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 اغشية ثنائي اوكسيد القصدير واغشية ثنائي اوكسيد القصدير المشوبة بالحديد باستخدام الترسيب كيميائي الحراري. بينت نتائج حيود الاشعة السينية أن كافة الاغشية كافة من ذات طبيعة متعددة البلور ورباعية التركيب. وقد وجد أن معدل الحجم الجيبي قد انخفض من 51Å الى 40Å نتيجة التشويب بالحديد.

سجل طيفي الامتصاصية والنفاذية من معرفةأجل نوع الانتقال وحساب الثوابت البصرية. أذ وجد أن فجوة الطاقة البصرية تقل بعد التشويب بالحديد وان طاقة الثوابت البصرية قد تاثرت نتيجة التشويب.

Introduction:

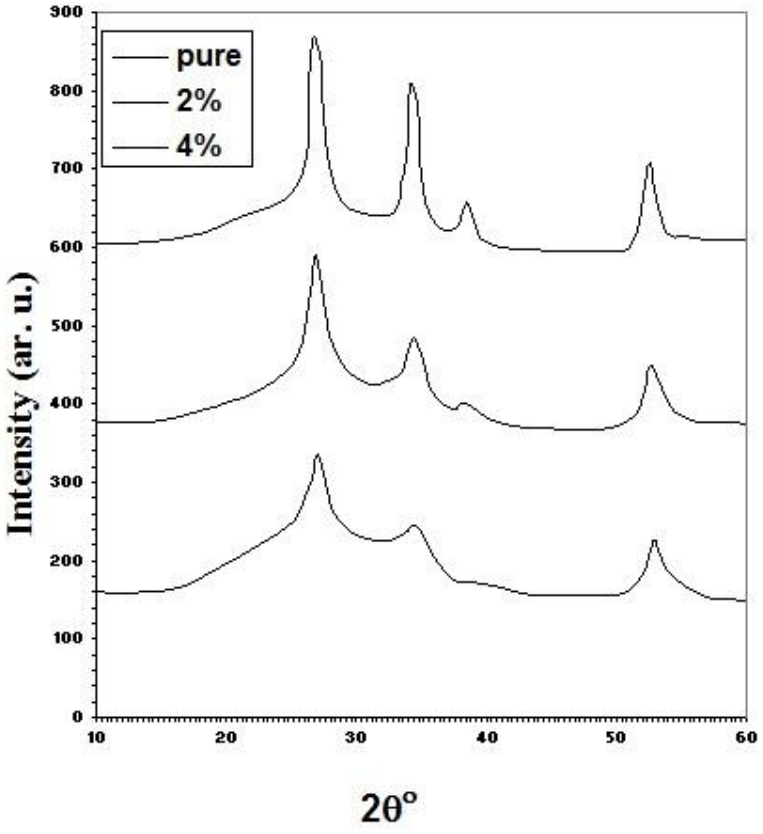
Tin oxide which is considered as transparent conducting oxide, is of considerable interest due to its unique properties such as, wide band energy gap, high donor concentration, large mobility, high transparency in the visible part of spectrum, superior chemical stability, mechanically strong, in expensive, 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 $SnCl_4.5H_2O$ and $FeCl_3 .2H_2O$ 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^oC 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_α radiation with a wavelength of 1.54Å. The scanning range of 2Θ is restricted to the range $10\text{-}60^o$ .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^o, 34.03^o, 38.01^o and 51.92^o respectively. The XRD measurements do not reveal the existence of Fe_2O_3 phase, indicating that



Fig(1): XRD spectra of the samples under investigation

Fe is cooperated into the tin oxide lattice. The average grain size of un-doped and Fe-doped thin films are estimated for the (110) plane using Scherrer's formula[6]:

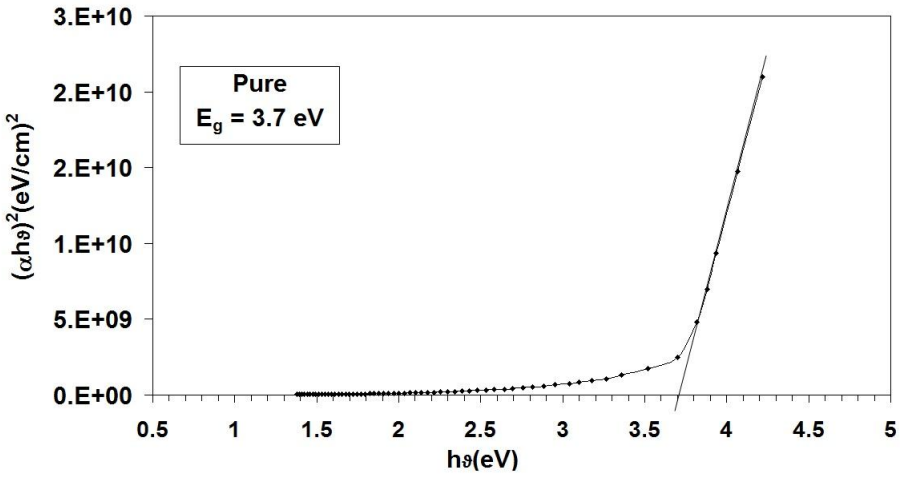
$$D = \frac{0.9\lambda}{B\cos\theta} \quad \text{.....} \quad (1)$$

Where *D* is the average grain size, λ is the x-ray wavelength; *B* is the Full Width at Half Maximum (FWHM) of XRD peaks and θ is the Bragg angle. The average grain size at crystalline orientation of (110) for the as deposited and Fe-doped SnO_2 is $51A^o$, $46A^o$, and $40A^o$ 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.

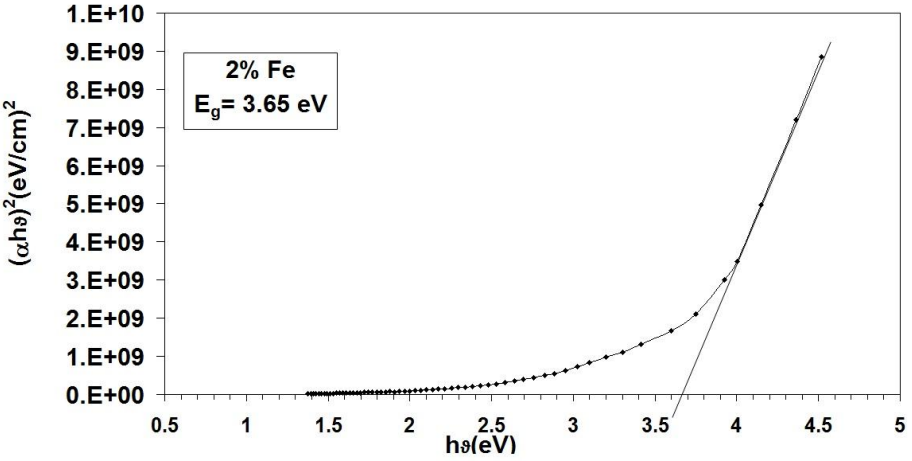
The absorption coefficient (α) and incident photon energy (hυ) is related by the following equation [17]

$$(\alpha h\upsilon)^2 = A\,(h\upsilon - E_g) \text{ ..... } (2)$$

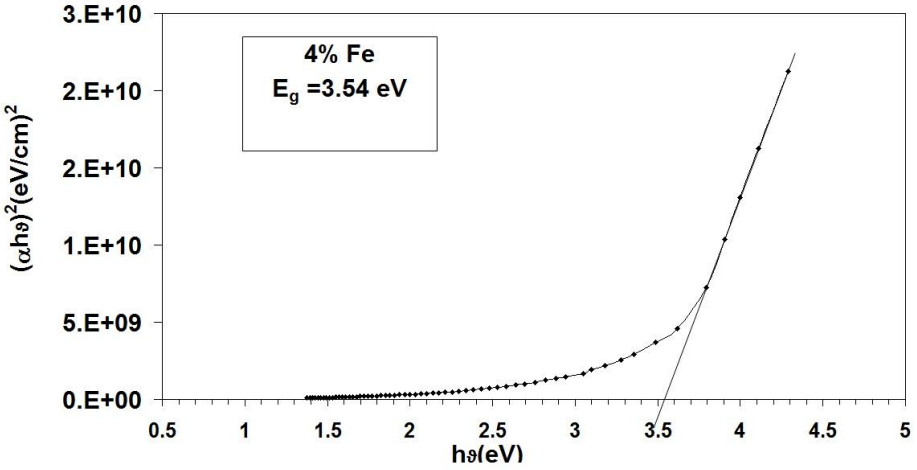
Where *A* constant, E_g optical energy gap. The E_g can be determined by extrapolations of the linear portion of the curve to the $h\upsilon$ axis. Figs (2-4) show the curve of $(\alpha h\upsilon)^2$ versus $(h\upsilon)$ for undoped and Fe-doped SnO_2 respectively.



Fig(2) $(\alpha\ h\ \upsilon)^2$ **versus photon energy for undoped** SnO_2



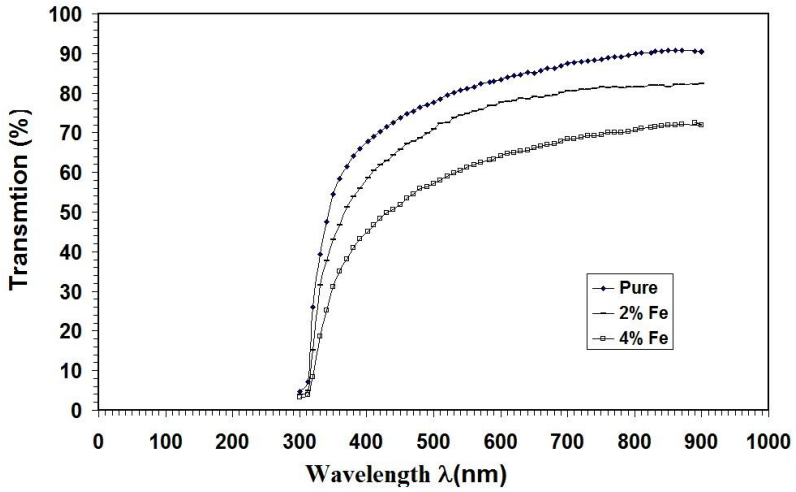
Fig(3) $(\alpha\ h\ \upsilon)^2$ **versus photon energy for SnO_2 doped 2% Fe**



Fig(4) $(\alpha\ h\ \upsilon)^2$ **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.

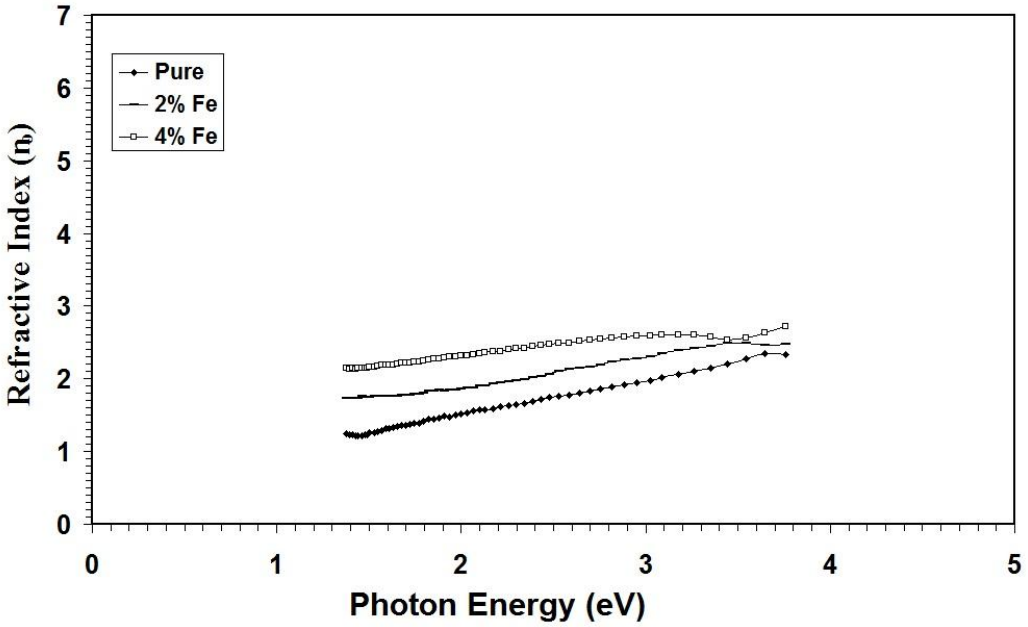


Fig(5) The transmittance for the undoped SnO_2 and Fe doped SnO_2

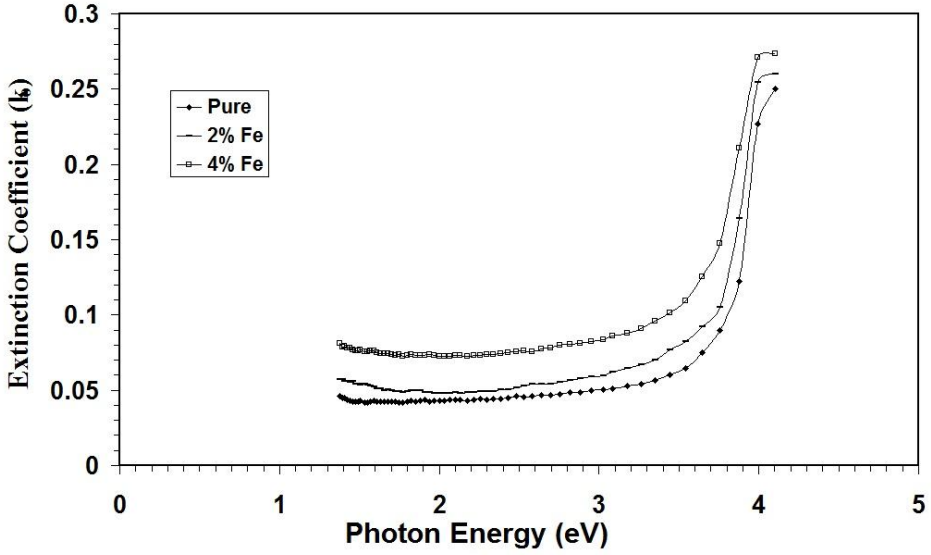
The refractive of the films under investigation is determined by using the following relation[18]:

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

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



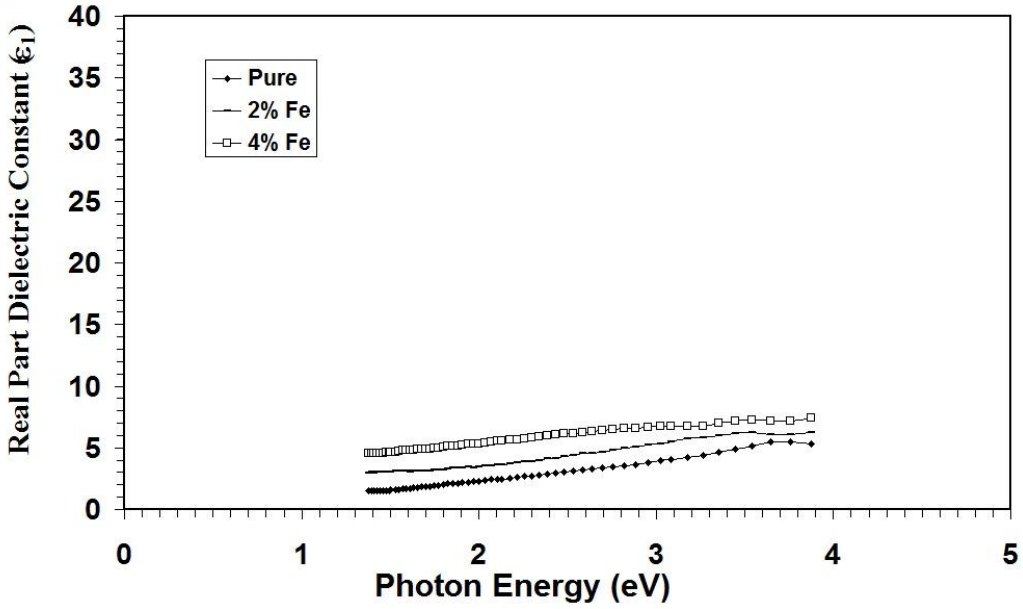
Fig(7) The extinction coefficient for the undoped SnO_2 and Fe doped SnO_2

These results agree with XRD result. The real ε_1 and imaginary part ε_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]

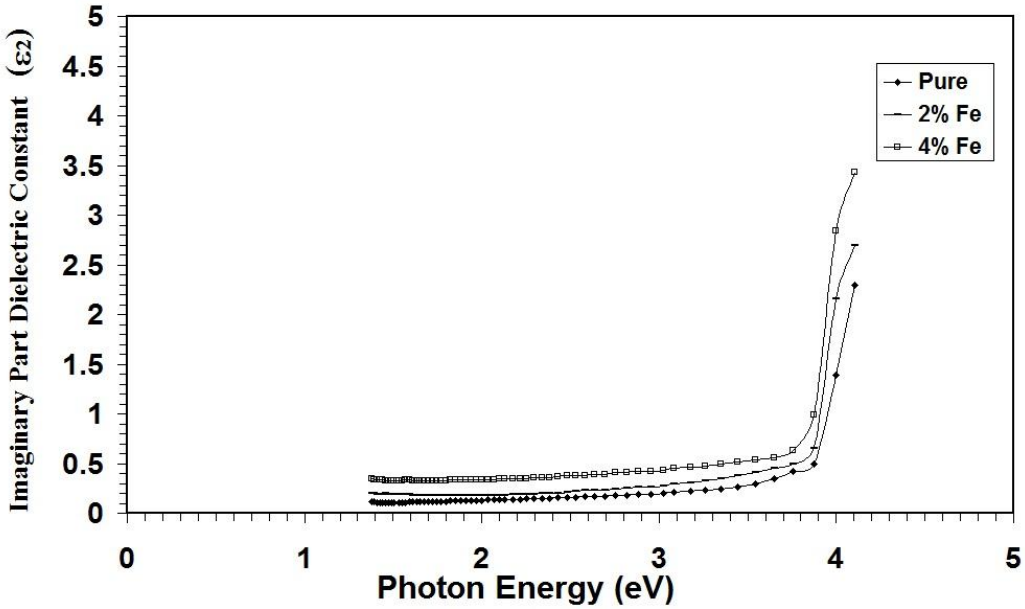
$$\varepsilon_1 = n_o^2 - K_o^2 \quad \text{..... (4)}$$
$$\varepsilon_2 = 2n_o K_o \quad \text{..... (5)}$$

Fig. (8) and fig.(9) show ε_1 and ε_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 ε_1 is associated with the term that how much it will slow down the speed of light in the material and the imaginary part ε_2 gives that how a dielectric absorb energy from electric field due to dipole motion.

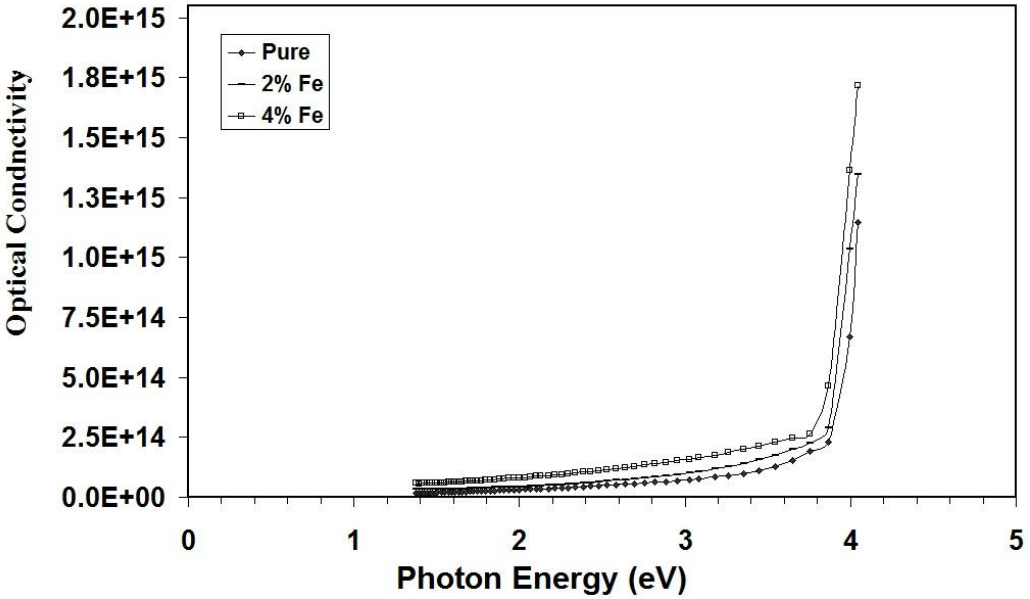
Fig.(10) shows the variation of optical conductivity with the incident photon energy. The optical conductivity is determined using the relation[20]



Fig(8) Real part of dielectric constant for the undoped SnO_2 and Fe doped SnO_2



Fig(9) Imaginary part of dielectric constant 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 σ 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.

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