Optical Properties And Electronic Transition Of Sno₂ Li Thin Films

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Abstract—In this paper , Undoped Tin Oxide and Lithium doped Tin Oxide with a percentage of doping (5%) to (0.05, 0.1 , 0.15, 0.2 ) M of the Concentration , and have been deposited on a glass substrate only at A substrate temperature of (400°C ) . The thickness of the deposited film Found to about (350 ± 15) nm . The optical properties SnO 2 has been studied transmittance and absorbance in the wave lengths rang (360 - 950)nm . The optical energy gap in the allowed direct transitions values for the undoped (SnO2) Films were (2.8, 2.7 , 2.6, 2) eV respectively, for each concentration (0.05, 0.1, 0.15, 0.1 )M respectively, at the rate of doping . When (SnO2) films are doped with lithium by (5%) , we note that the optical energy gap values for the allowed transmission decrease when the doping is increased (2.7, 2.4, 2.3, 2.2 ) eV respectively for each concentrations. The absorbance that decrease with the increase indoping for each concentration and the transmittance increased per concentration and (extinction coefficient , reflectiance , refractive index , real and imaginary By increasing in the doping per concentration .

Keywords—SnO₂ :Li , Optical properties , direct allowed transition , chemical Spray Pyrolysis ,

Introduction : 

In this work , method was used chemical Spray pyrolysis technique (CSP) ,this method is characterized by low cost and high- melting material, films can be prepared and well – homogenous films can be prepared in large area , this method is also suitable of films of oxides and sulfate materials[1] . The researcher (Manifacieret . al ) [2] studied thin (SnO₂) who prepared in two ways they the thermal Evaporation in vacuum and chemical Spray pyrolysis , he studied their optical and electrical properties ,where it was found that the method of thermal evaporation is the edge of absorption (2.4 eV) and the quality resistance (2×10⁵ Ω . cm ) , either in chemical Spray pyrolysis method the edge of the absorption (3.7 eV) and the quality (5×10⁵ Ω . cm ) , the reason for this difference is due to the process of crystallization of the prepared film , in the method of thermal evaporation the films were amorphous to crystallization ,in the chemical Spray pyrolysis method , the films were polycrystalline.Tin oxide (SnO₂) is a sensitive material for various gases , which has led to a lot of research in the field of gas sensors [3].It has recently been used in the design of ultraviolet (UV)and Laser diodes [4] .

Experimental Work :-

Lithium was doped by 5% and by concenteration (0.05, 0.1,0.15,0.2)M , thin (SnO₂) films are prepared using a chemical Spray pyrolysis device as Shown in figure (1) . By using Tin chloride (SnCl₂ . 2H₂O) and the concentrations (0.05, 0.1, 0.15 , 0.2) M were dissolved in (100ml) per
Figure (1) shows the chemical Spray pyrolysis unit

Percentage of doping (5%) distilled water by using mixer glass at normal atmospheric pressure, then the solution was sprayed with a fixed distance on the glass substrates of films was heated at a temperature of (400°C). Thickness of (350 ± 15) nm. The lithium was used as a doping agent with a volumetric concentrations of (0.05, 0.1, 0.15, 0.2) M. The thickness of the films of the equation:

\[ t = \frac{\Delta m}{\rho A S} \]  \hspace{1cm} (1)

the absorbance and the transmittance were recorded using a spectrophotometer type (shimadzu UV – 1650 PC) in the wavelength range (360 – 950) nm and all reading were recorded at room temperature.

Results and dissection :-

Figure (2-a,b) shows the relationship between absorbance and wavelengths(360 – 950) nm of the SnO₂ films, (a) undoped of the concentrations (0.05, 0.1, 0.15, 0.2) M , (b) doped with lithium by percentage (5%) and concentrations (0.05, 0.1, 0.15, 0.2) M . We observe a decrease in absorption by the increasing of wavelength, because the falling photon could not irate the electron and move it from the balance to the conductor beam and so on photon energy is less than the value of the forbidden gap [5], we also note that absorption at wavelength leads to an increase in the optical energy value when increasing doping concentrations.
Figure (2-a,b) absorbance as a function of wavelength for Tin oxide (SnO$_2$) films (a) undoped different concentrations (0.05, 0.1, 0.15, 0.2)M (b) Lithium and different concentrations with doping (5%).

Figure (3-a,b) represents the relationship between the transmittance and the wavelength of the tin oxide films (a) undoped (SnO$_2$), (b) doped of lithium (SnO$_2$:Li) with percentage of doping (5%) increased transmittance with increased wavelength. As well as increasing transmittance by increasing doping concentrations with lithium. This is due to the lower roughness of the surface that has been increased by doping concentrations (SnO$_2$:Li). The roughness of the surface reduces the dispersion of light and improves transmittance[6].
The absorption coefficient can be calculated in the absorption region of the relationship [6].

$$\alpha = \frac{2.303 \ A}{d} \quad (2)$$

d : the thickness of the films.
A : absorbance.

When the absorption coefficient value is ($\alpha > 10^4 \ cm^{-1}$) is the occurrence of the allowed direct transitions [7]. Figure (4 – a, b) shows the change in the absorption coefficient by photon energy for tin oxide, (a) undoped (b) doped with lithium for Concentrations (0.05, 0.1, 0.15, 0.2) M and by doped (5%). Not that the Coefficient absorption decreases with the increase of the oercentage of doped concentrations which are consistant (Bagheri) [8].
Figure (4 - a,b) shows absorption coefficient as a function of photon energy of Tin oxide films (a) undoped, (b) doped lithium and different concentrations (0.05, 0.1, 0.15, 0.2) M of the percentage of doping (5%).

The optical gap can be calculated ($E_g^{opt}$) for direct allowed transition according to this relationship [9].

\[ \alpha(hv) = p (hv - E_g^{opt})^r \]

where:
- $\alpha$: constant depends on the type of material.
- $E_g^{opt}$: optical energy gap.
- $r$: 1/2 value.

Figure (5 – a,b) represents the relationship between photon energy and the $(\alpha hv)^2$ of Tin oxide for as deposited. Thin films of concentrations (0.05, 0.1, 0.15, 0.2) M. The optical energy gap was decreasing up on Doping ratio. The reason for this is the formation of local levels in the conduction bond there leading to decrease the optical energy gap($E_g^{opt}$).
Figure (5-a,b) optical energy gap for direct transmission allowed Tin oxide films is (a) undoped and (b) doped lithium and different concentrations (0.05, 0.1, 0.15, 0.2)M of the percentage of doping (5%)
**Table (1) Optical energy gap for direct transitions allowed values for Tin oxide films undoped and doped lithium for the concentrations (0.05, 0.1, 0.15, 0.2 ) M Of percentage of doping (5%) .**

<table>
<thead>
<tr>
<th>sample</th>
<th>Optical energy gap values ($E_{g}^{opt}$) for direct transmission allowed (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(SnO$_2$) (0.05) M</td>
<td>2.8</td>
</tr>
<tr>
<td>(SnO$_2$) (0.1) M</td>
<td>2.7</td>
</tr>
<tr>
<td>(SnO$_2$) (0.15) M</td>
<td>2.6</td>
</tr>
<tr>
<td>(SnO$_2$) (0.2) M</td>
<td>2</td>
</tr>
<tr>
<td>(SnO$_2$: Li) (0.05) M</td>
<td>2.7</td>
</tr>
<tr>
<td>(SnO$_2$: Li) (0.1) M</td>
<td>2.4</td>
</tr>
<tr>
<td>(SnO$_2$: Li) (0.15) M</td>
<td>2.35</td>
</tr>
<tr>
<td>(SnO$_2$: Li) (0.2) M</td>
<td>2.2</td>
</tr>
</tbody>
</table>

Figure (6- a,b) represents the relationship between the wavelength and the reflectance of the undoped and lithium doped Tin oxide for different concentrations (0.05, 0.1, 0.15, 0.2 )M for the percentage of doping (5%). We can note that the reflectance decrease with increase in wavelength. The reflectance of the doping thin films were decreased for increasing doping concentrations.

![Figure 6a](image1.png)  
**Figure 6a:** Reflectance as a function of wavelength for tin oxide films (a) undoped , (b) doped lithium and different concentrations (0.05, 0.1, 0.15, 0.2) M of the percentage of doping (5%).
The Refractive index ($n_0$) calculation through the following relationship[11].

$$n_0 = \left[\left(\frac{1+R}{1-R}\right) - (K_0^2 + 1)\right]^{\frac{1}{2}} + \frac{1+R}{1-R} \quad \text{--------- (4)}$$

Figure (7-a,b) represents the relationship between the wavelength and the Refractive index of the (a) undoped, (b) Lithium doped Tin oxide different concentrations (0.05, 0.1, 0.15, 0.2) M of the percentage of doping (5%). We can notice that the refractive index decrease with the increase in wavelength. The refractive index of the thin films will decrease when the concentrations ratios increase as a result of the change of crystalline surfaces. We also note that the refractive index diagram is similar to the reflective diagram.

Figure (7-a,b) shows Refractive index as a function of photon energy of Tin oxide films (a) undoped, (b) doped lithium and different concentrations (0.05, 0.1, 0.15, 0.2) M of the percentage of doping (5%).

Extinction coefficient ($k_0$) calculation through the following relationship [12]:

$$k_0 = \frac{a\lambda}{4\pi} \quad \text{------------------ (5)}$$
Figure (8- a,b) represents the relationship between the photon energy and The Extinction coefficient of the, (a) undoped, (b) Lithium doped Tin oxide for different concentrations (0.05, 0.1, 0.15, 0.2) M of the percentage of doping (5%), we can notice that the Extinction coefficient Decrease with the increase in photon energy for the undoped of the concentrations (0.05, 0.1, 0.15, 0.2) M and lithium doped for the concentrations

![Graph](image)

(a)

![Graph](image)

(b)

Figure (8 - a,b) shows Extinction coefficient as a function of photon energy of Tin oxide films (a) undoped, (b) doped lithium and different concentrations (0.05, 0.1, 0.15, 0.2) M of the percentage of doping (5%).

Real dielectric constant ($\varepsilon_1$) and imaginary dielectric ($\varepsilon_2$) can be calculated using the following relationships:

$$\varepsilon_1 = n^2 - k^2$$  \hspace{1cm} (6)

$$\varepsilon_2 = 2n k$$  \hspace{1cm} (7)

Figure (9- a,b) represents the relationship between the real ($\varepsilon_1$) part of Dielectric constant and the photon energy of the (a) undoped, (b) Lithium doped Tin oxide for different concentrations (0.05, 0.1, 0.15, 0.2) M of the percentage of doping (5%). The real dielectric constant can be
Notice with the refractive index because the real part depend on refractive index according to the equation (6). We can notice that the real part decrease with the increase in photon energy for the undoped same the real part of the doping thin films were decreased as the doping concentrations.

![Graph](image)

Figure (9 - a,b) shows Real dielectric constant as a function of photon energy of Tin oxide films (a) undoped, (b) doped lithium and different concentrations (0.05, 0.1, 0.15, 0.2) M of the percentage of doping (5%).

Figure (10- a,b) represents the relationship between the imaginary (ε₂) part of Dielectric constant and the photon energy of the (a) undoped, (b) Lithium doped Tin oxide for different concentrations (0.05, 0.1, 0.15,0.2) M of the percentage of doping (5%). The imaginary dielectric constant can be Notice with the refractive index because the real part depend on
Figure (9 - a,b) shows Imaginary dielectric constant as a function of photon energy of Tin oxide films (a) undoped , (b) doped lithium and different concentrations (0.05, 0.1, 0.15, 0.2 ) M of the percentage of doping (5%).

**Conclusion:**
Absorbance , optical energy gap , absorption coefficient, refractive Index , real dielectric constant and imaginary dielectric constant are Decreased , but also value of the transmittance was increased with doping concentrations of thin films prepared . The type of transition observed was direct allowed transition in this work.
References