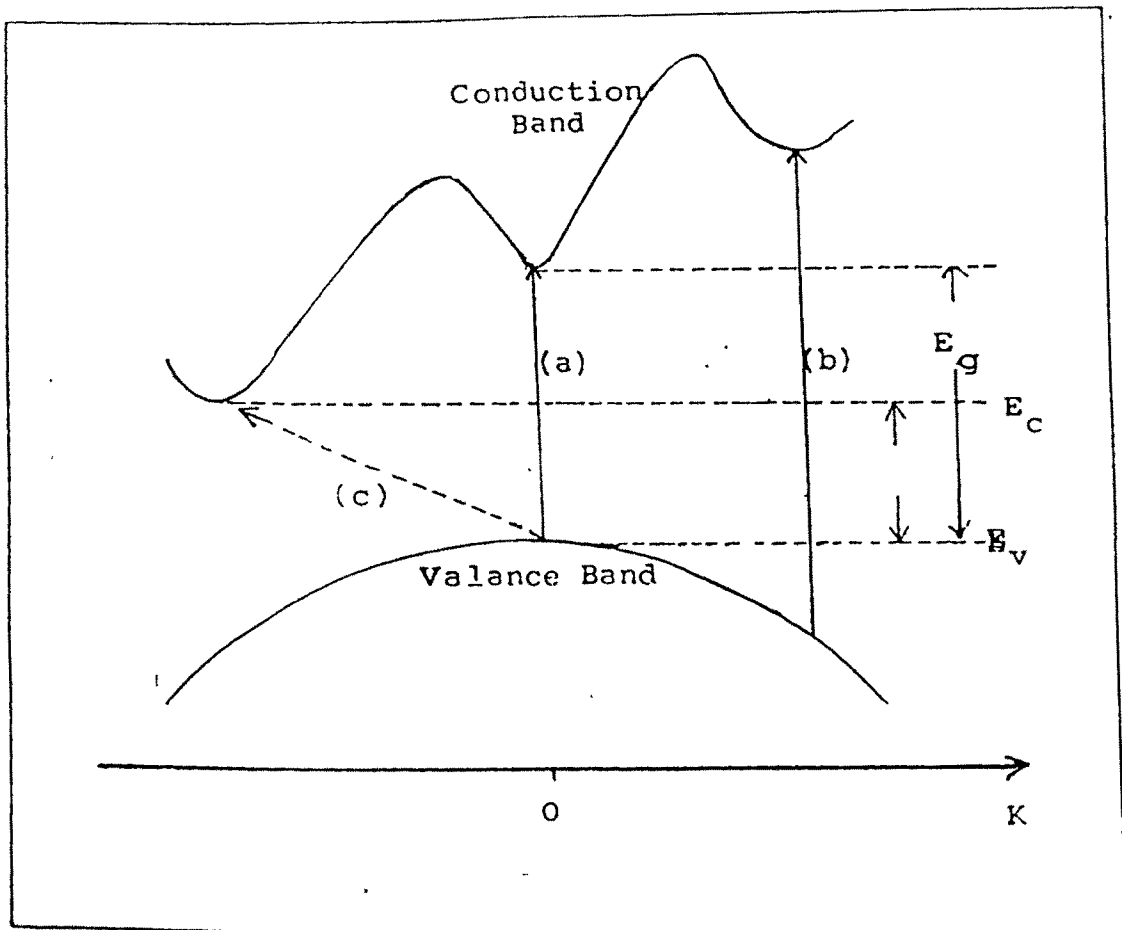


Figure - 3 : Optical transitions.

(a) and (b) Direct transitions.

(c) Indirect transition involving phonons.

2. Excitonic.
3. Between sub-bands.
4. Between impurities and bands.
5. Transition by free carriers within a band.
6. Resonance due to vibrational states of lattice and impurities.

The absorption is expressed in terms of a coefficient which is defined as the relative rate of decrease in light intensity $L(h\nu)$ along its propagation :

$$\alpha(h\nu) = -\frac{1}{L(h\nu)} \frac{dL(h\nu)}{dx} \quad \text{.....3}$$

where, $L(h\nu)$ is incident light intensity. α is the absorption coefficient [19-20].

The basic theory of direct and indirect transitions in semiconductors was formulated by Bardeen et al [21]. The direct transitions are generally supposed to be taking place from valence band to conduction band under the selection rule :

$$\mathbf{K} - \mathbf{K}^1 + \frac{2\pi \mathbf{i}}{\lambda} = 0 \quad \text{.....4}$$

where \mathbf{K} and \mathbf{K}^1 are the wave vectors of electron before and after transition, respectively, λ is the wavelength of the photon and \mathbf{i} is the unit vector along the

direction in which the photon travelled before it is absorbed. This can be simplified to $K^1 = K$, since $2\pi/\lambda$ is small compared to either K or K^1 . This shows that only vertical transitions are allowed; other transitions, if taking place, will be of very small probability. Thus the steep edge in absorption spectra is attributed to the highly probable direct transitions. The weak lingering absorption in the tail region is considered to be due to indirect transitions involving the participation of phonons in the process and this will happen when the wave-vectors at the minima of the conduction band energy surface do not coincide. A phonon is emitted or absorbed depending on whether the energy of photon is more or less than the indirect band gap energy.

For direct transition, the absorption coefficient relates to the photon energy as

$$(\propto h\nu) = B (h\nu - E_g)^x \quad \dots\dots 5$$

where $x = 1/2$ for allowed transitions and $x = 3/2$ for forbidden transitions; E_g is the direct energy gap and B is a parameter that depends on the transition probability. For the indirect transition,

$$(\propto h\nu) = A (h\nu - E_g \pm E_p)^x \quad \dots\dots 6$$

where $x = 2$ for indirect allowed transitions and $x = 3$ for forbidden transitions, E_g is the band gap and E_p is the absorbed or emitted phonon energy [22-24]. At room

temperature, transitions, both with phonon emission and phonon absorption, will contribute to the absorption.

An ample study can be found reported in literature on the transport properties of pure Bi_2Te_3 crystal and thin films. There are scarce reports so far on transport properties of doped Bi_2Te_3 crystals and thin films. The results obtained of measurements of transport properties of $\text{In}_{0.1}\text{Bi}_{1.9}\text{Te}_3$, $\text{In}_{0.2}\text{Bi}_{1.8}\text{Te}_3$ and $\text{In}_{0.5}\text{Bi}_{1.5}\text{Te}_3$ crystals and their thin films carried out by the author are presented in chapter no.8 & 9.

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