# STUDY OF OPTICAL AND PHYSICAL PROPERTIES OF BISMUTH-ANTIMONY THIN FILMS


*Submitted by*

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**Adm. No.: 08 PHY/19**


***A Thesis submitted in partial fulfillment of the requirements***

***For the award of the degree of M.Sc. in Physics under***

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# CERTIFICATE – I

This is to certify that the thesis entitled, **"Study of optical and physical properties of bismuth-antimony thin films"** is submitted in partial fulfillment of the requirements for the award of the degree of **Master of Science** in **Physics** of the **Orissa University of Agriculture and Technology**, Bhubaneswar, is a faithful record of bona fide research work carried out by **Shubhasmita Pattanaik** under my guidance and supervision and that no part of this thesis has been submitted for any other degree or diploma or published in any form.

It is further certified that the help and sources of information availed of during the course of study have been duly acknowledged.

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# CERTIFICATE – II

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# DECLARATION

I hereby declare that the project work entitled "**Study of optical and physical properties of bismuth-antimony thin films**" submitted by me for the partial fulfillment of the master of science to the **CBSH, Orissa university of agriculture and technology, Bhubaneswar** is my own original work and has not been submitted earlier to OUAT or to any other institution for the fulfillment of the requirement for any course of study. I also declare that no chapters of this manuscript in whole or in part in lifted and incorporated in this report from any earlier work done by me or others.

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# ABSTRACT

The formation of solid solution in semiconductor is of interest since of results in no of other semiconductor material .it has huge application in electronics and opto-electronic devices. Bismuth Antimony undergoes semimetal transitions. We have successfully grown BiSb alloys on glass substrate over a wide range of Sb compositions. The aim of the experiment is to study the optical and physical properties of BiSb. Little work has been done on BiSb thin film deposition on glass slab done by thermal evaporation method followed by thermal annealing .henceforth the optical and physical properties has been studied. Afterwards the comparison has been done before and after annealing. We found that using UV spectroscopy, optical properties like absorbance, extinction coefficient, refractive index, dielectric constant and the optical conductivity increases after annealing with increase in Sb content. The transmittance, optical bandgap, dielectric loss deceases after annealing with increase Sb content. Theoretical studies were made for studying the physical properties.

## THESIS OUTLINES

The thesis is composed of 4 chapters.

| | |
|---|---|
| CHAPTER-I | Depicts about the properties of bismuth and antimony and bismuth antimonide. |
| CHAPTER-II | Discuss about the preparation of sample using different method thermal evaporation method, thermalannealing, UV spectroscopy, various optical properties and physical properties of bismuth antimonide. |
| CHAPTER-III | Discuss about the results i.e the optical and physical properties and various graphs. |
| CHAPTER-IV | Summarizes the thesis and recommends for future work. |

# CHAPTER-I

# INTRODUCTION

The exhibition of the solid solutions in semiconductors is of curiosity as it outcomes in an abundance of other semiconducting materials. One specific category of these type materials is the binary alloy of compound semiconductor, which are of tremendous technological concern in electronic and opt-electronic equipment. The Bismuth-Antimony thin films undergo semi metal–semiconductor transition. The BiSb thin film exhibit “ordinary size effect” and “quantum size effect”. BiSb alloys ($Bi_{1-x}Sb_{x)}$ comprise a material structure which has been fascinating significant notoriety in recent days .That category of materials is assumed as a promising materials prospects for thermoelectric, refrigeration in cryogenic temp. Spectra.

Little work has been done on BiSb thin film deposited on glass slab. This deposition has been done by thermal evaporation method. Henceforth, the physical and optical properties has been studied. Also, the annealing has been done for the same deposition on the thin film and its properties has been also studied. Afterwards a comparison has been made about what happens to the properties before and after annealing. The BiSb glasses tempted extremely in numerous research areas that is in photoconductors and transport, phase optical storage medium. Numerous BiSb alloys are super conductor at a inadequate temperature, are semiconductors and are used in thermos electric equipment.

The present paper reports optical and physical properties of $Bi_{1-x}Sb_{x}$ assuming x=0.025, 0.05, 0.075, 0.1 forming thin films. And the optical properties includes extinction coefficient ,refractive index , absorption coefficient with optical bandgap, that details are researched in spectra of 200nm to 800nm by verifying transmission ranges. And this optical behavior correlated with physical properties likely cohesive energy, co-ordination number and lone-pair electrons and optical band gap.

Bismuth antimony in their respective composition have been one of the greatly intriguing substances structures for several decades, with considering their high anisotropic transportation behavior and delicate effective mass and elevated mobility carriers. Those materials category supposed to be one among most effective thermoelectric equipment for cooling purpose within lower extent below 100 K. In the earlier 1990s, Dresselhaus and Hicks acknowledged that Nano structured substances can have strengthened their thermoelectric figure of excellence as related to their majority equivalents. [2] [3]

By the growth of the $Bi_{1-x}Sb_x$ in the shape of quantum detention , nanowires are initiated in that directions those are remain normal along the wire which initiates those 3 parameters of the (1) orientation of the wire with association to axes of the crystal (2) the width of the wire (3) the cross-section ratio , that indicating the ratio among the long side width and therefore resulting the short side width having the cross-section is therefore forming a rectangular shape which means This ratio is distinct from the ratio among the length of the nanowire and therefore the width of its cross section, if the cross section assumed to be a square structure). Those formed pair of parameters may be familiarized control the electronic begure and, particularly, the quantum confinements impact that has been just wont to enhance that thermoelectric accomplishment of Bismuth antimony film.

That topic including Nano-particles of $Bi_{1-x}Sb_x$ contains 2 fundamentals: the manner of one Nanoparticle and therefore the aspect of large substances which are comprised by Nano particles constituents. There has not eventually been ample investigation on the electronic properties of single Nano particles of $Bi_{1-x}Sb_{x.}$ The analysis regarding those bulk substances constructed by Nano particles of $Bi_{1-x}Sb_x$ is additionally at an extremely earlier stage. Ahead the explicit advancement of the nanotechnology field, researchers investigated that the thermoelectric performance of polycrystalline $Bi_{1-x}Sb_x$ materials of micro-sized grains may alter as a function of grain size. [5] Advantages of working with films are large area uniformity, better chance to make good electrical and thermal contacts, ability to nanostructure. [6]

Bismuth and antimony are semimetals and having structure of rhombohedral. And those possessing a little e energy overspread among the valence and conduction bands, increased carrier abilities with small effective masses. Due to those properties, Bismuth and antimony normally been utilized for quantum size effect studies. The Bi12xSbx alloy structure are often behaves as a semiconductor or semimetal reckoning on the antimony concentration. [8] There having various initial actions for the growth Bi thin films and super lattices. High vacuum thermal evaporation on mica substrates was initially employed for the growth epitaxial Bi films, Bi/Cd Te super lattices, and Bi/PbTe superlatives. [9] [10]

### I.1 PROPERTIES OF BISMUTH

Bismuth (Bi), the most metallic and therefore the least thick of the weather within the chemical element cluster (Group fifteen of the periodic table). The metallic element is hard, brittle, lustrous, and coarsely crystalline. It is distinguished from all different metals by its color grey-white with a ruddy tinge.

Fig I-Bismuth

Metallic element is employed in the main in alloys, to several of that it imparts its own special properties of low freezing point and enlargement on action (like water and antimony). Metallic element is so a helpful element of type-metal alloys, that build neat, clean castings; and it is a crucial ingredient of low-melting alloys, referred to as liquid alloys that have an oversized style of applications particularly in fire-detection instrumentality.

Bismuth show visible light from yellow to blue. Bi is a fragile metal with a white, silver pink pigmenting, usually having an polychromatic chemical compound which decay color.

Bismuth is diamagnetic and it's having high electrical resistance. Elemental Bi is denser at intervals the liquid part than the solid, a distinctive it shares with element, silicon, water, gallium. The sole primal atom of Bi, bismuth having mass no 209, was historically thought-about the enormous stable atom. Bi has the longest best-known decay half-life. Commercially, the radioactive atom bismuth having mass no 213 square measure usually made by colliding metal including bremsstrahlung photons from an atom smasher. Bi has been using in pharma industry, cosmetics and pigments, replacement of lead, low melting solders, melted alloys, artificial fibers, shots and shotguns.

## I.2 PROPERTIES OF ANTIMONY

Antimony (Sb) is a semi metallic element. It occupies 5th period and Group 15 of the table of chemical elements. As it is having semi metallic nature, it persist as both metal and non-metal. The color of antimony is silvery, bright, brittle, and hard and its non-metallic form shows greyish powder. Like other elements in group 15 of the periodic table, antimony is known as a bad conductor of both heat and electricity.

Fig II- antimony

As Antimony can constructs a highly advantageous alloy with lead, improving its hardness along with its mechanical strength. Antimony can be utilized in semiconductors as a dopant in non-type silicon wafers diodes, Hall- effect equipment and infrared detectors.

Antimony possess 2 stable isotopes those are sb having mass no 121 acquiring a natural abundance of 57.36% and Sb having mass no 123 sustaining natural abundance of 42.64%. There are 35 radioisotopes of sb are known out of which longest-lived is sb of mass no 125 having a half-life of 2.75 years. Besides this there are 29 metastable states which have been defined. The greatly stable of those is 120m1Sb having a half-life period of 5.76 days. The Isotopes which are considered to be lighter than the stable 123Sb prefer to decay by $\beta+$ decay, and those which are heavier prefer to decay by $\beta-$ decay, with some irregularities. [13]

Compounds in this category commonly are characterized as derivatives of $Sb^{3-}$. Antimony produces antimonides with metals, like silver nationwide ($Ag_3Sb$) with indium antimonide (InSb) .The alkali metal and zinc antimonides, like $Na_3Sb$ and $Zn_3Sb_2$, are considered better reactive.

Antimony constructs a extremely valuable alloy with lead, improving its hardness along with its mechanical strength. In lead acid batteries, Sb accumulation enhances plate strength and charging qualities. Antimony is increasingly being wielded in semiconductors as a dopant in n-type silicon wafers for diodes, Hall-effect appliance.

### I.3 BISMUTH ANTIMONIDE AND ITS USES

Bismuth and it's compound with antimony provide extraordinary properties and are assuring competitors do their thermoelectric applications. Bismuth with Antimony resulting alloys comprise a materials system that attracting significant compassion in recent days. Those group of substances is evaluated as the promising substances prospects for thermoelectric and refrigeration in the cryogenic temperature spectrum. There are much prosperous stages in thin film Bi1-xSbx referred to bulk Bi1-xSbx, since two additional parameters are introduced: film thickness with growth orientation that gives rise to the exploration on Bi1-xSbx thin films extremely fascinating. In particular Bi0.9 Sb0.1, were the first experimentally observed 3D topological insulators and those materials having conducting surface states but having an insulating interior. Numerous Bisb alloys furthermore superconductor at poor temp., are semiconductors, and those are utilized in thermoelectric equipment.

As bismuth and antimony possessing identical lattice parameters, it is not shocking that Bi-Sb alloys can establish a solid solution over the entire composition extent. As expected, the lattice parameters for the alloys are between those of Bi and Sb. Bismuth Antimonide (BiSb) is used as a significant equipment in the field of Nano electronics used as a topological insulator – offering unique opportunities to control electric currents and magnetism, and promising material for future spintronic applications. The highest temperature, at which thin film of thicknesses 150-1350A can super conduct is nearly 2Kelvin. Single-crystal has property that can super conduct at just higher temperatures. It has critical magnetic field of 1.6T at 4.2K. At 40K, the mobility of electron of Bismuth Antimonide (BiSb) varied from 0.49*106 /Vs at a Sb conc. Of 0 to .24*106 /Vs and at an Sb concentration of 7.2%. That is much enormous as compared to the electron mobility of other broad semiconductors like Si, which is found to be 1400 /Vs at room temperature. Its effective electron mass is supposed to be 0.002me for x=.11 and .0009me at x=.06. This is much smaller than the electron effective mass in several popular semiconductors (1.09 in Si at 300K, .55 in Ge, and .067 in GaAs). A low EEM is decent for thermos-photovoltaic appeals.

BiSb are utilized as the n-type legs in several thermoelectric appliances below room temperature. At 80K, the figure of merit for peaks at 6.5*/K when x = 15%. Furthermore, the See beck coefficient at 80K of is -140μV/K, much less than the Seebeck coefficient of pure bismuth, -50μV/K. [15]

## I.4 OPTICAL PROPERTIES

The optical property of a matter is defined, how it interacts with light. Certain optical properties are-absorption, transmittance, refractive index, reflectance, extinction coefficient, dielectric constant with optical conductivity. We shall now have a brief discussion on these properties and from they have been derived.

1. Absorption- this term means a substance captures and transforms energy and it measures attenuation.

2. Transmittance- Transmittance (T) describes how the light passes through a sample unchanged.

3. Reflectance- it is the light incident on the surface of a material that is reflected at an interface. The reflectance spectrum curve is the plot of the reflectance vs wavelength.

4. The optical band gap is the excitation energy which determines the onset of vertical interbank transitions.

5. Refractive index- In optics, it is the ratio of the speed of light in vacuum. Mathematically.

6. Extinction coefficient- it is defined as an extent of the absorption of light at a given wavelength in a medium.it is of 2 types such as mass extinction coefficient and molar extinction coefficient.

7. Dielectric constant-A dielectric is a material that has conductivity very low but inherits an ability to store an electrical charge (due to Dielectric polarization). The complex dielectric constant has two parts i.e real and imaginary. the real part is the evidence of the extent up to which a substance could be polarized and the imaginary part attributed with dielectric losses.

8. Optical conductivity- This is approximately associated to the dielectric function, the abstraction of the dielectric constant is to irregular frequencies. It is also interpreted as the conduction manner happening from the activity of charges for the differing (alternating) electric field of incident light

So now we shall find the formulas for these optical properties and correlate them to use them for calculation purposes.

From Wood and Tauc's formula,

$$(\alpha h\nu)\ n = B\ (h\nu - E_g)$$

Here B is a const.,

Eg = the optical band gap energy,

n = constant that having values of 1/2 and 2 which are assigned for the allowed direct allowed and indirect allowed transition.

In the above formula,

A = the absorption coefficient

$$\alpha=2.303*absorbance/thickness$$

Optical properties such as extinction coefficient, optical conductivity with dielectric constant of the semiconductors are significant. The complex optical refractive index is

$$m = n + i k$$

Here

n= real part which refers refractive index

K= the imaginary part which refers the extinction coefficient

$$k = \alpha\lambda /4\pi$$

$$n = (2-T)/T+\sqrt{((4(1-T))/T^2 -K^2 n)}$$

Where

α = the absorption coefficient

T = transmittance

The both real and the imaginary parts of that complex optical dielectric constant can be evaluated by extinction coefficient and refractive index by the subsequent two mathematical equations

$$\varepsilon 1=n2-k2$$

$$\varepsilon 2=2nk$$

Where

ε1 =the real part and

ε2 = the complex part of the dielectric constant.

The dielectric loss (tanδ) depicts the inefficiency of material to hold energy or behave as an insulating material.

$$\tan \delta = \varepsilon 2 / \varepsilon 1$$

Optical conductivity is a complex number so calculated by using real and imaginary parts

$$\sigma 1 = \omega\ \varepsilon 2\ \varepsilon 0$$

$$\sigma 2 = \omega\ \varepsilon 1\ \varepsilon 0$$

## I.5 PHYSICAL PROPERTIES

A distribution of thin-film properties is essential for the research of thin-film substances and equipment. Certain physical properties like theoretical bandgap, coordination number, cohesive energy, and lone pair electron are mandatory in the research of thin film produced by BiSb compound.

Theoretical Band gap- It is stated as the energy difference between the conduction and valence band. Virtually, bandgap represents the energy employed to promote a valence e bound to an electron to evolve conduction electrons.

Cohesive energy- it is otherwise called as binding energy which is required to break all the bonds gas. Insulators and semiconductors are bound together strongly and have good mechanical strength also so they possess a huge amount of cohesive energy.

Coordination number- This is the number of ligands connecting to the central metal atom.it is established by physical measurements.

Lone pair electron-The unshared pair of valence electrons is known as lone pair. The coordination number is assigned by the 8 N rule, for N is the no. that represents of outer shell electrons in a given atom. The average coordination no. is interpreted as the atom averaged covalent coordination of the constituents.

Now we shall use mathematical formulation to find the required formulae to find certain values for coordination number, theoretical bandgap, lone pair electron, and cohesive energy.

The average coordination number $\langle r \rangle$ is evaluated by employing the following formulae –

$$\langle r \rangle = (x*NSb + (1-x)*NBi) / (xx) \ldots\ldots\ldots\ldots (1)$$

Where x= concentration of antimony

1-x=concentration of bismuth

NSb=coordination number of bismuth=3

NBi=coordination number of antimony=3

The theoretical band gap can be calculated by using the following formulae-

Eg(total)=Eg(Bi) *(1-x)+Eg(Sb)*(x)……….. (2)

Here Eg(Bi)=0.22eV and Eg(Sb)=0.17eV

The lone-pair electron for the given compound can be found using the following formulae-

L=V-〈r〉…………………………………. (3)

Where V=valence electron

〈r〉=average coordination number

## Objective

1. To produce a thin film of bismuth antimonide using thermal evaporation method.
2. To study the optical properties of bismuth antimonide (bisb) by using thermal annealing.
3. To study the physical properties of bismuth antimonide (bisb) by using thermal annealing.
4. To study the optical as well as physical properties by uv spectroscopy.

# CHAPTER-II

## II.1 THERMAL EVAPORATION METHOD

Thermal evaporation method can enclose vast number of lab applications including preparation of thin film for optical and their electronic application. This thermal evaporation method involves a technology known vacuum technology used for coatings of pure materials to the surface of different objects. Thermal evaporation is also designated as Physical Vapor Deposition (PVD). Their objective is to be coated is illustrated because the substrate, may be any different of a good sort of aspects namely solar cells, semiconductor wafers, optical ingredients, or several additional chances. Inside the vacuum, even a comparatively short vapor pressure is adequate to boost a vapor cloud inside the chamber. That evaporated substance now comprises a vapor stream, which crosses the chamber and blows the substrate, clasping thereto as a covering or film.

This vacuum coating unit comprises of a box shape structure that consists of pumping unit along with necessary electric component required. The system consisted of a rotary pump and a condensation pump. Some important accessories of this unit are

1. Boats-

Boats are basically thin sheet metal slabs containing adequate higher-temperature metal with formed incisions or grooves to which the substance is positioned. The filament citation proposes the security of intense voltage, as if extremely elevated current is expected, usually numerous 100 amps.

2. Diffusion Pump

This is a kind of vacuum pump constructed to attain adequately vacuum pressures (10-10 -10-2 mbar) than apparent by the aim of automatic pumps independently. Using either airflow or a water line, the outside of the pump is cooled. As the vapor jet influences, the outer refrigerated shell of the condensation pump the gas entrained within the jet flow coalesces, holding up the entrained pumped gases to the bottom of the pump.

3. Rotary Pump-

Rotary vane pumps are available in 2 categories, those wont to develop crude vacuum levels (760 to 1 torr) and people wont to produce tough vacuum levels (760 to 10-3 torr). The technique of those pump types varies based on the amount and tolerance of varies within the pump. The rotary pump is accomplished to deposit substrate regularly on large plane

Thin Film Evaporation techniques propose the advantages of somewhat increased deposition rates, and thickness supervision, and (with adequate manual arrangement) decent evaporated stream directional control for mighty objectives as take-off processing to realize directly patterned layers and can be relatively easily fabricated during a single deposition procedure.

Fig III. Vacuum coating unit

## II.2 SAMPLE PREPARATION

Thin films with different compositions of Bi1-xSbx (x=0.025,0.050,0.075,0.100) were composed by thermal evaporation procedure by utilizing Hind High vacuum coating unit over glass substrate rates at a base pressure of~5 *104 Torr. The substrate temperature was retained at room temperature and the rate of deposition was adjusted at 5 nm/s during the deposition procedure. To urge the homogeneous and identical film, the substrates were rotated gradually. The film thickness of the samples was investigated by a crystal thickness monitor and was formulated about 500 nm in to prevent the thickness effect.

### II.2.1 THERMAL ANNEALING

Thermal annealing is a usual process used to reduce stress, increases ductility, and reduce its hardness. In such a process the thin film is carefully placed in a glass container and placed inside the hot oven. Then a required temperature limit is set for the annealing process. After the temp is required temperature is reached it is allowed to heat the thin film for 3-4 hours according to the requirement. Then after cooling the material is taken out. Due to annealing, the properties of the thin film get changed, henceforth further studies are carried out by UV spectroscopy and XRD to determine required physical and optical properties.


Fig IV. Box type Furnace for Annealling

### II.2.2 UV SPECTROSCOPY

The ultra-violet visible spectroscopy is a very useful tool for the investigation of electronic transition and the energy band gap of any material. When UV-visible radiation interacts with the matter, it gets absorbed by the matter, resulting in the increase of its energy. The wavelength of the absorbed light is always equivalent to the energy required to move an electron from lower energy band to the higher energy band. This results in a sharp absorbance edge in the absorption spectra of the material. The energy associated with this edge gives the band gap of the material. In general broad edge represents glassy state of material. The broad edge may represents the presence of more than one band edges in the compound as well as give insight to the presence of possible imperfection.

The UV-visible spectroscopy is primarily utilized to specify the energy band gap of semiconducting materials. The broadening of band edge helps in prediction of splitting of bands. Isolating a thin band of radiation from a continuum light source for absorption measurements, or estimation of the emission from excited atoms or molecules is considered as one of applications. Specifically UV-visible spectroscopy can be used to identify an unknown compound by a comparative analysis. UV-visible spectra of the unknown with respect to a known spectra can be compared. The light source is usually hydrogen or deuterium lamp for UV-visible measurements.

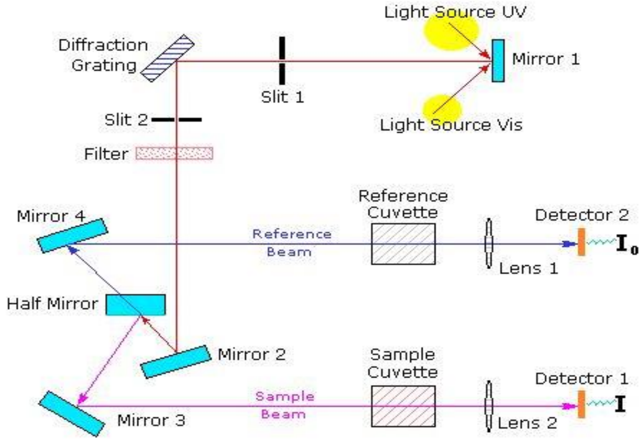



Fig V Schematic diagram illustrating UV-Vis spectroscopy

The optical band gap (Eg) can be evaluated employing the Tauc relation

$$\alpha h\upsilon = A\,(h\upsilon - Eg)^{m}$$

Fig VI. UV Spectroscopy

# CHAPTER-III

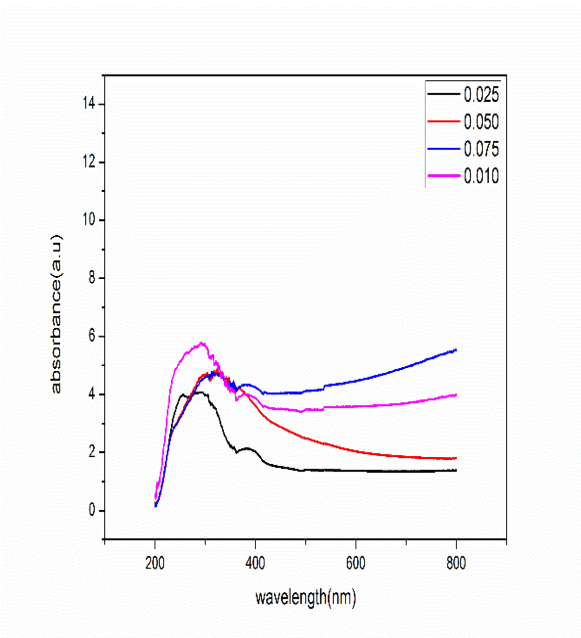
## III.1 OPTICAL PROPERTIES

The UV visible spectroscopy was carried out to find reflectance of the sample Bi 1-xSb x with the values of x= 0.025, 0.050, 0.075, 0.100. Now from the reflectance data, the absorbance is found out in the spectrometer itself. Moreover, the transmittance value is also calculated in the same process. Henceforth bandgap was calculated from Tauc's plot and rest of the optical properties were calculated.

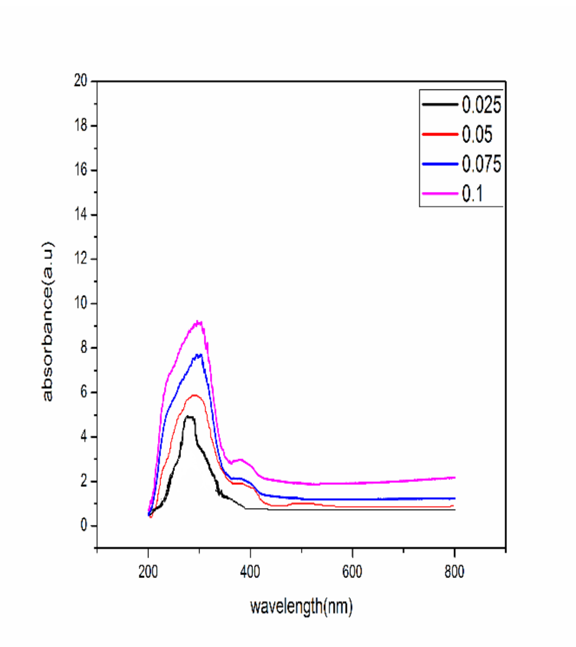
### III.2 ABSORBANCE

Absorbance increases with increase in concentration of Sb from 0.025 to 0.100 due to Lambert's-Beer law. According to Lambert's-Beer law, absorbance of a light absorbing material is proportional to its concentration in the compound. If concentration is increased then there are more molecules to hit when light passes through it and hence get absorbed.

After annealing, it is observed that annealed absorbance is increased.




(Before annealing)




(After annealing)

Fig VII. Absorbance vs wavelength (nm)

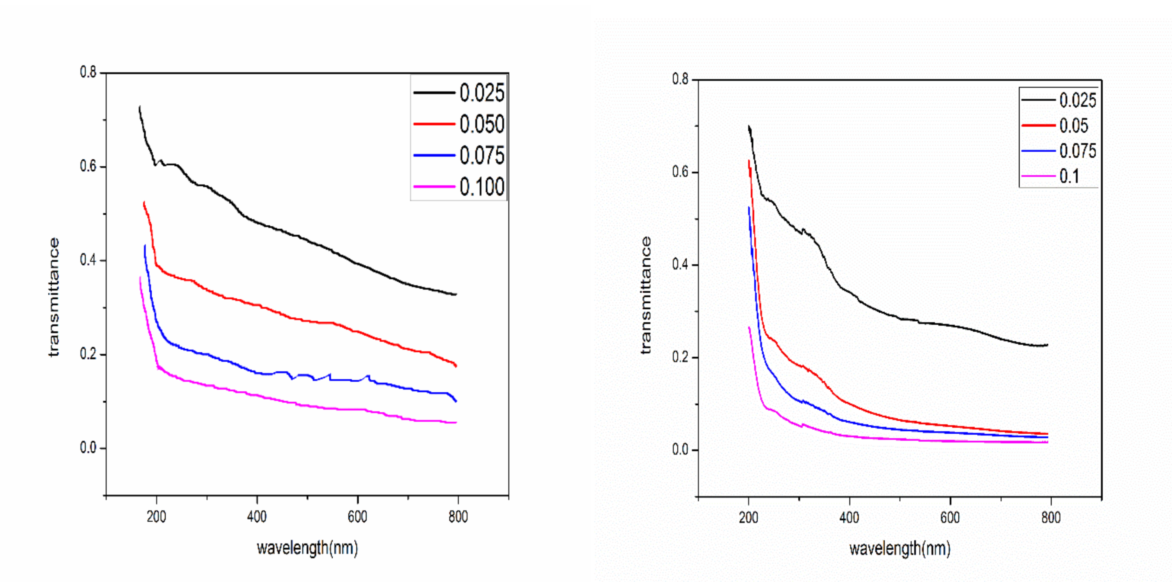
**Table III.a** Absorbance

| | **As prepared** | **After annealing** |
|---|---|---|
| **X=0.025** | 0.4 | 0.5 |
| **X=0.050** | 0.45 | 0.6 |
| **X=0.075** | 0.5 | 0.8 |
| **X=0.100** | 0.6 | 0.9 |

## III.3 TRANSMITTANCE

Transmittance decreases with increase in concentration of Sb from 0.025 to 0.100 because as the absorbance increases. Mathematically A=2-log T.

After annealing, it is observed that annealed transmittance is decreased




(Before annealing) (After annealing)

Fig VIII. Transmittance vs wavelength (nm)

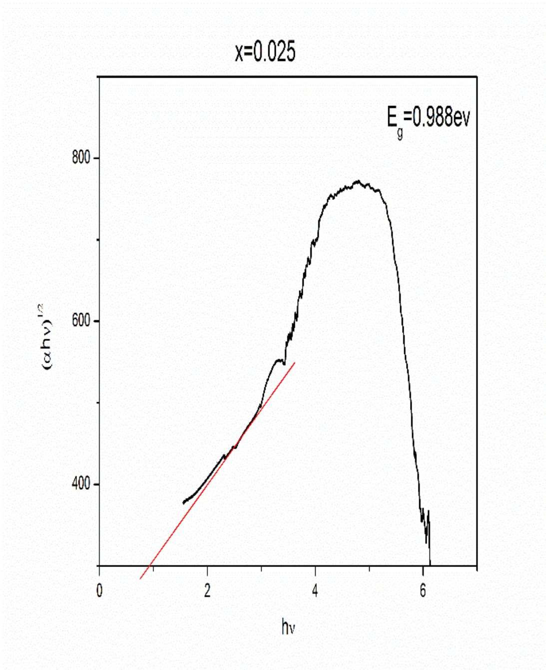
**Table III.b** Transmittance

| | As prepared | After annealing |
|---|---|---|
| **X=0.025** | 0.6 | 0.5 |
| **X=0.050** | 0.4 | 0.25 |
| **X=0.075** | 0.3 | 0.2 |
| **X=0.100** | 0.2 | 0.1 |

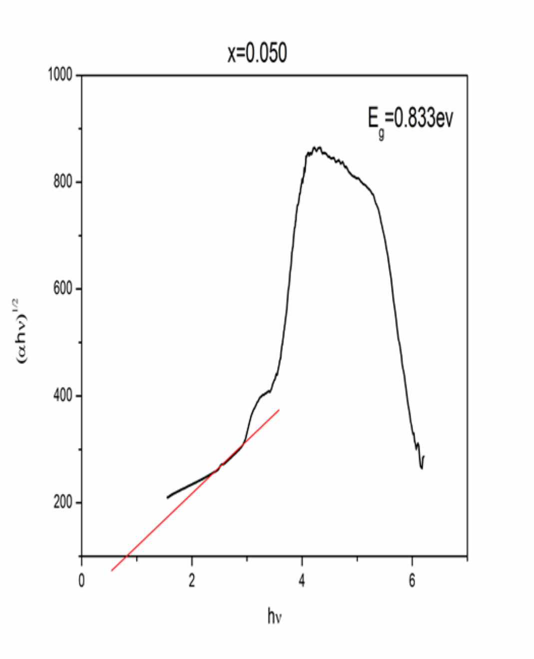
## III.4 OPTICAL BAND GAP

By using Wood-Tauc's formulae, the optical band gap energy is being found. The graph is being plotted between hυ is taken along x axis and (αhυ) 1/2 along y axis. The band gap energy is estimated by extrapolating the linear portion of the curves. It is being found that the band gap reduces with gain in concentration of Sb from 0.025 to 0.100. The band gap may be an area in energy having no allowed states. When Sb is doped higher and higher in concentration, then the chemical composition of the compound is changed due to doping. Commonly those contaminants establish a superficial state in the band gap. Superficial states retain minor ionization energy and while doping density is increased, the dopant state generates a band structure. In that case, the shallow band is near to conduction band and so the band gap will reduce.

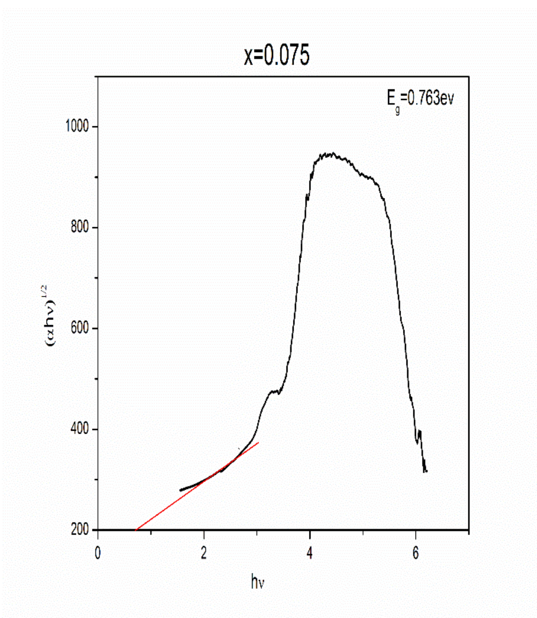
After annealing, the band gap decreases as compared to as prepared material due to dangling bond formation i.e an unsatisfied immobilized atom.



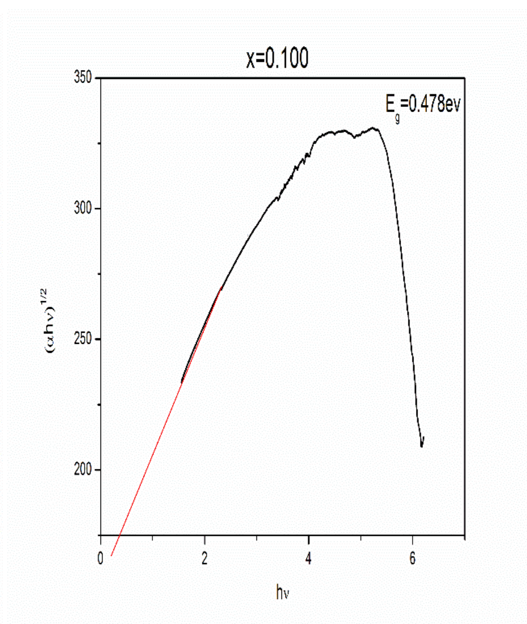

(a)




(b)

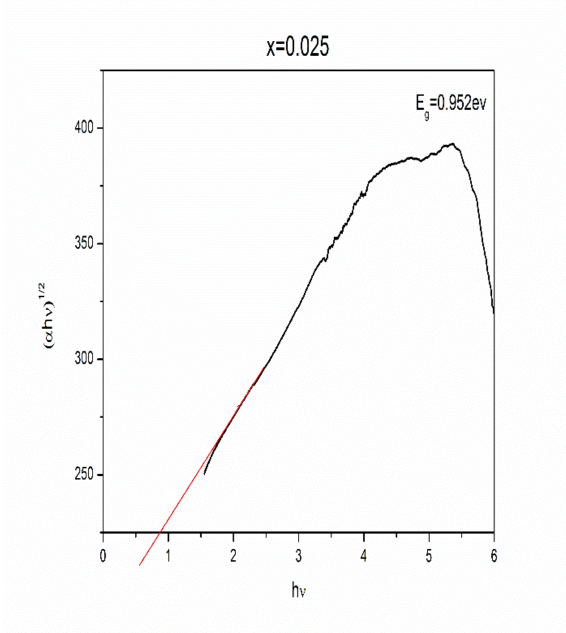



(c)

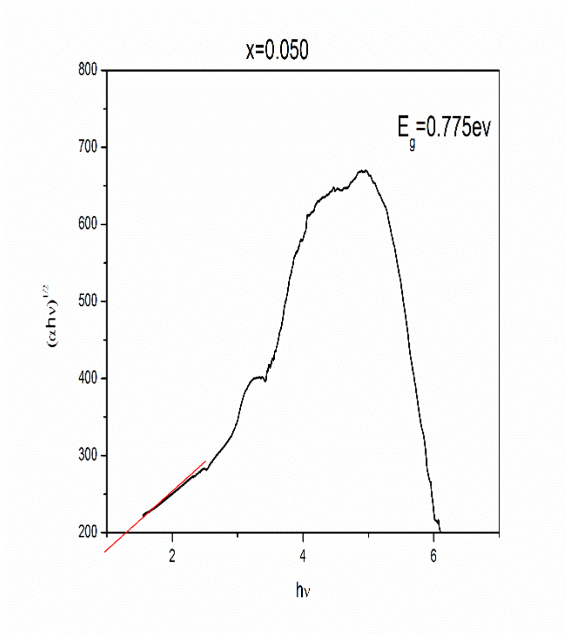



(d)

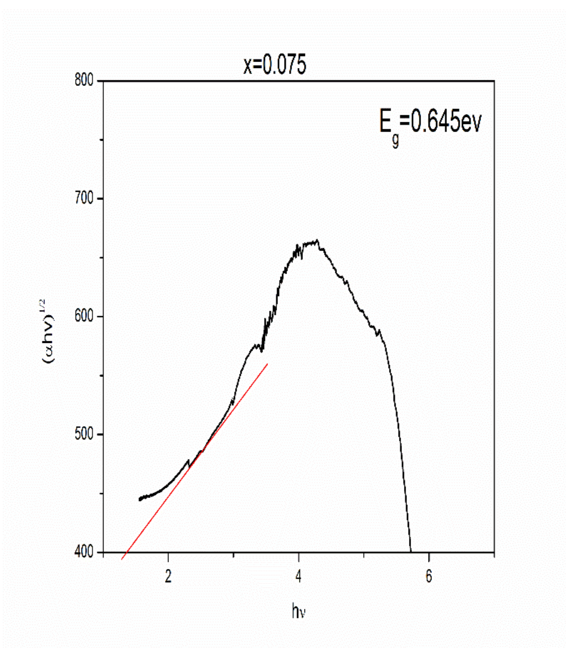
Fig IX. (a,b,c,d) Band gap at different x value before annealing



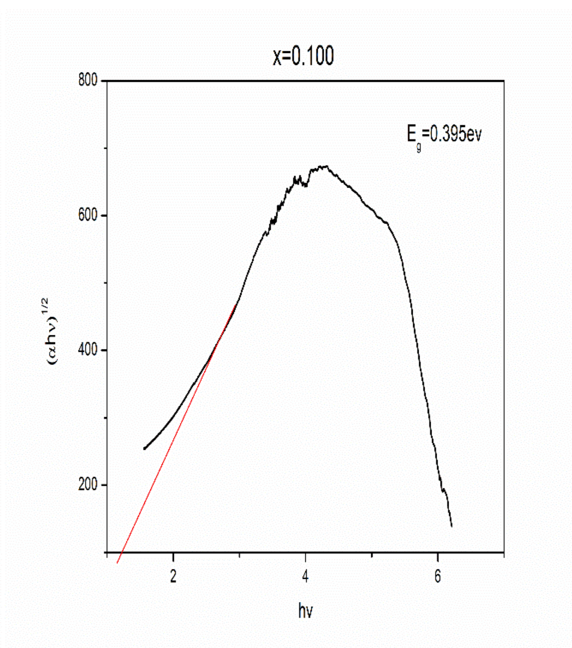

(e)




(f)




(g)

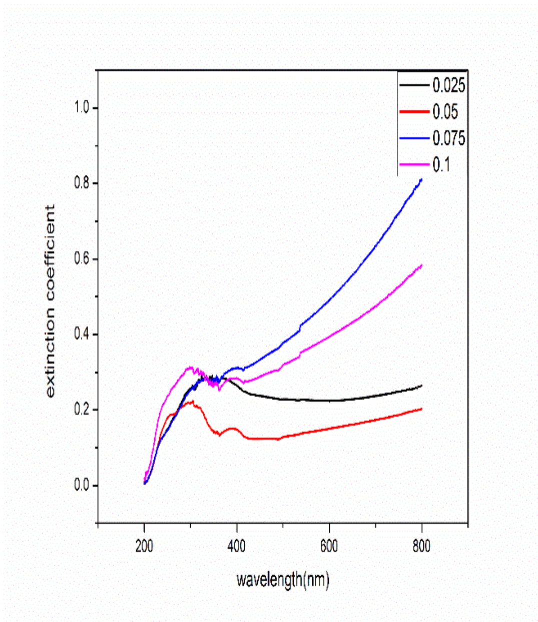



(h)

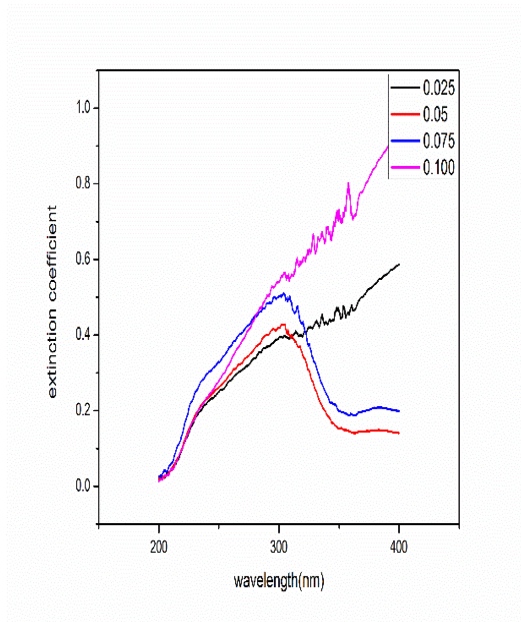
Fig X. (e,f,g,h) Band gap at different value of x after annealing

### III.5 EXTINCTION COEFFICIENT

The extinction coefficient provides the quantity of absorption expense when the wave propagates through the substance. As we know extinction coefficient is directly proportional to the absorption coefficient. So extinction coefficient boosts with an improvement in the concentration of antimony from 0.025 to 0.100. After annealing, the extinction coefficient increases.




(Before annealing)

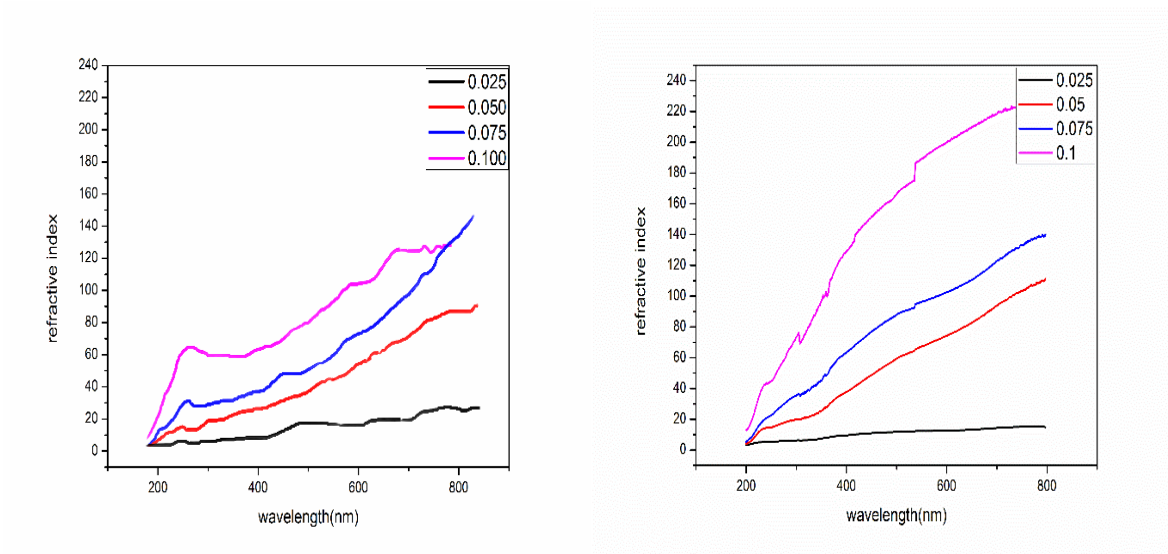



(After annealing)

Fig XI. The extinction coefficient vs wavelength (nm)

### III.6 REFRACTIVE INDEX

The refractive index increases with improvement in conc. Of antimony from 0.025 to 0.100. This is due the reason that by Moss's law, the band gap very inversely to the 4th power of the refractive index. After annealing, the refractive index increases.



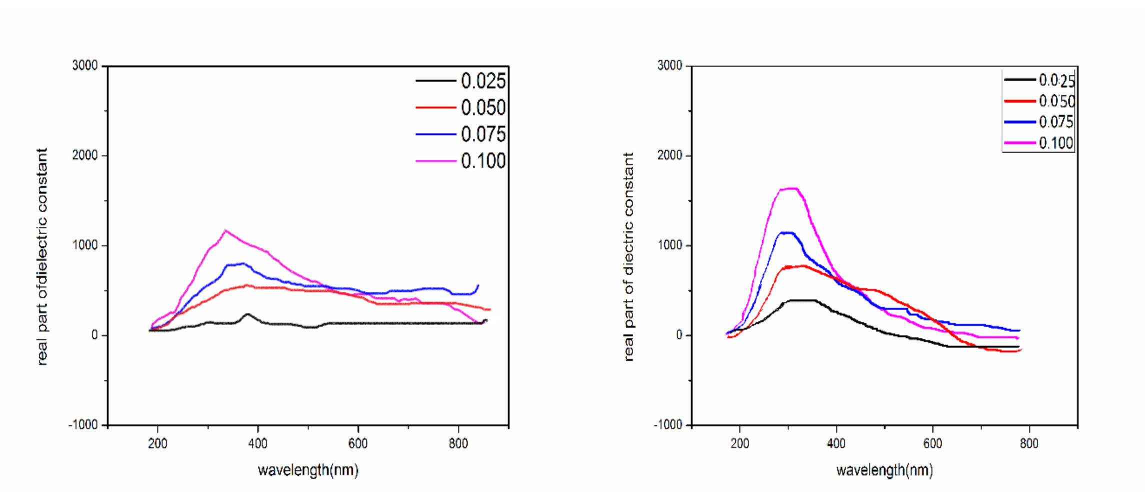

(Before annealing) (After annealing)

Fig XII. The refractive index vs wavelength (nm)

## III.7 DIELECTRIC CONSTANT

Real part –It rises with the gain in the conc. Of antimony from 0.025 to 0.100. This is because the absorbance increases, so also the energy storing capacity increases. However, it can be related to the refractive index, where also it shows that it is directly proportional to the refractive index.

After annealing, the dielectric constant is also increased.

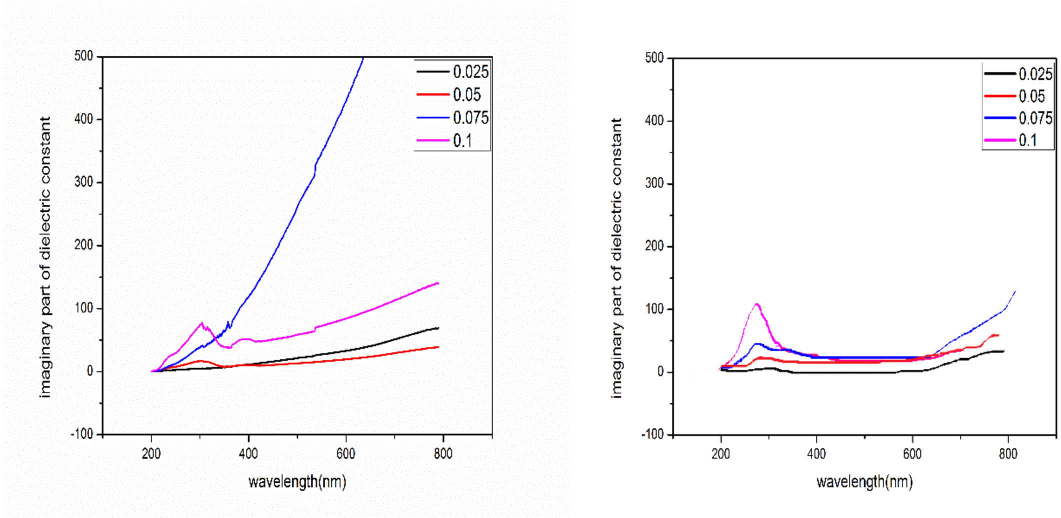



(Before annealing) (After annealing)

Fig XIII. Real part of dielectric constant vs wavelength(nm)

Imaginary part-It also increases with increase in concentration of Sb from 0.025 to o.100.

After annealing, the dielectric constant also increases.

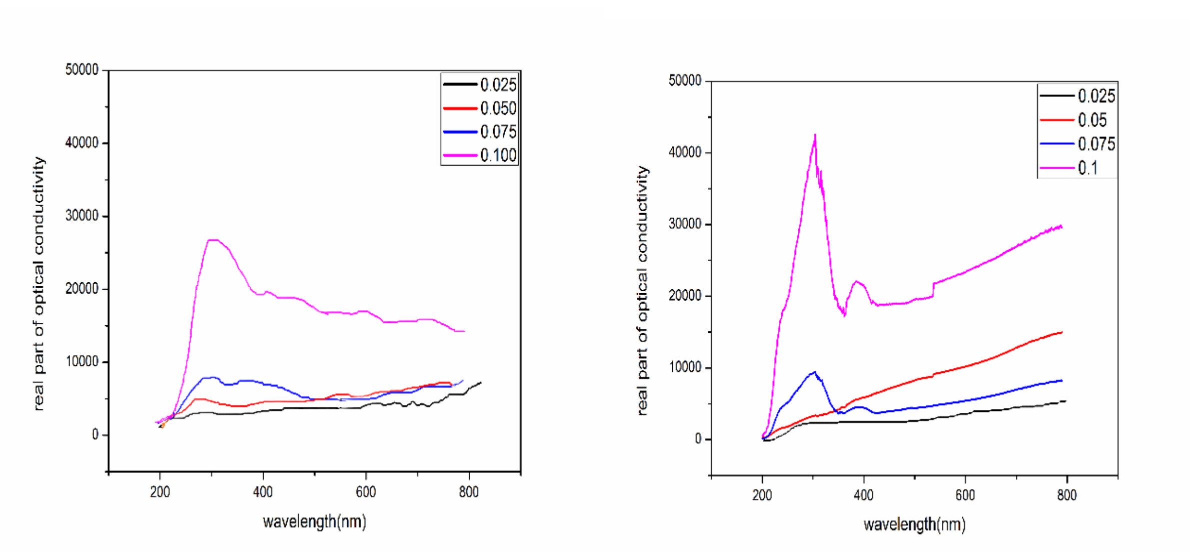



(Before annealing) (After annealing)

Fig. XV. Imaginary part of dielectric constant vs wavelength(nm)

## III.8 OPTICAL CONDUCTIVITY

Real part-It increases with increase in concentration of Sb from 0.025 to 0.100. After annealing, the optical conductivity increaes as band gap is decreaed.

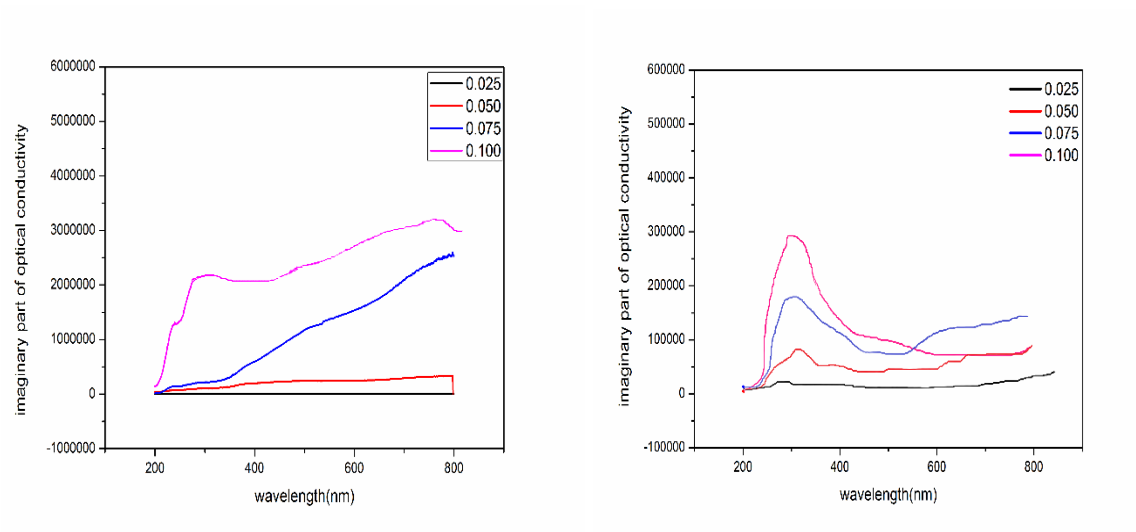



(Before annealing) (After annealing)

Fig XVI Real part of optical conductivity

Imaginary part-It increases with increase in concentration of Sb from 0.025 to 0.100.

After annealing, the conductivity increases as the band gap is decreased.



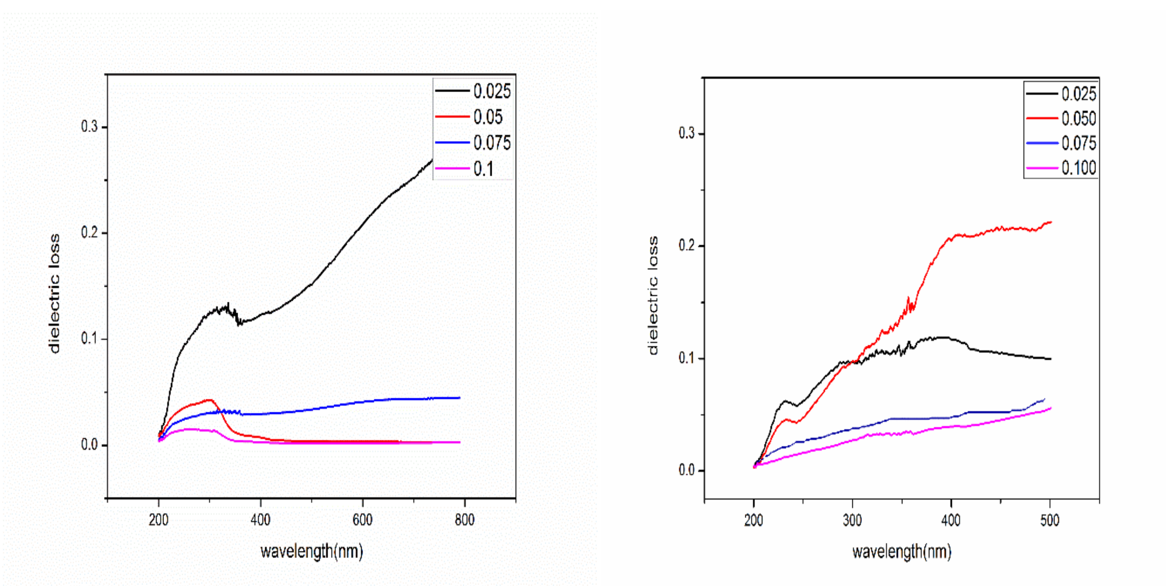

(Before annealing) (After annealing)

Fig XVII Imaginary part of optical conductivity vs wavelength(nm)

**III.9 DISSIPATION FACTOR/ DIELECTRIC LOSS-**

It decreases with an increase in the concentration of Sb from 0.025 to 0.100.

After annealing, the dielectric loss decreases.




(Before annealling) (After annealing)

Fig XVIII Dielectric loss vs wavelength(nm)

## III.10 THEORETICAL CALCULATIONS

The coordination number ⟨r⟩ of $Bi_{1-x}Sb_x$ is found to be 3 from formulae used in equation number (1).

Similarly, the theoretical band gap is calculated for different values of x using equation number (2). Then the lone pair electron is calculated using formulae in equation number (3).

**Table III.c** Theoritical Calculation

| Composition | Theoritical band gap ($E_g$) | Valence electron (V) | Lone pair electron (L) L=V-$\langle r \rangle$ |
|---|---|---|---|
| X=0.025 | 0.21875 | 4.95 | 1.95 |
| X=0.050 | 0.21750 | 4.90 | 1.90 |
| X=0.075 | 0.21625 | 4.85 | 1.85 |
| X=0.100 | 0.21500 | 4.80 | 1.80 |

Hence, it is concluded that theoretical band gap decreases with a gain in concentration Sb from x=0.025 to 0.100, and also the optical band gap decreases which have been experimentally proved. The decline in optical bandgap may be attributed with a decline in cohesive energy of the operation with an increase in Sb content. The no. of lone pair electrons also diminishes with a rise in Sb content that s due to the exchange of Sb with the lone pair of Bi atoms.

# CHAPTER-IV

# CONCLUSION

In my current paper, we have discussed both the theoretical and the experimental results attained from the $Bi_{1-x}$ $Sb_x$ thin film. First of all experimental study has been done to study the optical properties like transmittance, absorbance, extinction coefficient, refractive index, dielectric constant, optical conductivity, and dissipation factor. Using UV spectroscopy, the absorbance was found out which increases with the increase in concentration, so also the extinction coefficient increases. However, the transmittance decreases with a gain in Sb content. But the optical band gap decreases with the improvement in the concentration of Sb content which could be understood by the dangling bond concept. The refractive index gains with a gain in Sb conc. by Moss's law. After annealing, the absorbance of the compound increases and the bandgap decreases. Apart from this, theoretical studies were made for studying the physical properties. It was found that optical properties are benefited by physical properties i.e decline in optical band gap is favored by a lowering in cohesive energy of the operation. Lone pair electron was also organize to decrease with an increase in Sb content. From this study of optical and physical property, the BiSb compound can be beneficial in many ways.

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