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Optical and Structural Properties of ZnO:Au Nanocomposite Thin films

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ABSTRACT

Zinc Oxide (ZnO) nanoparticles were mixed carefully with gold (Au) nanoparticles. These chemical-compounds were used to make nanocomposite thin films by using the technique of spray pyrolysis. This work studies the XRD spectra of nanocomposite thin film of ZnO:Au, there two peaks with the orientation of (100) and (002) for the ZnO nanoparticles were found at 2θ = 31.5582 and 34.1617, which are specified by the reference of ZnO powder diffraction of card number (96-901-1663), and one peak with (111) orientation of gold nanoparticles at 2θ = 38.5799 by the reference of Au powder diffraction of card number (96-901-2431) was found. The AFM images of ZnO, Au and ZnO:Au nanocomposite thin films showed that all the specimens have a grainy nature. The results of optical properties were clearly demonstrated that when the wavelength increases the transmission increases, while the absorption coefficient, attenuation coefficient and energy gap decreases. Finally the dielectric constant measurements proved that real part dielectric constant and imaginary part dielectric constant of all trials decreases rapidly when the frequency is increasing.

Keywords: Zinc Oxide, Gold, Nanocomposite, Thin Film.

1. INTRODUCTION

In recent years, researchers in the electrical engineering fields, chemistry and physics have focused the attention to the development and characterization of nanocomposite materials [1]. Zinc oxide (ZnO) is an n-type metal oxide semiconductor of a great band-gap energy (3.3 eV) and large excitation restricting energy (~60 m eV) at room temperature [2]. The wide band gap of this material makes it an excellent visible light transparent and the UV absorbing material [3]. ZnO nanostructures show different sizes depend on effects, good electrical properties and high luminescence. ZnO thin films have the potential to be utilized as thin solar cells, field effect transistors, gas sensors antibacterial treatment, UV absorption, photo catalyst, catalyst [4,5]. ZnO is transparent to visible light and can be very conductive by doping, Wurtzite zinc oxide has a hexagonal structure (space group C6mc). The ZnO structure can be simply defined as a variety of alternating planes consisted of tetrahedrally coordinated O^{-2} and Zn^{+2}ions, combined alternately along the c-axis as shown in figure (1) [6,7].

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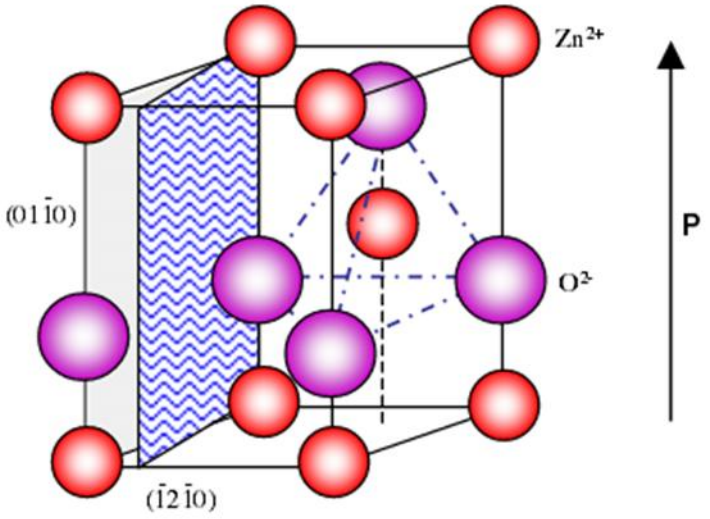

Figure 1. The wurtzite structure model and the Lattice constant values of the ZnO [3].

ZnO exhibits high catalytic efficiency, ability of absorption is strong, high point of isoelectric, and fast kinetics transfer of electrons [8]. For thin film deposition various chemical and physical techniques have been utilized, such as spray pyrolysis, thermal evaporation, conventional sputter deposition technique, electrodeposition and chemical vapor deposition (CVD) [9]. The noble metal of gold was used due to the high electron affinity behavior, Au is the most inert metallic elements with interesting properties as a heterogeneous catalyst [10].

In the present investigation, we report the synthesis of Au-ZnO nanocomposite by a simple, cost-effective spray pyrolysis technique. The effect of Au doping on the structural, surface morphological and optical properties of thin films has been investigated.

2. EXPERIMENTAL

The raw materials of Zinc Oxide (ZnO) nanoparticles with a purity of 99.999 and particle size ranged in 73.74nm, gold nanoparticles with purity of 99.999 and the particle size ranged in 53.63nm. All compounds were supplied from Fluka company Swiss product. Propanol solution ($CH_3.CH_2.CH_2OH$) with a purity of 99.999 and double distilled deionized water were used.

About 0.01 g of ZnO nanoparticle was dissolved in 20 ml propanol solution for 1 hour by using ultrasonic technique. The ZnO: Au thin films were deposited on glass substrates by spray pyrolysis technique. The deposition procedure contains the precursor solution, carrier air gas assembly connected to a spray nozzle, reaction chamber in which substrate was heated and controlled by a variac. Firstly precursor spray solution was entered in a syringe with a metallic needle and then transmitted to hot substrate kept at the deposition temperature of 250°C using a chromel-alumel thermocouple established digital temperature controller. Pressure of the carrier air gas was fixed at one bar. The distance between the substrate and spray nozzle was set to 30 cm. The spray rate of solution to the hot substrate was kept at 5 ml/min throughout the experiment. After deposition, films were allowed to cool at an ambient temperature slowly. Then all samples were placed in furnace at temperature 400 ^{0}C for one hour to get a good crystalline phase. Finally, the samples were allowed to cool at room temperature after 15 minutes.

For the characterization of samples, the films structure was studied utilizing the high-resolution X-ray diffraction (HR-XRD), (X'Pert Pro MRD PW3040 system diffractometer, PANalytical Company, Netherlands) system equipped with Cu-K α-radiation of wavelength λ = 0.15418 nm, at 40 kV and 30 mA. The morphology of the surface was studied to examine the particles size of ZnO, Au and ZnO:Au thin film utilizing atomic force microscopy (AFM) (SPM-9600, Scanning Probe Microscope, Shimadzu, Japan) was used for investigating the roughness of ZnO, Au and ZnO:Au thin film. The optical properties were investigated using the double-beam Ultr-Violet (UV-vis) spectrophotometer (Shimadzu UV-Vis 1800, Japan).

3. RESULTS AND DISCUSSION

3.1 Structural Results

Figure (2) shows the XRD spectra of the nanocomposite thin film of ZnO: Au. From the figure, it may be noticed that there are two peaks with the orientation of (100) and (002) for the ZnO nanoparticles were found at 2θ = 31.5582 and 34.1617, which are specified by the reference of ZnO powder diffraction of card number (96-901-1663), and one peak with (111) orientation of gold nanoparticles at 2θ = 38.5799 by the reference of Au powder diffraction of card number (96-901-2431), were also found. The XRD outcomes appear that the film were polycrystalline Wurtzite hexagonal and cubic structure and have no distinguished orientation. The displayed result are agreement with previous study [11].

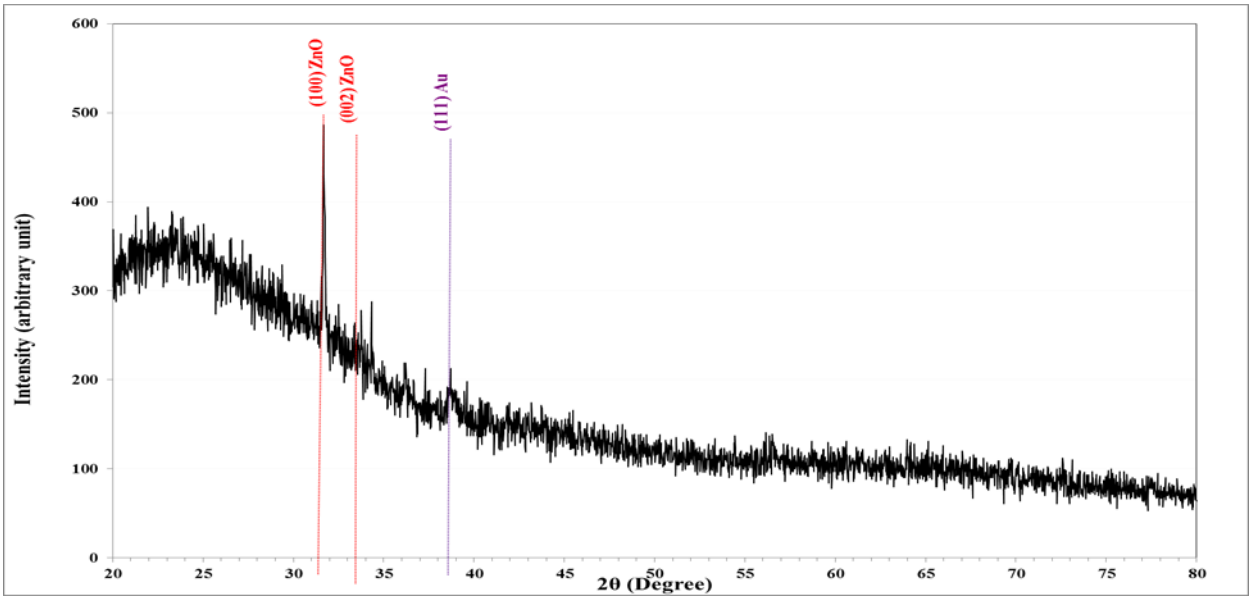

Figure 2. XRD spectra1 for ZnO:Au nanocomposite thin film prepared by spray pyrolysis method.

Table 1 XRD data of ZnO: Au nanocomposite thin films prepared by spray pyrolysis method

2θ (Deg.)	FWHM (Deg.)	d_{hkl} Exp.(Å)	C.S (nm)	d_{hkl} Std.(Å)	Phase	hkl	card No.
31.6581	0.1401	2.8240	58.9	2.8137	Hex. ZnO	(100)	96-901-1663
33.6198	0.2522	2.6636	32.9	2.6035	Hex. ZnO	(002)	96-901-1663
38.6922	0.5885	2.3253	14.3	2.3500	Cub. Au	(111)	96-901-2431

3.2 Atomic Forces Microscopy (AFM)

Figure (3) shows two and three-dimensional atomic forces microscopy-images for ZnO nanoparticles thin film. While gold nanoparticle prepared by Turkevich method is shown in figure (4). Figures (5) displays two and three-dimensional atomic forces microscopy-images of ZnO:Au nanocomposite thin films. The average grain size and the films average surface roughness are shown in table 2. The AFM images of ZnO:Au nanocomposite thin films showed that all the specimens have grainy nature, these types of fine grain sizes are uniformly distributed along the film surface .

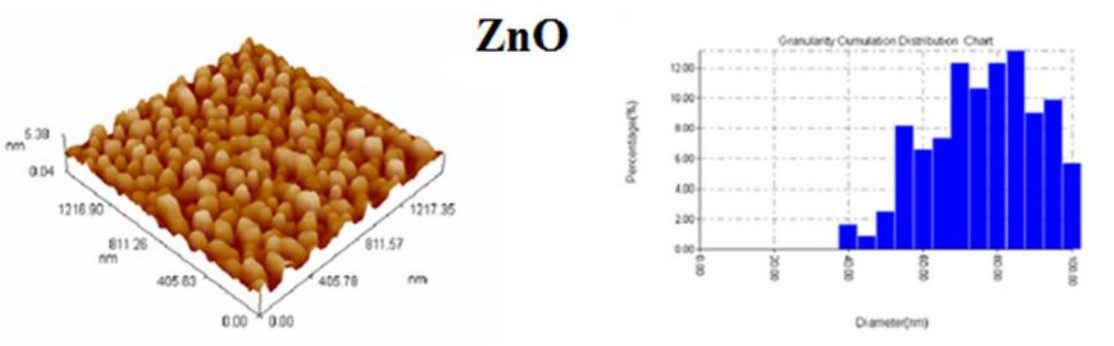

Figure 3. AFM images of ZnO nanoparticles thin film prepared by spray pyrolysis method.

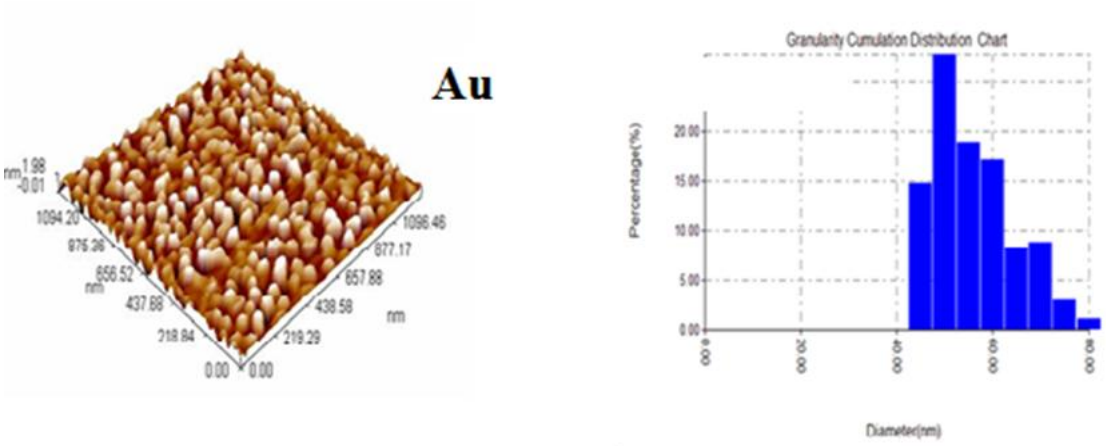

Figure 4. AFM images of Au nanoparticles thin film prepared by spray pyrolysis method.

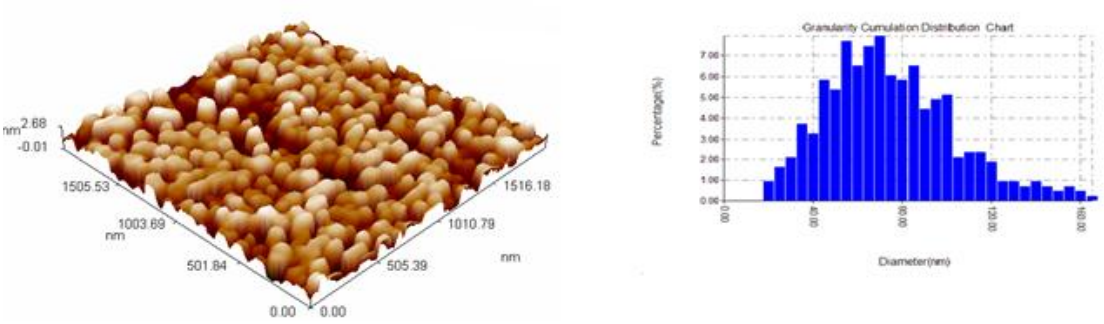

Figure 5. AFM images of the concentration ZnO:Au nanocomposite thin film prepared by spray pyrolysis method.

Table 2 Average grain size and average roughness of ZnO, Au and ZnO:Au nanoparticles thin films

Sample	*Ave. diameter (nm)*	*Roughness average (nm)*	*Root mean square (nm)*
ZnO	73.74	0.617	0.722
Au	53.63	0.386	0.46
ZnO:Au	71.78	0.523	0.621

3.3 Optical Properties

Figure (6) shows UV-Vis measurements on ZnO:Au nanocomposite thin films, provided the optical transmission spectra. Nanocomposite thin film of ZnO:Au showed a weak transmission at a wavelength 310-330 nm and a strong transmission band in the wide spectral range of 340–1100 nm. Figure (7) shows the optical absorption spectra of ZnO:Au nanocomposite thin films. The absorption coefficient appears at high value in the spectral range of 300-350 nm for the films, and later reduce until reaches to zero at the visible region, it is evident that the absorption band is due to the Au nanoparticles. The extinction coefficient values of the ZnO:Au nanocomposite thin films exhibited the same behavior of the absorption coefficient as shown in figure (8). While Figure (9) represents the energy band gap of the ZnO: Au nanocomposite thin films, the thin films energy band gap has the value of 3.2 eV [12,13]. Figure (10) shows the variation of the real part of the dielectric constant values (ε_r) and the imaginary part of the dielectric constant value (ε_i) with wavelength for (ZnO: Au) nanocomposite thin films. It can be seen that the real and imaginary part has a large value in the range of 300-550 nm then start to decrease until zero at the wavelength of 1100nm.

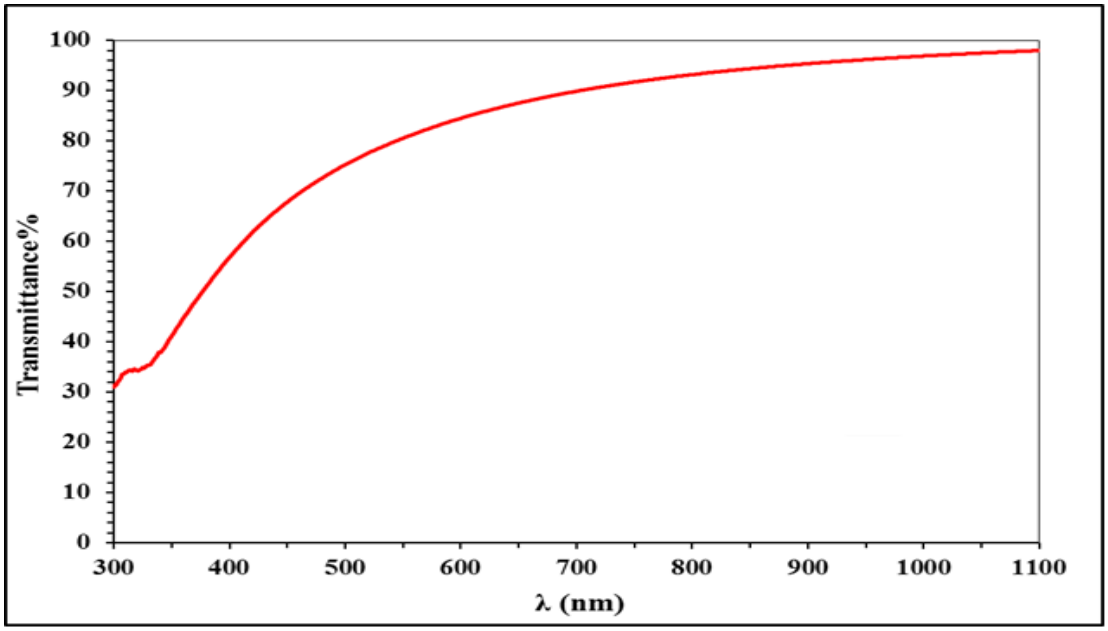

Figure 6. Transmittance as a function of wavelength for ZnO:Au nanocomposite prepared by spray pyrolysis method.

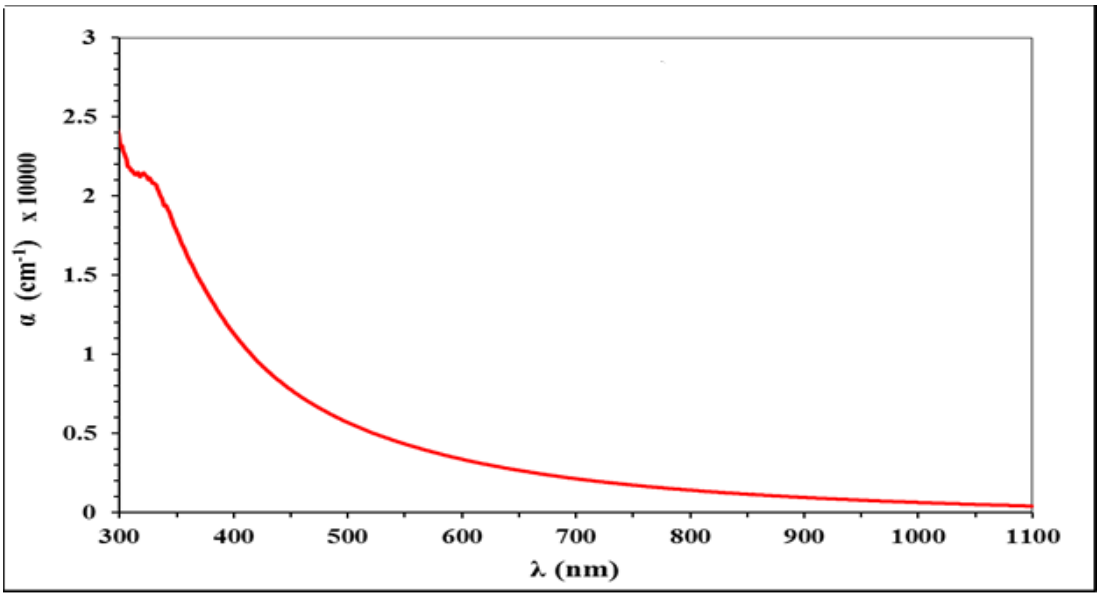

Figure 7. Absorption coefficient (α (cm^{-1})) versus wavelength of the ZnO:Au nanocomposite thin films prepared by spray pyrolysis method.

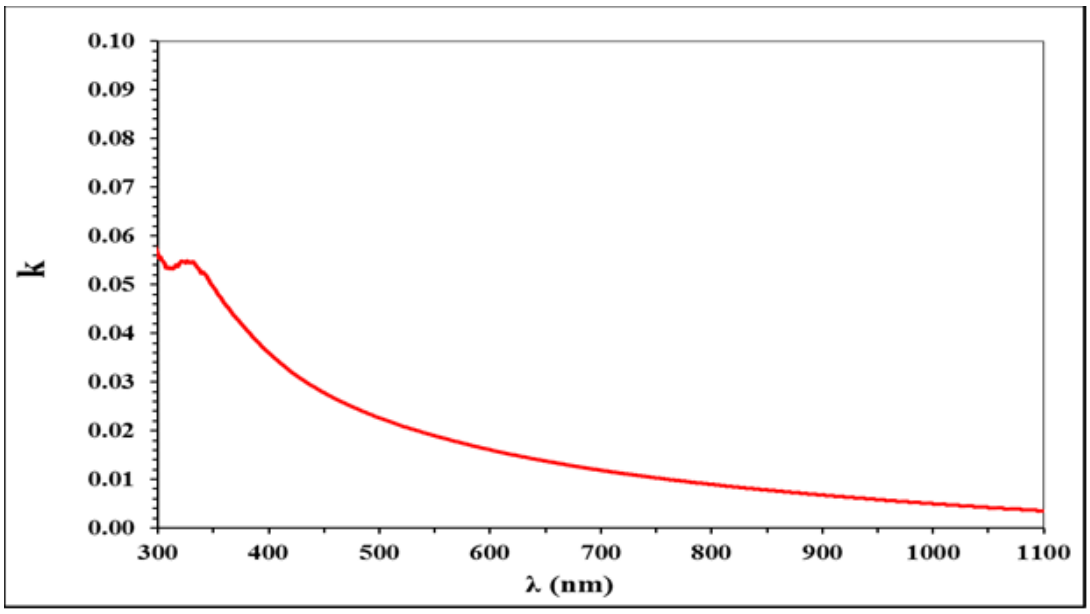

Figure 8. Extinction coefficient versus wavelength of the ZnO:Au nanocomposite thin films prepared by spray pyrolysis method.

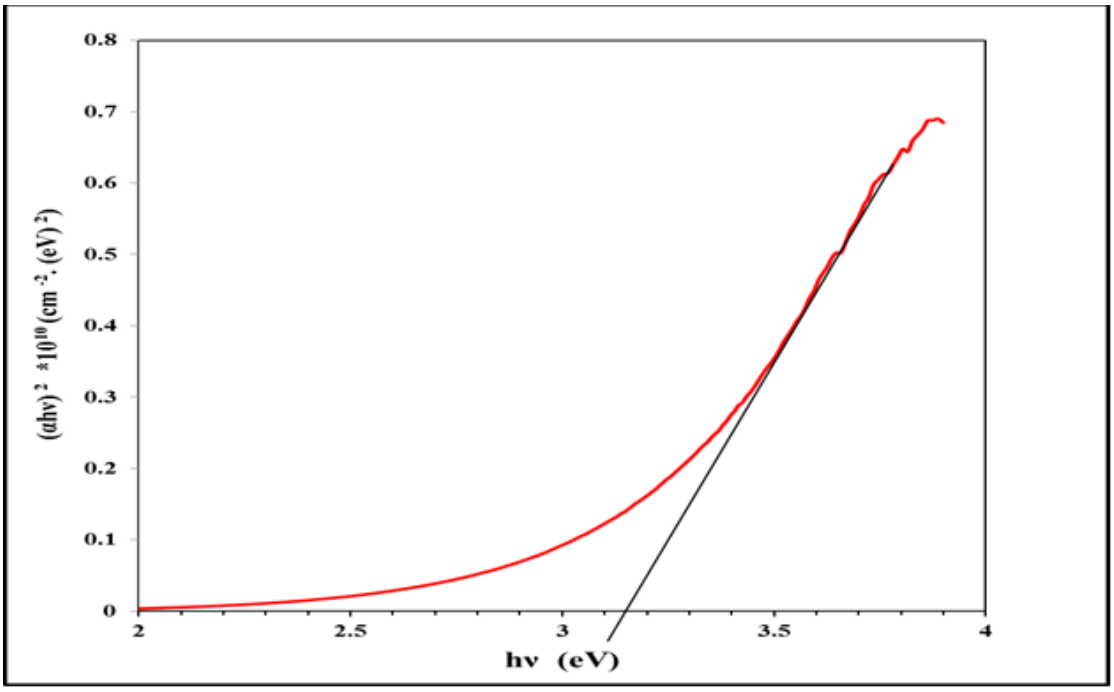

Figure 9. Energy band gaps at Rom Temperature of the ZnO:Au nanocomposite thin films prepared by spray pyrolysis method.

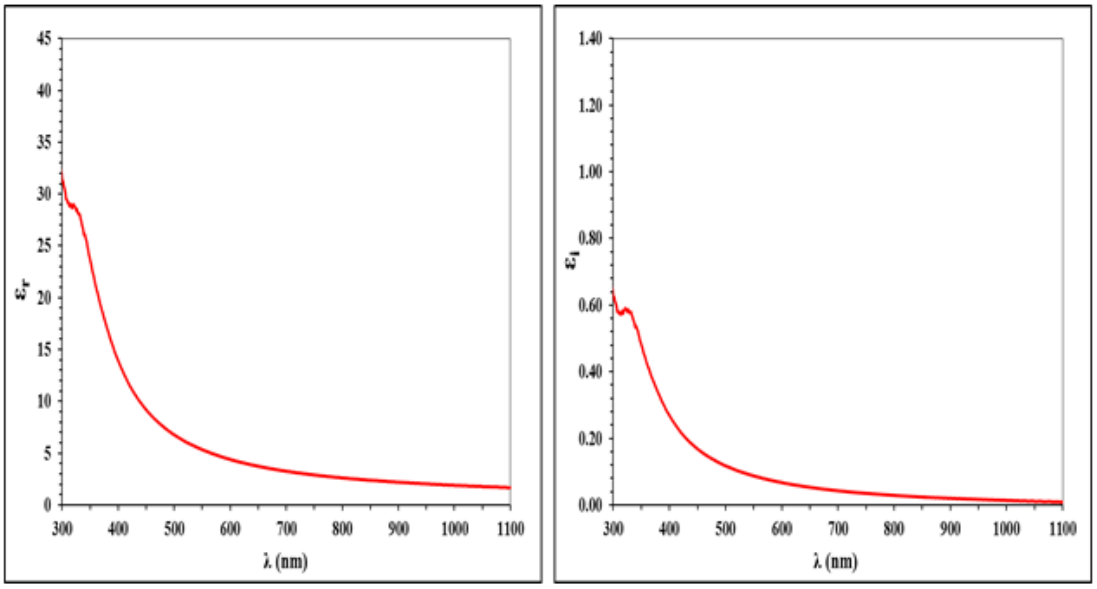

Figure 10. Variation of real (ε_r) and imaginary (ε_i) parts of dielectric constant versus wavelength of ZnO:Au nanocomposite thin films prepared by spray pyrolysis method.

4. CONCLUSION

Polycrystalline composition (ZnO:Au) has been successfully synthesized by spray pyrolysis method. The transmittance increases with increasing wavelength, while the optical band gap, absorption coefficient and extinction coefficient reduces with the increment wavelength. The dielectric constant variation with the frequency shows the conventional dielectric dispersion in the low frequency region and remains regular in the high rate of recurrence region. The average

grain size of ZnO is 73.74 nm, the average grain size of Au is 53.63, while for ZnO: Au the size is 71.78 nm due to the gold nanoparticle concentration.

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LIST OF SYMBOLS

Symbol	Description
d	Distance
λ	Wave length
a	Lattice constant
dhkl	Interplanar distance
hkl	Miller indices
C.S	Crystalline size
α	Absorption coefficient
A_0	Absorbance
t	Thickness
E_g	Energy gap
T '	Transmittance
n	Refractive index
K	Extinction coefficient
ε_r	Real part of dielectric constant
ε_i	Imaginary part of dielectric constant