Structural and Optical Constants of Fe-doped SnO$_2$ Thin Film

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**Abstract:**

Tin oxide and Fe-doped tin oxide have been prepared using chemical spray pyrolysis. XRD analysis reveals that all the films are polycrystalline with tetragonal structure. The average grain size is found to decrease from 51Å to 40Å due to Fe-doping. Absorbance and transmittance are recorded in order to calculate kind of transition and optical constants. It is found that optical energy gap decrease after doping and all the optical constants are affected by Fe-doping.

المقدمة:

حضرت أغشية ثنائي أوكسيد القصدير وأغشية ثنائي أوكسيد القصدير المشوية بالحديد باستخدام الترسيب الكيميائي الحراري. بنتجت نتائج حيود الأشعة السينية بأن كافة الأغشية من ذات طبعة متعددة البلور ورباعية التركيب. لقد وجد بعد القدر الحجم الجيبي قد انخفض من 51Å إلى 40Å نتيجة التشويب بالحديد. سجل طيفي الامتصاصية والفاندانا نعوض معرفة نوع الانقلال وحساب الثوابت البصرية. لقد وجد بأن فجوة الطاقة البصرية تقل بعد التشويب بالحديد وأن طاقة الثوابت البصرية قد تأثرت نتيجة التشويب.
Introduction:

Tin oxide which is considered as transparent conducting oxide, is of considerable interest due to its unique properties such as, wide band energy gap, high donor concentration, large mobility, high transparency in the visible part of spectrum, superior chemical stability, mechanically strong, in expensive, non-stoichiometric semiconductor and behaves more or less as a degenerate n-type with low n-type resistivity \[1-6\]. Tin oxide may be used as electrode material in several processes of technological interest like, liquid crystal display, solar cells, electro chromic devices, gas sensors, chemical sensors and antireflection coatings \[7-10\]. Several methods have been adopted to prepare un-doped and doped SnO\(_2\) including, electron beam evaporation, r.f. spattering, filtered vacuum arc, pulsed laser deposition and spray pyrolysis technique \[11-15\]. In this work we study the effect of (Fe) on the structural and optical properties of SnO\(_2\).

Experimental:

Tin oxide and Fe (volume concentration 2 and 4%) Tin oxide has been prepared on a glass substrates using chemical spray pyrolysis. 0.1M of SnCl\(_4\).5H\(_2\)O and FeCl\(_3\).2H\(_2\)O with deionised water to prepare the required solution. For un-doped SnO\(_2\) and Fe doped SnO\(_2\) the preparation conditions are: the distance between the spray nozzle and substrates 30cm, the spray rate 5ml/min, the glass substrate temperature was maintained at 500°C during the hole spraying process using chromel-Alumel thermocouple which is used to measure the temperatures of the hot-plate. After the completion of spraying process the sample is rapidly let to cool down to room temperature. The films are highly reproducible which is confirmed from the repeated experiments of each concentration. The thickness of the film is obtained by weighing method and it is found to be 300±30nm. The x-ray diffraction studies are carried out using x-ray diffractometer type shimadzu, power diffraction system with CuK\(_{\alpha}\) radiation with a wavelength of 1.54Å. The scanning range of 2\(\Theta\) is restricted to the range 10-60°. Optical absorbance and transmittance are obtained by double beam spectrophotometer (shimadzu uv-1650pc) in the wavelength range of (300-900nm).

Results and Discussion:

Fig.(1) shows XRD patterns of the (as) deposited and Fe-doped SnO\(_2\). It is quite clear from the figure that the diffraction peaks appear, exhibiting polycrystalline with tetragonal structures, the diffraction peaks oriented along the (110), (101), (200), (211) at 26.74°, 34.03°, 38.01° and 51.92° respectively. The XRD measurements do not reveal the existence of Fe\(_2\)O\(_3\) phase, indicating that
Fe is cooperated into the tin oxide lattice. The average grain size of undoped and Fe-doped thin films are estimated for the (110) plane using Scherrer’s formula$^{[6]}$: 

Fig(1): XRD spectra of the samples under investigation
\[ D = \frac{0.9 \lambda}{B \cos \theta} \]  \hspace{1cm} (1)

Where \( D \) is the average grain size, \( \lambda \) is the x-ray wavelength; \( B \) is the Full Width at Half Maximum (FWHM) of XRD peaks and \( \theta \) is the Bragg angle. The average grain size at crystalline orientation of (110) for the as deposited and Fe-doped SnO\(_2\) is 51A\(^\circ\), 46A\(^\circ\), and 40A\(^\circ\) respectively. The addition of Fe\(^{3+}\) significantly influenced the crystallinity of SnO\(_2\), suggesting a decrease of crystallinity in the Fe-doped SnO\(_2\) Thin films in comparison with un-doped SnO\(_2\). This could be clearly seen in fig.(1) by the decrease in the intensity and increase FWHM of the planes.

The absorption coefficient (\( \alpha \)) and incident photon energy (\( h\nu \)) is related by the following equation \([17]\)

\[(\alpha h\nu)^2 = A (h\nu - E_g) \]  \hspace{1cm} (2)

Where \( A \) constant, \( E_g \) optical energy gap. The \( E_g \) can be determined by extrapolations of the linear portion of the curve to the \( h\nu \) axis. Figs (2-4) show the curve of \((\alpha h\nu)^2 \) versus \((h\nu)\) for undoped and Fe-doped SnO\(_2\) respectively.

**Fig(2)** \((\alpha h\nu)^2 \) versus photon energy for undoped SnO\(_2\)
Fig(3) \((\alpha h \nu)^2\) versus photon energy for SnO\(_2\) doped 2\% Fe

Fig(4) \((\alpha h \nu)^2\) versus photon energy for SnO\(_2\) doped 4(\%) Fe
Optical energy gap for un-doped SnO$_2$ is 3.7eV while for 2% and 4% Fe-doped are 3.65eV and 3.54eV respectively, this decrement might be due to appearance of the Fe-Sn metallic compound which results to reduce the degree of crystallinity. The transmittance in the wavelength (300-900nm) of undoped and Fe-doped SnO$_2$ are shown in fig.(5), the transmittance are found to decrease as the doping percentage increases whereas, the average transmittance decreases from >80% at 550nm to ~60% for 4% Fe-doped SnO$_2$ for the same wavelength, which is related to reduction of crystalline size and escalation of light scattering.

Fig(5) The transmittance for the undoped SnO$_2$ and Fe doped SnO$_2$

The refractive of the films under investigation is determined by using the following relation\(^{[18]}\)

\[
n_o = \left[\frac{1+R}{1-R}\right] + \sqrt{\frac{4R}{(1-R)^2} - K_o^2} \quad \text{(3)}
\]

Where R is the reflectance, $K_o(K_o = \alpha \lambda / 4\pi)$ is the extinction coefficient. The $n_o$ and $K_o$ values dependence of photon energy are shown in figs (6) and (7) As seen in the figures, the $n$ and $K$ values increase with increasing doping ratio it has been well
established that the refractive index is closely correlated with film density, a higher refractive index implies a denser film, the increase in refractive index is attributed to the decreasing in the value of grain size with the Fe-doping concentration.

Fig(6) The refractive index for the undoped SnO$_2$ and Fe doped SnO$_2$

Fig(7) The extinction coefficient for the undoped SnO$_2$ and Fe doped SnO$_2$
These results agree with XRD result. The real $\varepsilon_1$ and imaginary part $\varepsilon_2$ of the dielectric constants ($\varepsilon = \varepsilon_1 + i\varepsilon_2$) may be related to the real part of refractive index and the extinction coefficient $^{[19]}$

\begin{align*}
\varepsilon_1 &= n_o^2 - K_o^2 \quad \ldots (4) \\
\varepsilon_2 &= 2n_oK_o \quad \ldots \ldots (5)
\end{align*}

Fig. (8) and fig.(9) show $\varepsilon_1$ and $\varepsilon_2$ values dependence of photon energy for all the samples under investigation. The values of the real part are higher than the imaginary part, it can be seen that the real and imaginary parts of the dielectric constant increase with Fe-doped. The real part $\varepsilon_1$ is associated with the term that how much it will slow down the speed of light in the material and the imaginary part $\varepsilon_2$ gives that how a dielectric absorb energy from electric field due to dipole motion.

Fig.(10) shows the variation of optical conductivity with the incident photon energy. The optical conductivity is determined using the relation $^{[20]}$

![Fig(8) Real part of dielectric constant for the undoped SnO$_2$ and Fe doped SnO$_2$](image)

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Fig(9) Imaginary part of dielectric constant for the undoped SnO$_2$ and Fe doped SnO$_2$

Fig(10) Optical conductivity for the undoped SnO$_2$ and Fe doped SnO$_2$
where $c$ is the velocity of light. The optical conductivity directly depends on the absorption coefficient and found to increase sharply for higher values due to large absorption coefficient of these values. We can also notice that $\sigma$ increase for Fe-doped SnO$_2$.

**Conclusion:**

The effect of Fe-doping on SnO$_2$ has been investigated. XRD analysis shows that all the samples are polycrystalline and Fe-doping affected the crystallinity disorder by increasing it. The result show that Fe decrease the optical energy gap and increase the refractive index, Extinction coefficient, real and imaginary parts of dielectric constant and optical conductivity .From these result one can conclude that Fe-doped SnO$_2$ can be used as semiconductor, in electronic devices applications.

**References:**


