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Methodology of Optical studies for Semi-conducting thin films of Ternary compounds

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ABSTRACT
Ternary alloys of II-VI group semiconductors prepared by using binary semiconductors can thus be grouped as a class of tailored and engineered materials in which energy band gap lattice parameters and other functional parameters could be continuously varied by selecting binary constituents and their relative compositions accordingly. The use of thin film polycrystalline semiconductors has attracted much interest in an expanding variety of applications in various electronic and optoelectronic devices. The optical properties of thin films mainly depend upon the thickness, doping and deposition technique used to prepare thin films. The characterization of the thin films is very important for their efficient application in various solid-state device fabrications. The thin films can characterize through their optical, structural, mechanical, surface morphological, magnetic and electrical properties. Absorption coefficient, optical band gap, nature of band gap of the materials of films can be determined by absorption spectra while the optical constants (refractive index, extinction coefficient and dielectric constants) and thicknesses of the films can be determined using transmission spectra of the films.
Key words: *optical properties, absorption spectra, transmission spectra, ternary compounds.*

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INTRODUCTION

The defining property of a semiconducting material is that it can be doped with impurities that change its electronic properties in a convenient way. Because of their application in devices like transistors, IT devices and lasers, the search for new semiconducting materials and the improvement of existing materials is an important field of study in materials science. The most commonly used semiconductor materials are crystalline inorganic solids. These materials can be classified according to the periodic table groups from which their constituent atoms come. Semiconductor materials are differing by their properties. Compound semiconductors have advantages and disadvantages in comparison with silicon. For example gallium arsenide has six times higher electron mobility than silicon, which allows faster operation; wider band gap, which allows operation of power devices at higher temperatures. It gives lower thermal noise to low power devices at room temperature. Its direct band gap gives it more favorable optoelectronic properties than the indirect band gap of silicon. It can be alloyed to ternary and quaternary compositions with adjustable band gap width, allowing light emission at chosen wavelengths and and with lowest losses in optical fibers. The major applications of thin films are found in optoelectronics devices (e.g. solar cells and photovoltaic cells), optical devices (e.g. LED), solid state devices and in many other electronic appliance. In communication systems, various type of catalysis process coating of all kinds, and in energy generations and conservations strategies thin films technology is widely using these days. Multilayer optical filters are widely used which are constructed by multilayer thin films. AR (Antireflection) coatings are used on the lenses

of virtually all optical equipments, including cameras, microscopes, telescopes etc. One of the most critical applications of hard coating has been in ball bearings, used in virtually precision rotating machinery. Characterization of optical properties helps in determination of features such as band gap (E_g), nature of band gap. The II-VI group compounds are widely used in solid-state devices such as photovoltaic cells, infrared detectors, nuclear radiation detectors and windows for IR laser etc. This group is much more important for photoconductive and photo electric device [1]. The binary and ternary semiconductors have been attracting much more interest in photovoltaic [2-6]. Ternary compounds provide a possibility of tailoring their properties as per requirements and hence project themselves as important semiconducting materials for future advancement in the field of device fabrication. Currently this development goes hand-in-hand with explosion of scientific and technological break-troughs in microelectronics, optics and nanotechnology [7]. A second major field comprises process technologies for films with thickness ranging from one to several microns. These films are essential for multitude of production areas, such as thermal barrier coatings and wear protections, enhancing service life of tools and to protect materials against thermal and atmospheric influences [8,9].

MATERIALS AND METHODS

Experimental: The optical properties of vacuum evaporated thin films deposited onto highly cleaned glass substrates is to be studied from the measurement of absorption and transmission spectra taken from Hitachi Spectrophotometer Model U-3400 at room temperature. Absorption coefficients, optical band gap, nature of band gap of the materials of films are determined by absorption spectra while the optical constants (refractive index, extinction coefficient and dielectric constants) and thicknesses of the films are determined using transmission spectra of the films.

Optical Absorption: In the absorption process a photon of known energy excites an electron from a lower to a higher energy state. In other manner we can say that absorption is also resulted from interaction between atoms and electromagnetic radiations. The conduction and valence band are the regular features of all the solids. Only difference is upto which they are occupied and vertical separation between them i.e. energy band gap. Thus energy band may be defined as the gap or region between the valence and conduction. The measurement of absorption spectra is the direct method for probing the band structure of semiconductors band. The band gap may be classified as direct and indirect band gap depending upon the electron transition.

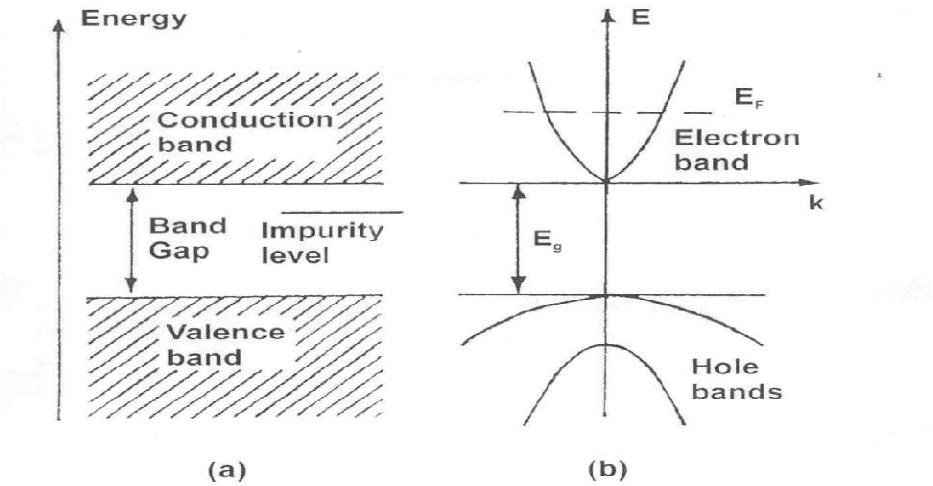

Figure 1.1 (a) Representation of Conduction and Valance Bands in a Semiconductor (b) Energy Vs Wave-Vector Diagram.

Direct and Indirect Bad Gap:

As the photon of incident light is absorbed by the material, an electron is excited from lower to upper energy state. This transition of electron can be direct or indirect shown in figure 1.2.

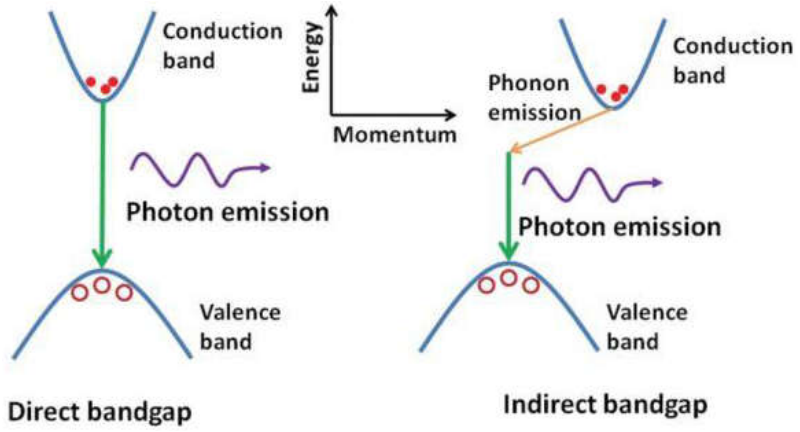

Figure 1.2: Direct and Indirect Band Gap.

In a direct transition an electron in the conduction band can fall to an empty state in the valence band giving off the energy difference E_g as photon of light. On the other hand, if an electron in the conduction band cannot fall directly to the valence band but must undergo a momentum change as well as changing its energy. The difference between direct and indirect band structure is very important for deciding that which semiconductor can be used in device requiring light output.

RESULTS AND DISCUSSION

Determination of Energy Band Gap (E_g) : The absorption spectrum of the material is an important technique, which is used for measuring the energy band gap (E_g) of a semiconductor. An important feature of this method is that it is applicable for any range i.e narrow or wide band gap material. In this experiment photon of selected wavelength are incident on the sample and the relative transmission of the various photon is observed. Let a photon beam of intensity I0 (photons/cm^2 sec) is incident at the sample of thickness t and the intensity of light transmitted is I_t, then;

$$I_t = I_o e^{-\alpha t} \quad \text{.....(1)}$$

Where α is the absorption coefficient and has unit cm^{-1}. The coefficient varies with photon wavelength and also with the materials. Discrimination between direct and indirect transition is possible on the basis of the dependence of absorption coefficient on photon energy. The various type of transition give rise to different frequency dependencies absorption coefficient near the fundamental absorption edge for direct transition, we have [10]

$$\alpha h\nu = A\left(h\nu - Eg\right)^{n} \quad \text{.....(2)}$$

Where hν = photon Energy,

α = Absorption coefficient,

E_g = Energy band gap

A = Constant,

n=1/2 (Allowed direct transition), n = 3/2 (Forbidden direct transition)

N = 2 (Allowed indirect transition) and n = 3(Forbidden indirect transition)

The indirect transition gives rise to relation

$$\alpha h\nu = A\left(h\nu - E_g^{'}\right)^{1/2} \quad \text{.....(3)}$$

Where $E_g^{'}$ = $E_g \pm h\nu_{pn}$ and υ_{pn} is frequency of photon n = 2 provides the allowed transition.

In case of direct band gap the allowed transitions could be find out by using n = 1/2 in equation (2).

A plot of $(\alpha h\nu)^2$ versus $h\nu$ when extrapolation of the straight line to $(\alpha h\nu)^2 = 0$ axis give the value of the energy band gap.

While in case of indirect band gap the allowed transitions could be find out by using n = 2 in equation (3).

A plot of $(\alpha h\nu)^{1/2}$ versus $h\nu$ when extrapolation of the straight line to $(\alpha h\nu)^{1/2} = 0$ axis give the value of the energy band gap.

Optical Transmission:
Let a light beam of intensity I_0 be made incident on a surface and I be intensity of transmitted beam then the ratio of transmitted to incident intensity I/ I_0 is termed as the transmission coefficient. If α is the absorption coefficient, t is the thickness and R is the reflectivity then the radiation traversing the first interface is $(1-R) I_0$. The radiation reaching the second interface is $(1-R)I_0 \exp(-\alpha t)$ and only a fraction of $(1-R)(1+R) I_0 \exp(-\alpha t)$ emerges. The internally reflected portion comes out after a considerable attenuation. Thus the resultant i.e. the overall transmission is given by;

$T = (1-R)^2 \exp(-\alpha t)/(1-R^2) \exp(-2(-\alpha t))$ .....(4)

When the product αt is large, we can write

$T = (1-R)^2 \exp(-\alpha t)$ .....(5)

Determination of optical constants: The optical behavior of a material is generally used to;

- determine the optical constants
- n (refractive index)
- k (extinction coefficient)
- ε (dielectric constant)
- t (thickness)

Transmission Method for Determination of n, k, ε & t:
The measurement of the transmission T of light through a parallel-faced dielectric film in the region of transparency is sufficient to determine the real and imaginary parts of the complex refractive index $\eta = n - ik$, as well as the thickness t. J.C. Manifacier et.al (1976) derived the expressions to calculate the optical constants of thin film material by using transmission spectra (envelope method) as given below [11]. If we assume that the film is weakly absorbing and substrate is completely transparent, then using Manifacier envelope method the refractive index (n) and extinction coefficient (k) of the film on a transparent substrate can be evaluated from the transmission spectra.

$$n = \left[N + (N^2 - n_0^2 n_1^2)^{1/2}\right] \quad \text{.....(6)}$$

Where

$N = ((n_0^2 + n_1^2) / 2) + 2 n_0 n_1 (T_{max} - T_{min}/T_{max} - T_{min})$

$$P = \frac{\left[1-(T_{max}/T_{\min})^{1/2}\right]}{\left[1+(T_{max}/T_{min})^{1/2}\right]} \frac{C_1}{C_2} \quad \text{.....(7)}$$

Where $C_1 = (n + n_0)(n_1 + n)$ and

$C_2 = (n - n_0)(n_1 - n)$

$$\kappa = \left(-\lambda/4\pi t\right) \ln P \quad \text{.....(8)}$$

Equation (6) shows that n is explicitly determined from T_{max}, T_{min}, n_1 and n_0 at the same wavelength. From equation (7) we can find α. The thickness t of the layer can be calculated from using equation (9)

$$t = \frac{M \lambda_1 \lambda_2}{2 [n_{\lambda_1} \lambda_2 - n_{\lambda_2} \lambda_1]} \quad \text{.....(9)}$$

Where M is the number of oscillations between the two extrema (M = 1 between two consecutive maxima or minima); λ_1, $n_{\lambda 1}$ and λ_2, $n_{\lambda 2}$ are the corresponding wavelengths and indices of refraction. Knowing t and α , we are able to calculate the extinction coefficient k

from equation (8). It is worthwhile noting those expressions (6), (8) and (9) can be easily calculated using a programmable pocket calculator.
Complex dielectric constant is given by

$\varepsilon^* = \varepsilon' - i\,\varepsilon''$ .....(10)
we know the relation between complex di-electric constant and complex refraction index is given by

$\varepsilon^*(\lambda) = n^2(\lambda)$
or
$\varepsilon^*(\lambda) = (n-ik)^2$ .....(11)

$\varepsilon'-i\varepsilon'' = n^2-k^2-2ink$
Equating real and imaginary parts, we get
$\varepsilon' = n^2-k^2$ .....(12)

And $\varepsilon'' = 2nk$ .....(13)

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