Structural and Optical properties of Polymers(PVA / PVP) doped with V_2O_5 composites films

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Abstract

Study the effect of doping V_2O_5 on polymers poly vinyl alcohol (PVA), poly vinyl pyrrolidone (PVP) on the optical and structural properties for film prepared by using Casting method at thickness(300±20)nm ,All the materials dissolved in distilled water by magnetic mixer for one hour .The optical parameters measured by using UV-VIS spectrometer ,and the structural parameters measured by X-ray diffraction .when measured the energy gap found that the value was decreases from 4.6 eV to 2.98 eV with doping .The refractive index ,extinction coefficient ,absorption coefficient ,real and imaginary dielectric constants of (PVA/PVP) are increasing with doping by V_2O_5 and with increase the ratio of doping .

Key words: PVA , PVP, doping ,structural and optical properties,V_2O_5

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Introduction

Composites of Polymer have been become on .account of simple process ability ,relatively in expensive ,very pest quality surface and simple fabrication of thin and thick samples [1,2].There are several factors which affect polymer properties such as optical ,structural ,electrical and doping ,It is possible to control the type of polymer through control of concentration ,interplay with the polymer chains doping [3].Interest in the study of electronic transitions of polymers gives a clear idea about the optical properties and that knowledge useful in many applications including protective coatings ,optical filter, Semiconductor and a cover Solar collection [2,4].

Poly (vinyl pyrrolidone)(PVP) and poly (vinyl alcohol)(PVA) are possess distinctive qualities from arrange of polymers are the possessing high polar ,simple processability and friends of environment ,And also characterized Superb thermo stability ,good electrical properties ,a loft mechanical strength and water Solubility [6,7].

From previes studies ,which focused on composites PVA/PVP doping are [8]."that they concluded for their studies polymer PVA and PVP thin films deposited onto SAW substrates by using spin coating .all samles show high sensitivity to relative humidity with range (5-95)%RH.and the other result that the better parameters of the PVP-senser" ."The Shen Hong ,C.Bolin et al [9] studied colloidal Au with PVP composite films prepared by spin-coating method ,then found that large optical nonlinearities of Au/PVA films".Poly (vinyl pyrrolidone)PVP andPoly(vinyl alcohol)PVA,are in the list of synthetic polymers which are used in medicine.[4].Vanadium Pentoxide is used in many applications such as gas sensing agent , a window for solar cells and the important application of V_2O_5 is the positive material of lithium ion batteries..[5]

The aim of the work preparation of (PVA-PVP-V_2O_5) films and study their structural and optical properties.

Method and Materials

In this research ,putting 4gm of PVA with (w_t =30000 gm/mol) and 4gm of PVP with (w_t=70000gm/mol) dissolved in 100mil distilled water by magnetic mixer for one hour ,NH_4NO_3 dissolved in distilled water at concentration 2% and 6% by magnetic mixer for one hour .Two dropes of each solution is put in glass petri deshes at dimeter (4cm) and left to dry in the room temperature for 72 hour ,the samples thickness were (300) nm ,which was measured by weighting method depending on the equation[6].

$th = \Delta m/\rho\, a$ ………………… (1)

when th:is thickness ,Δm : the different between weight substrate before and after the film deposition , ρ: the density, a:is the area of the film . The transmission measured by (UV-visible spectroscopic effect) As well as sampling X-ray diffraction by shemadzu XRD –diffractometer . The structural parameters was calculated such as :

the Grain Size [10]. By Scherrers equation can be calculated

$G.S = M\,\lambda/\beta \cos\theta$ …………………………….. (2)

Where M is constant equal to (0.94), λ is the wavelength of X-ray (1.5406A°) , β is the full width at half maximum (FWHM) and θ is the Braggs angle .

Using The dislocation density (η) also calculated by " Williamson and Smallmans equation [11]".

$\eta = 1/(G.S)^2$ …………………………. (3)

Also the number of crystals ($N_\circ$) calculated by using the equation .[12].

$N_\circ = th/(G.S)^3$ …………………….. (4)

At the end of structural parameters the strain (S) calculated by the formula . [13]

$S = \beta \cos\theta/4$ ………………………. (5)

All these parameters put in the table (1) The value of the number of crystals and dislocation density and the strain was increase at doping ratio 6% .
The energy band gap (Eg) could be calculated by equation . [14] and show in shape (4) .
$\alpha h\nu = L(E-Eg)^J$………………………….. (6)
where α is the absorption coefficient , ν is the incident photon frequency, L is constant and h is planck constant ,if J equal (1/2) the allowed direct transition ,but if equal to (2) the allowed in direct transition , the value of Eg recorded in table (2)
The energy E can be calculated by the relation . [15]
$E = h\nu = 1240/\lambda$" …………………….. (7)"
The reflectance R also calculated by the formula . [16]
R=1-(A+T)" ………………………………… (8)"
The extinction coefficient ($K_\circ$) can be calculated by the equation .[17] and show in shape (5).
$K_\circ = \alpha\lambda / 4\pi$ ….. (9)
After calculated R and $K_\circ$ can be easly to calculated refractive index by the relation [18].and draw in fig (6) .
$n = \frac{1+R}{1-R} + \left(\frac{4R}{(1-R^2)} - K_\circ^2\right)^{1/2}$ (10)
The dielectric constant into two types ; real (ε_r)and imaginary (ε_i) can also evaluated by the relation [19].and show in figure (7,8) .
" $\varepsilon_r = n^2 - k_\circ^2$ " ………………………………. (11)
" $\varepsilon_i = 2nk_\circ$ " ……… (12)
The optical conductivity as a function of photon energy can be also calculated by the relation [20].and show in shape (9).
$\delta = \frac{\alpha n c}{4\pi}$ …………………………. (13)
Where c: the velocity of light .
By using the relation no. (13) can be found the absorption coefficient [21].and show in figure (10).
$\alpha = 2.303(A/th)$ ………………………….. (14)

Discussion of Results

Figure (1) show the XRD for PVA , PVP , PVA:PVP:V_2O_5(2%) and PVA:PVP:V_2O_5 (6%) . we found that the samples of V_2O_5 is orthorhombic structure , then the peaks of [600] plane at 37.8° ,[002] plane at39.08° and[020] at 37°.

The optical parameters was studied like the spectra of absorption A% and transmission as shown in shape (2-3) we note the absorption spectra of the samples as a function of wave length decrease with increasing of doping ratio. This behavior due to absorbs the incident light depit the V_2O_5 particles ,opposite the transmission which is increases with increase the doping ratio from 2% to 6% then is very high equal to≅ (95%) from these samples that is good to use in solar cell and other applications.

The optical band gap (Eg) which is clear in shape (4) decreases with doping in V_2O_5 and with increasing the ratio of doping ,this decrease of band gap due to the decrease in crystal size of original solution ,(Hussein 2015).

The observe increment of extinction coefficient in figure (5) at high wave length with doping and increasing of doping ratio of V_2O_5 due to more scattering of photons (Tintu 2010) [3] .

In the shape (7,8) we observed that ε_r behaves just like refraction index and extinction coefficient because they joined with it in relations .the real part of dielectric constant as a function of photon energy is increase at doping with V_2O_5 because increase the absorption of incident light .(Ahmed 2007).[22].

.we observed the optical conductivity was increase with increases of photon energy and this behavior is same as the absorption coefficient because it depending on it by the relation number (13) .

In the figure (10) we show the increase of absorption coefficient as a function of photon energy with increasing the ratio of doping because increase number of carries charges .and because the absorption coefficient less than 10^4 so the band gap is indirect . .

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Table (1): The structural parameters from grain size ,dislocation density ,number of crystals and strain .

Sample	G.S(nm)	$^{-2}$) (nm	N∘ (nm$)^{-2}$	S
PVA	0.8362	1.4302	513.17	0.4143
PVP	0.4690	4.5475	2909.79	0.7387
PVA:PVP:V_2O_5(2%)	0.7727	1.675	650.33	0.4484
PVA:PVP:V_2O_5(6%)	0.3273	9.337	8571.42	1.058

Table (2): The value of energy gap from the samples

Sam.	Eg(eV)
PVA	4.6
PVP	4.42
PVA:PVP:V_2O_5(2%)	3.49
PVA:PVP:V_2O_5(6%)	2.98

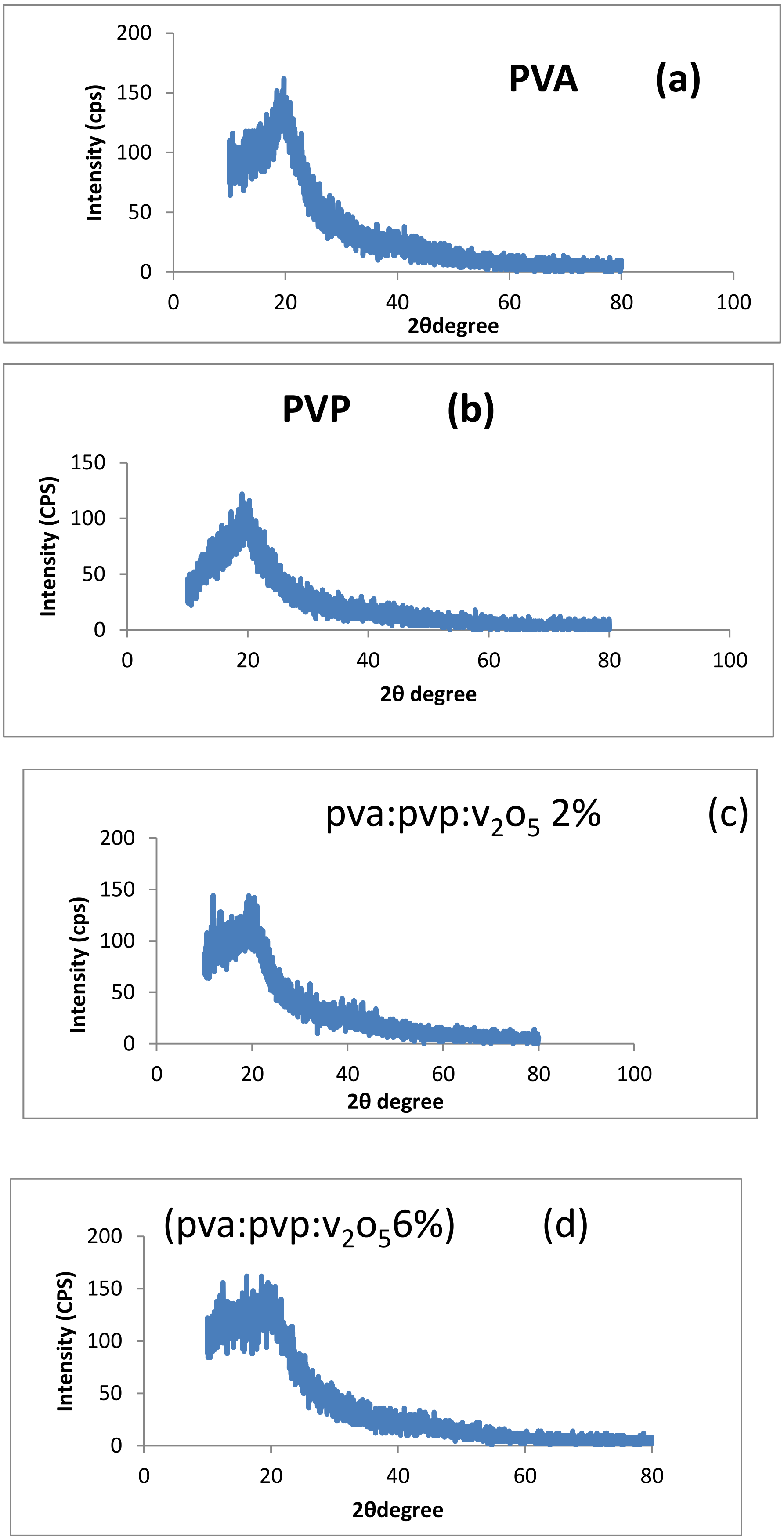

Figure (1) :(a,b.c.d) X-ray diffraction for the thin film.

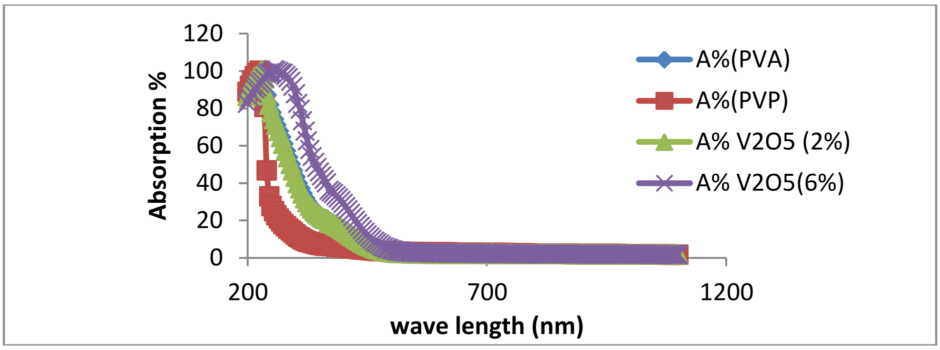

Figure (2):The Absorption ratio as a function of wavelength

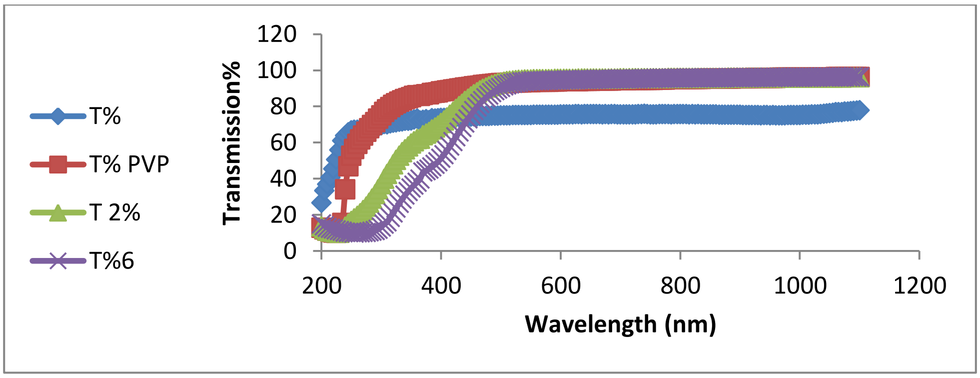

Figure (3): The Transmission ratio as a function of wavelength

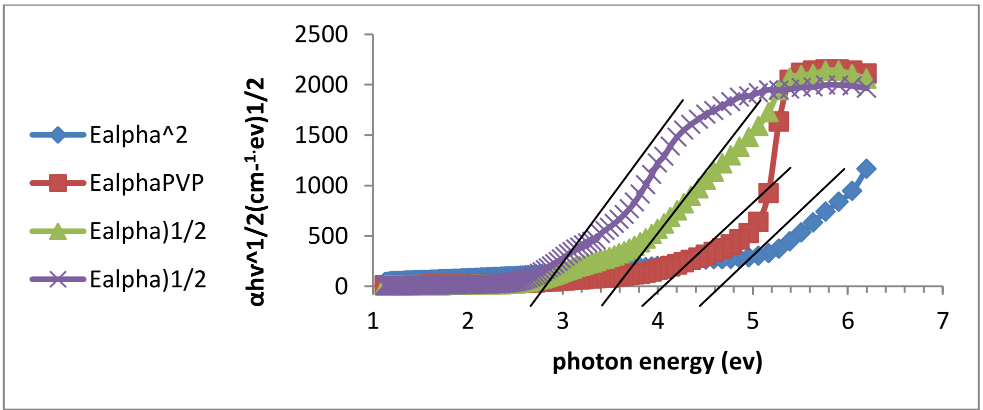

Figure (4):The realation between($\alpha h\nu)^{1/2}$ and photon energy .

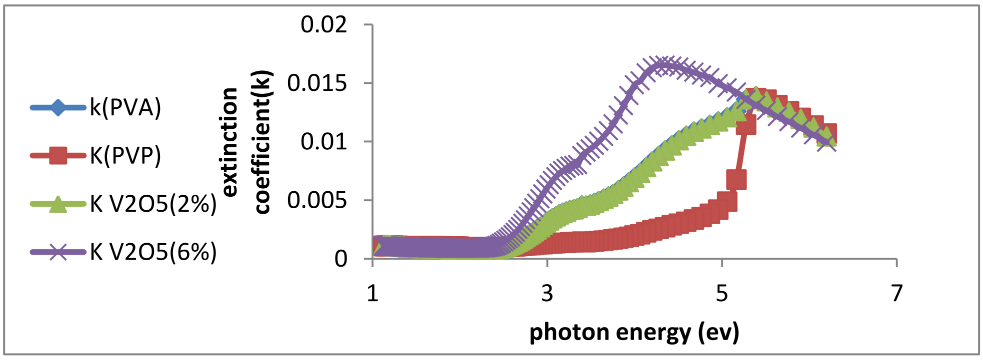

Figure (5): The Extinction coefficient as a function of photon energy.

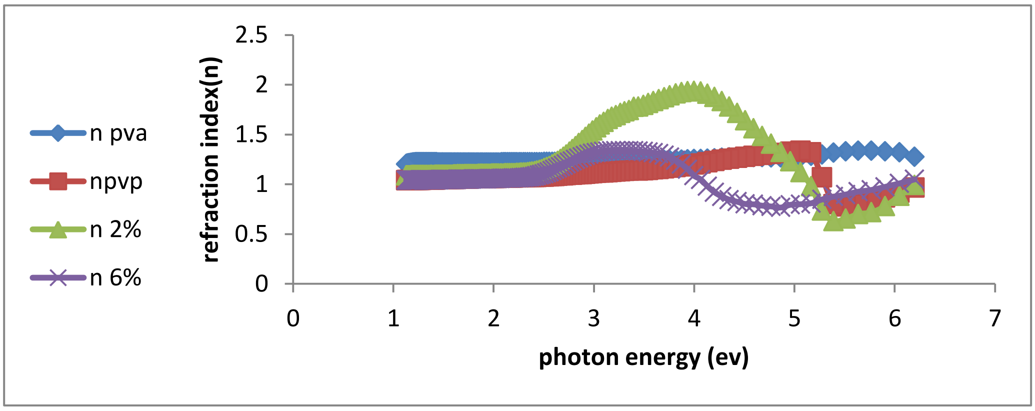

Figure (6) :The refractive index as a function of photon energy

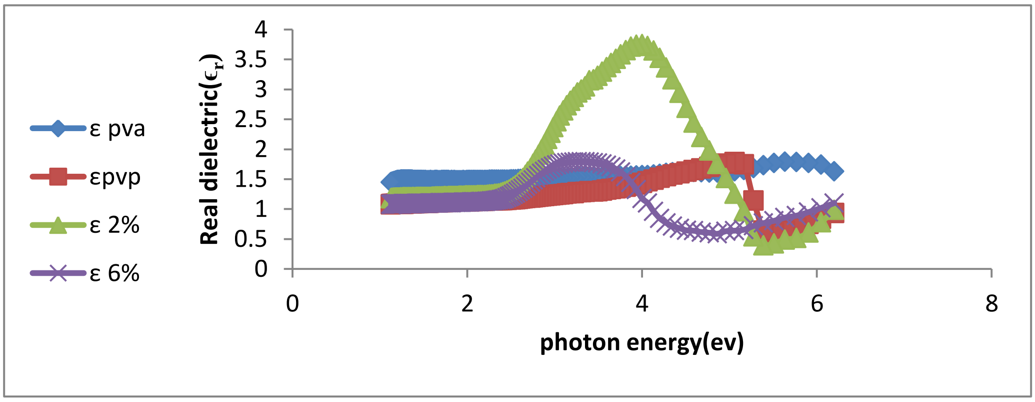

Figure (7): The real dielectric as a function of photon energy

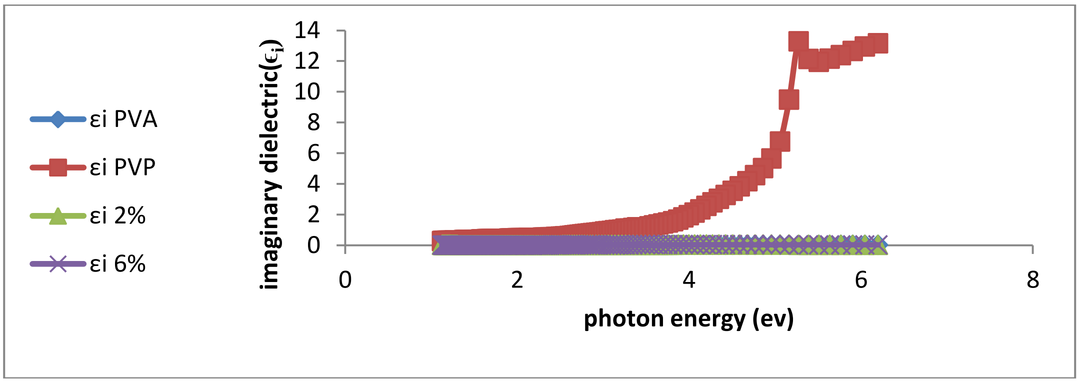

Figure (8):The imaginary dielectric as a function of photon energy .

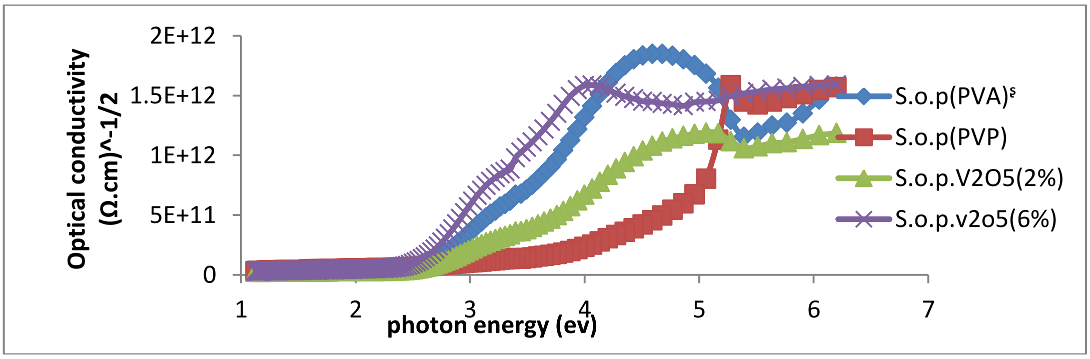

Figure (9):The optical conductivity as a function of photon energy .

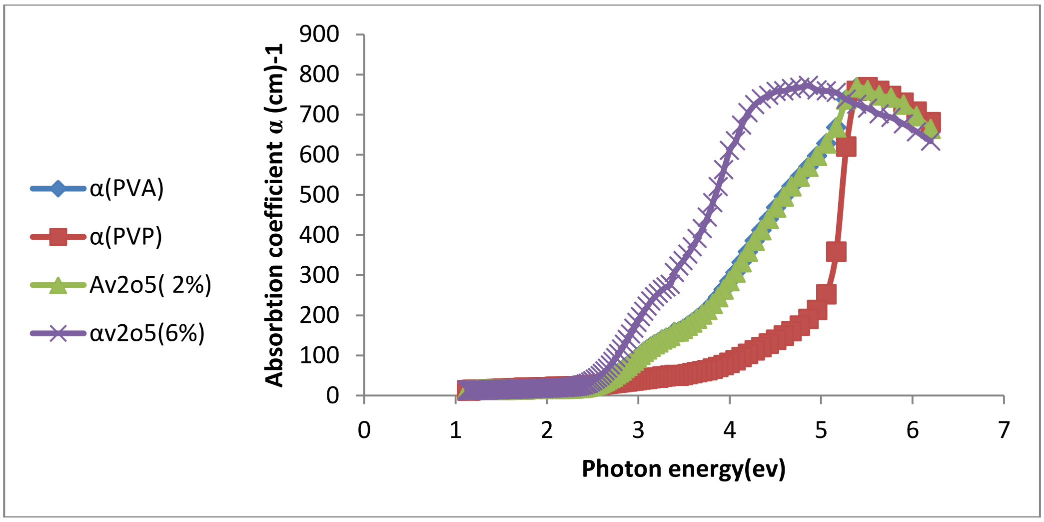

Figure (10):The Absorption coefficient as a function of photon energy.