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Optical Properties of $CuInS_2$ Films Produced By Spray Pyrolysis Method

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ABSTRACT

$CuInS_2$ Semiconductor Films have been produced by the Spray Pyrolysis method on to the glass substrate by using different molarity solutions. Optical Characteristics of the $CuInS_2$ Films have been analysed using Spectrophotometer in the wavelength range 380-1000 nm. The optical band gap energy has been obtained from the plot of $(\alpha h\upsilon)^2$ Vs $h\upsilon$. The absorption spectra of the Films Showed that this Compound is a direct band gap material and gap values varied between 1.51-1.80 ev, depending on the molarity solutions. The X-rays diffraction (XRD) spectra of the films have shown that the films produced are polycrystalline and chalcopyrite in structure.

Key Words : $CuInS_2$ Thin films, XRD, SEM.

INTRODUCTION

The development of contemporary, sophisticated technologies which increase the quality of human life is closely related to the Semiconducting materials. The science and technology of Semiconducting thin films have a Crucial role in high tech industry. Thin Film of Semiconducting materials are applicable in the field of microelectronic, Optical electronic, in Communication technologies, as well as in energy generation and Conservation Strategies, etc. .[1] $CuInS_2$ is one of the I-III-VI_2 type semiconductor which crystallizes in the chalcopyrite or sphalerite structure.[2] It has direct band gap of 1.3-1.5 ev, high absorption coefficient (10^5 cm^{-1}).[3] An environment viewpoint, $CuInS_2$ does not contain any toxic Constitutents that makes it suitable for terrestrial photovoltaic applications.[4]

A variety of techniques have been applied to deposit $CuInS_2$ thin films, such as single source evaporation, coevaporation from elemental sources, sulfurisation of metallic precursors. [5] diffusion of Cu and S into InxS Precursor, electrode deposition and spray pyrolysis [2, 6-8] Spray Pyrolysis is an attractive method for large area thin films production because it is a low-cost and easy to make process [8-10]

Several methods are reported for the preparation of $CuInS_2$ thin film such as electrodeposition,[11], Pulse lasor deposition[12], Physical vapor deposition[13], vaccum evaporation[14], close space sublimation[15], But all these methods have sophisticated requirement in other to precise temperature control, high pressure etc. Besides all above methods Spray pyrolysis techniques simple, convenient and cheaper.

In this study, preparation techniques as well as the optical properties of $CuInS_2$ Films have been investigated by using different molarity solutions

MATERIALS AND METHODS

All reagents used are of analytical purity, $CuCl_2$. $2H_2O$, $InCl_3$ and $CS(NH_2)$ which are purchased from LOBA chemical, Nagpur. Chemical Spray Pyrolysis method was used for the preparation of $CuInS_2$ thin Films.

Experimental Procedure :

$CuInS_2$ Films have been produced by spraying the aqueous solution of 0.01 M, 0.025 M and 0.05 M of $CuCl_2$. $2H_2O$, $InCl_3$ and CS $(NH_2)_2$ in a 1:1:2 (by volume) on the glass substrate at substrate temperature 300^0C The substrate temperature was maintained to within $\pm 5^0$c. Deionised water was used for preparing the solutions.

Spray pyrolysis is basically a chemical process, that is the spraying of the solution onto a substrate held at high temperature, where the solution reacts forming the desired film [16-25] The Spray rate was measured by a flowmeter. The flow rate of the solution during spraying was adjusted to be about 2.5 $mlmin^{-1}$ and Kept constant through the experiment. The normalized distance between the spray nozzle and substrate is 29 Cm. The temperature of the substrate was controlled by an iron-Constantan thermocouple.

The thickness of the films was determined using the weighing method. Crystal structure was investigated by means of a X-ray diffraction (XRD) and scanning electron microscopy (SEM).

RESULTS AND DISCUSSION

3.1 Optical Properties

3.1.1 Transmittance Measurements :

The optical band gap of the has been determined from the transmittance (T) Vs. wavelength (λ) plot shown in fig. 2a,2b & 2c. The fundamental absorption which corresponds to electron excitation from the valence band to the conduction band, can be used to determine the nature and value of the optical band gap.

3.1.2 Absorption Coefficient :

The absorption coefficients α of the films have been calculated from the experimentally measured values of A and T according to the following relation.

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

Where R is the reflectance, T the transmittance, A the absorbance

And t the film thickness [26-29]

The optical absorption coefficient α is determined using the relation

$A = (2.303/t) [\log (1/T)]$ ------------ (2)

Where t is the thickness of the films and T is the transmittance [30-32] We have calculated the absorption coefficient for $CuInS_2$ Films having thickness values that varied between 0.4057 µm, 0.4968µm and 0.5032 µm. Absortption coefficient spectra verses the wavelength are presented in figure 4a, 4b & 4c.

3.1.3 Determination of the gap energy :

The optical band gap Eg, for the as deposited were calculated on the basis of the fundamental absorption using the well-known relation

$(\alpha h\upsilon)^{1/n}$ = constant $(h\upsilon-Eg)$----------(3)

Where hυ is the incident photon energy, α is absorption coefficient, and the exponent n depends on the type of transition. n=1/2, 2, 3/2, and 3 corresponding to allowed direct, allowed indirect, forbidden direct and forbidden indirect transitions respectively [33-34].

Optical absorption studies of the $CuInS_2$ films have been carried out in the wavelength range between 380-1000 nm and are shown in figures1a, 1b and 1c. The values of the energy band gap can be eastimated from the extrapolation to zero absorption in the $(\alpha h\upsilon)^2$ versus hυ plots which are shown. This compound is a direct band gap material with values of 1.65ev, 1.57 ev and 1.50 ev with thickness t = 0.4057µm, t=0.4968 µm and t=0.5032 µm. In the present study, the decrease of optical band gap could be attributed to the presence of unsaturated defects, which increase the density of localized states in the band gap and consequently decrease the optical energy gap. [31]

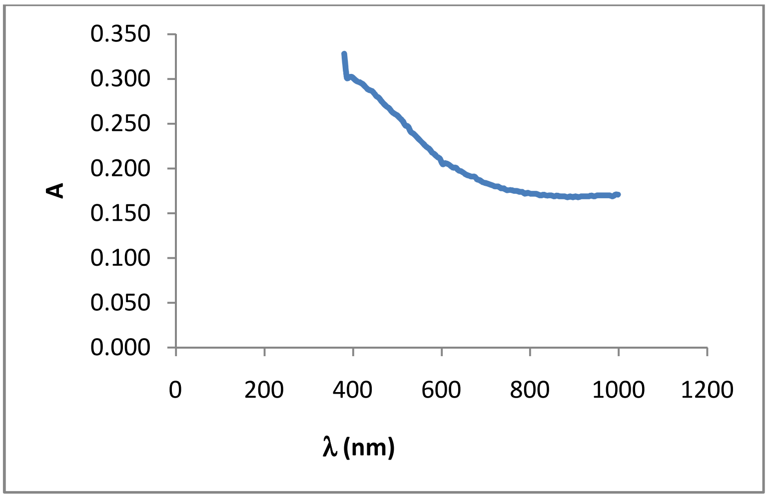

Fig. 1 (a) Absorption Spectra (A) of $CuInS_2$ Thin Film , t = 0.4057μm

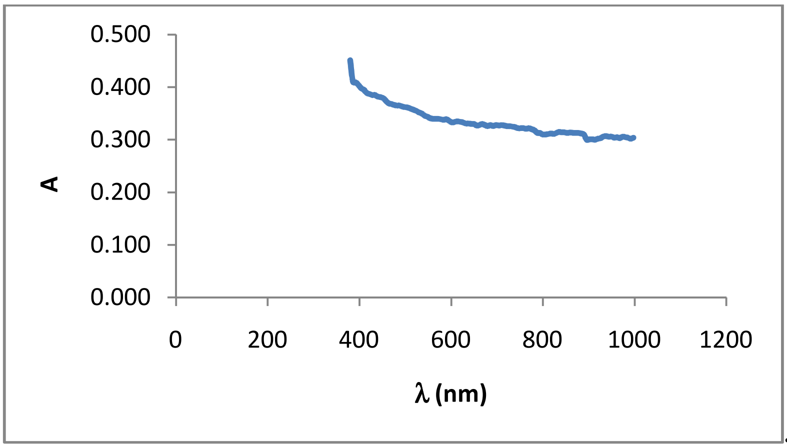

Fig. 1 (b) Absorption Spectra (A) of $CuInS_2$ Thin Film , t = 0.4968 μm

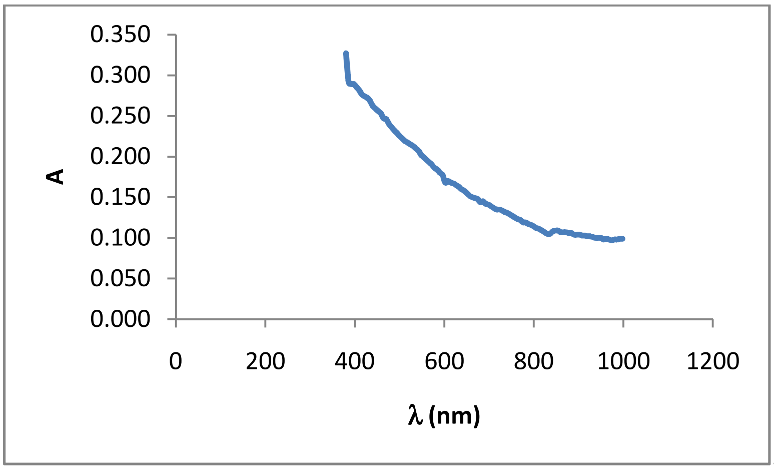

Fig. 1 (c) Absorption Spectra (A) of $CuInS_2$ Thin Film , t = 0.5032 μm

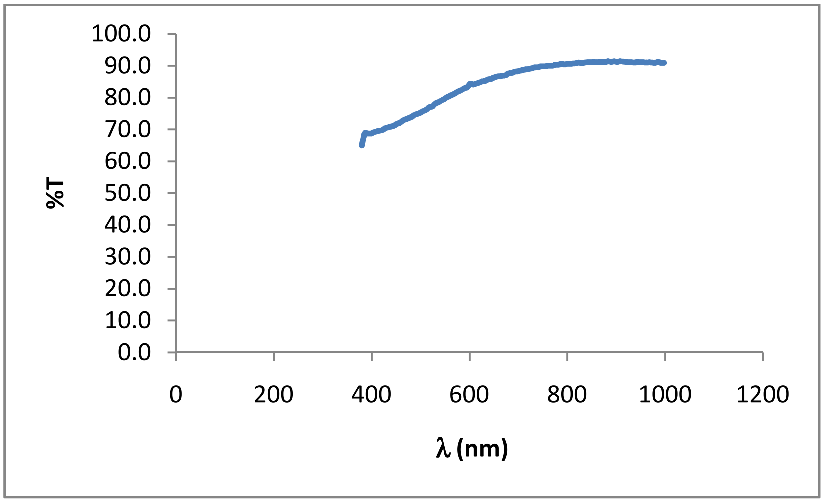

Fig. 2 (a) Optical transmission (%T) of CuInS2 Thin Film, t = 0.4057 µm

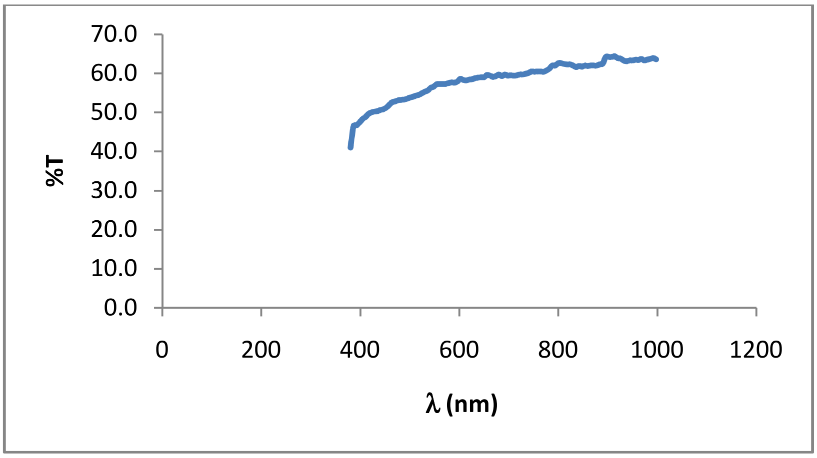

Fig. 2 (b) Optical transmission (%T) of CuInS2 Thin Film, t = 0.4968 µm

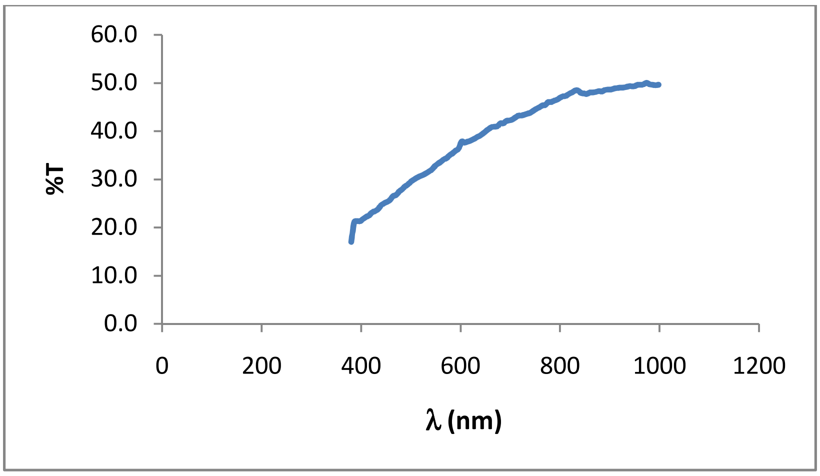

Fig. 2 (c) Optical transmission (%T) of CuInS2 Thin Film, t = 0.5032 µm

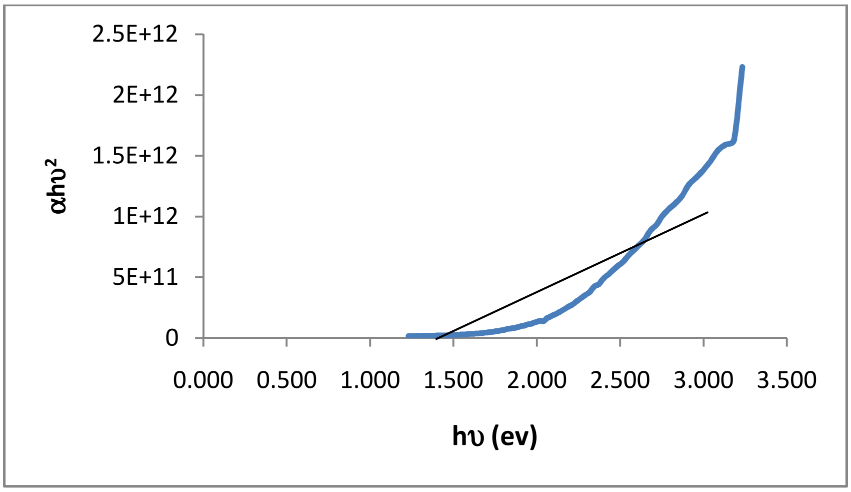

Fig 3 (a) Plot of (αhυ) ^{2} Vs Photon Energy (hυ), t = 0.4057 µm

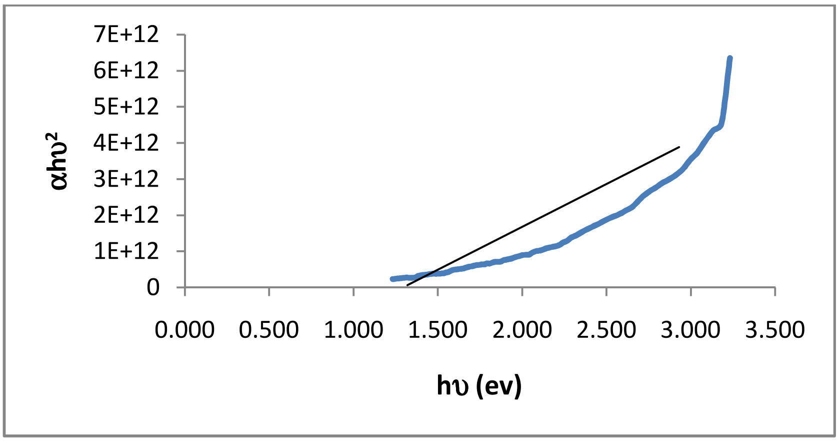

Fig 3 (b) Plot of (αhυ) ^{2} Vs Photon Energy (hυ), t = 0.4968 µm

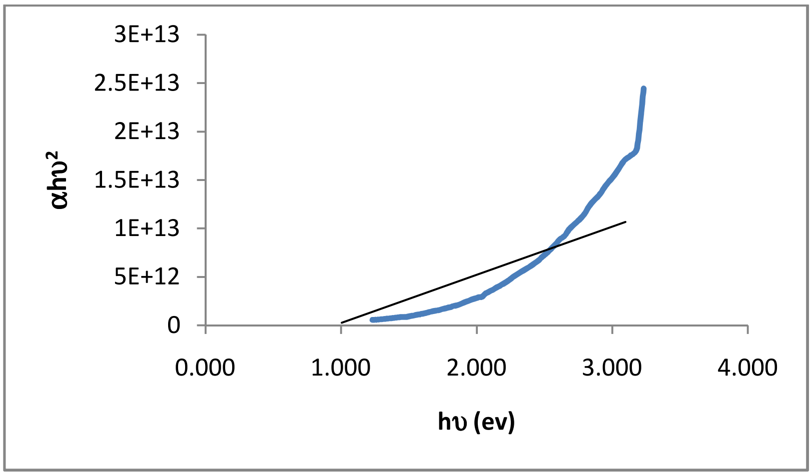

Fig 3 (c) Plot of (αhυ) ^{2} Vs Photon Energy (hυ), t = 0.5032 µm

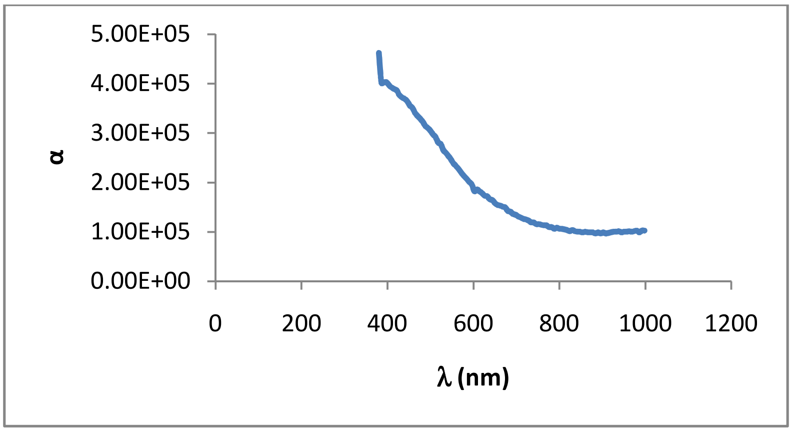

Fig 4 (a) Plot of Absorption (α) Vs Wavelength (λ), t = 0.4057 μm

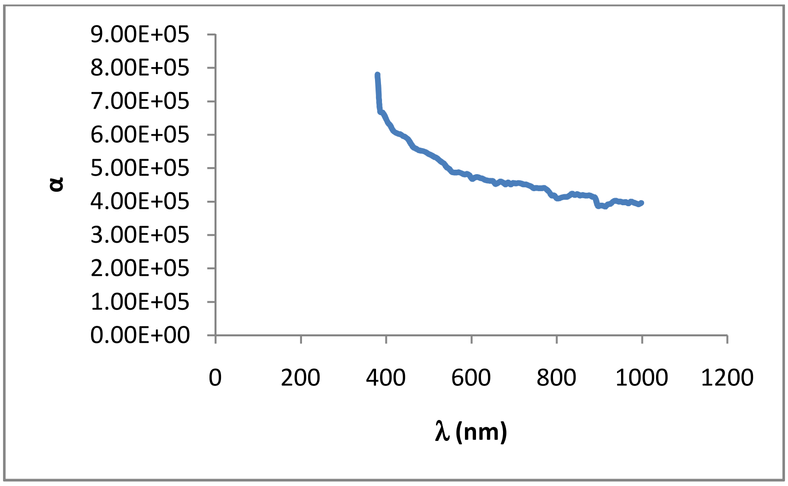

Fig 4 (b) Plot of Absorption (α) Vs Wavelength (λ), t = 0.4968 μm

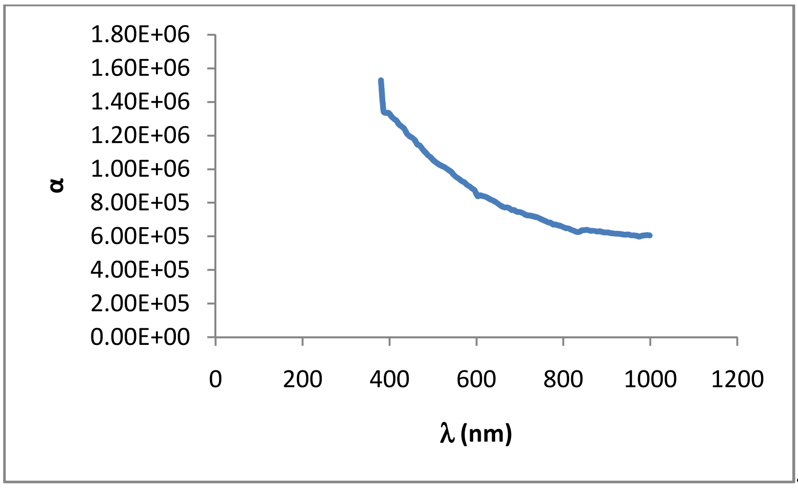

Fig 4 (c) Plot of Absorption (α) Vs Wavelength (λ), t = 0.5032 μm

Structural Properties

The XRD pattern of CuInS2 thin film was recorded with Philips X-ray Diffractometer.

X-ray diffraction of CuInS2 by spray pyrolysis method reveals that the film was polycrystalline in nature. X-rays reveals that the structure closely related to chalcopyrite structure [35]

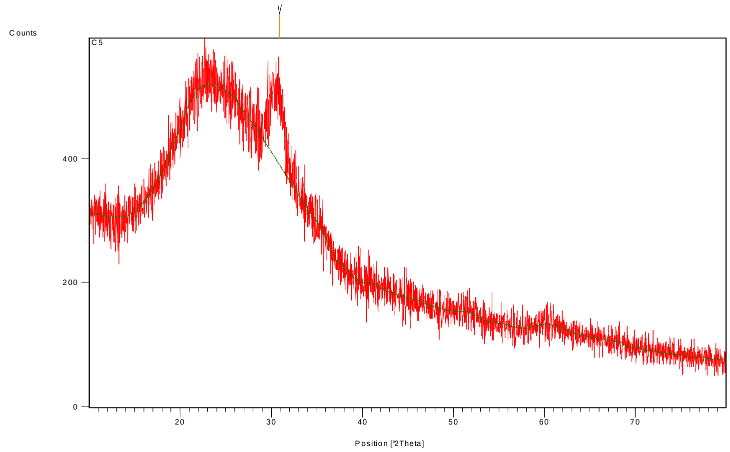

Fig 5 : The X-ray diffraction pattern of as-deposited $CuInS_2$ on glass substrate at 300^0C temperature.

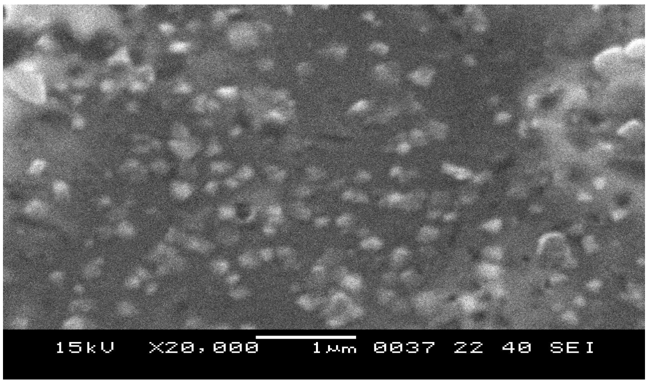

Fig. 6 : Scanning Electron Microscopy of as-deposited $CuInS_2$ on glass substrate at 300^0C temperature.

CONCLUSION

Films of $CuInS_2$ onto glass substrate with different molarity solutions, have been prepared using a spray pyrolysis method. The optical studies reveal that these films has a direct band gap and the band gap energy varies from 1.50 ev- 1.65 ev with different molarity solutions. It is observed that the band gap decreases with the increase of the molarity solutions. The determined optical parameters are in good agreement with previously reported results on similar films. In conclusion, spray Pyrolysis method for the production of thin solid films is a good method for the preparation of thin films suitable for scientific studies and for many applications in technology and industry.

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