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Effect of annealing temperature on the structural and optical properties of CdSe: 1% Ag thin films

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ABSTRACT

CdSe: 1% Ag thin films prepared by thermal evaporation method on glass substrates under vacuum technique with rate of deposition equal to 50 nm/min, the deposited films thickness (1μm) on glass substrates have been annealed at different temperatures for one hour. XRD measurement shows that the films have polycrystalline structure at R.T and change to single crystalline when annealed these films for different annealing temperatures (423, 473, 523 K). The optical measurement indicated that CdSe: 1% Ag films have direct optical energy gap, and it decreases with increasing annealing temperatures. The optical constant refractive index, extinction coefficient and dielectric constants were also studied.

Keywords**:** annealing; XRD; Optical; CdSe: 1% Ag; thin films

1. INTRODUCTION

Cadmium Selenide is an important member of the II-VI binary semiconducting compounds. This group of binary compounds belonging to the cadmium chalcogenide family (CdS, CdTe and CdSe) are considered to be very important materials for different optoelectronic devices [1,2] which including many applications such as solar cells [3], high efficiency thin film transistors, light-emitting diodes, gamma ray detectors, photo electrochemical cells (PEC) [4], thin film transistor and laser device [5]. Several deposition methods for prepared CdSe thin films such as thermal evaporation [6], chemical bath deposition [7], pulsed laser deposition technique [8], electron beam evaporation technique [9], successive ionic layer adsorption and reaction method (SILAR) [10]. In this paper we reported the structural and optical properties of CdSe:Ag thin films at different annealing temperatures.

2. EXPERIMENTAL WORK

The samples of Ag-doped CdSe thin films were prepared by thermal co-evaporation technique, in vacuum about 2×10^{-5} torr by using vacuum coating unit. A specific weight from Cadmium Selenid powder must be taken and put it in a molybdenum boat, take (1%) from this weight Silver and put it in other molybdenum boat. Glass slides were used as substrates which were cleaned chemically and ultrasonically, this slide was placed directly above of (CdSe and Ag) was used as source material at a distance of nearly 18 cm. The films thickness in the range of (1 µm) was measured by interference method and the deposition rate was 50nm/min. the films of CdSe: 1% Ag were annealed for different annealing temperatures in the range (423, 473, 523 K) for only one hour.

The optical band gap Eg can be estimated from the following relation known as the Tauc relation [11]:

$$\alpha h\nu = B(h\nu - Eg)^{n} \qquad (1)$$

where B is a constant, ν is the transition frequency and the exponent n characterizes the nature of band transition. N = 1/2 and 3/2 corresponds to direct allowed and direct forbidden transitions and n = 2 and 3 corresponds to indirect allowed and indirect forbidden transitions, respectively. For all the films the best straight line is obtained for n equal to ½, which is expected for direct allowed transition.

The optical constant absorption coefficient (α), refractive index (n), extinction coefficient (k) and real (ε_r) and imaginary part (ε_i) of dielectric constant can be calculated from the following equation [12].

$$\alpha = 2.303\frac{A}{t} \qquad (2)$$

where (t) is the film thickness and (A) is the optical absorbance.

$$k = \frac{\alpha\lambda}{4\pi} \qquad (3)$$

where (λ) is the wavelength of the incident radiation and (k) is the extinction.

$$\varepsilon_r = n^2 - k^2 \qquad (4)$$

$$\varepsilon_i = 2nk \qquad (5)$$

where (n) is the refractive index was obtained from the following relation [13].

$$n = \left[\frac{4R}{(R-1)^2} - k^2\right]^{1/2} - \frac{(R+1)}{(R-1)} \quad (6)$$

where *R* is the reflection.

3. RESULTS AND DISCUSSION

The XRD patterns of the CdSe and CdSe: 1% Ag films for different annealing temperatures having thicknesses (1µm) are shown in Figures (1:a and b) and Table (1). This figures shows that the structure are polycrystalline, Also which have a strong and sharp peak at reflecting (002) plane and small peaks at (103) plane as presented in Figures (1: a and b) with hexagonal structure for CdSe and CdSe: 1% Ag at RT ,according to the American standard for testing materials (ASTM) cards, but the structure of CdSe: 1% Ag are single crystal only of reflecting surface (002) when we annealed this films for different annealing temperature (423, 473, 523 K). This result an agreement with the result obtained by Eman et. al. [14] and Abbas [15].

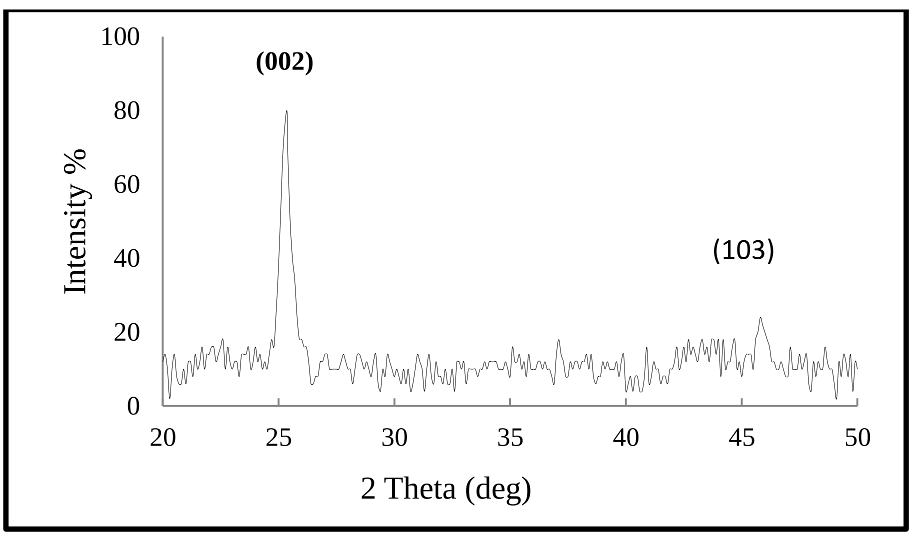


Figure 1(a). X-ray diffraction pattern of CdSe thin film as-prepared.

Figure (2: a) shows the optical energy gap values (Eg) for CdSe films while Figure (2: b) relive CdSe: 1% Ag films at different annealing temperatures 423, 473, 523 K from this Figures (2: a and b) we observed from plot $(\alpha h\upsilon)^2$ versus (hυ) the relation is linear plot as direct band gap nature of the films, also we notice the value of the optical energy gap of CdSe films is decreases from (1.75 eV) to (1.73 eV) after doped the films with (1%) Silver ,also we can see the value of optical energy gap decreases from (1.73 – 1.68) eV with increasing the annealing temperatures from (R.T – 523 K) and the values of (Eg) are equals to 1.73, 1.71, 1.70, 1.68 eV for CdSe: 1% Ag. This may be due to the increases of density of localized states in the energy gap which causes a shift to lower values [14], This result agree with the results reported by Abbas [15], Hider [16] and Nawfal et al [17].

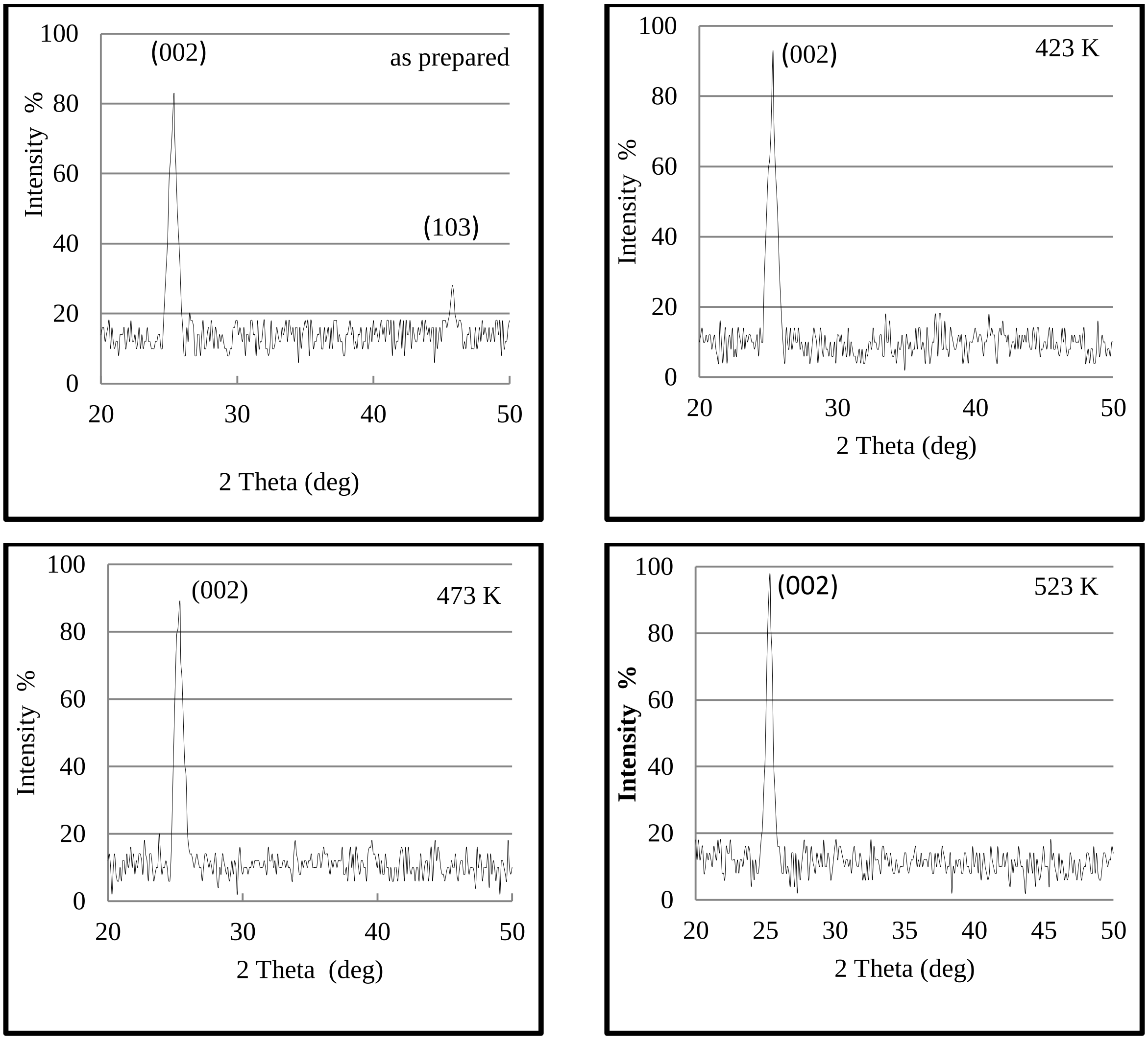


Fig. 1(b). X-ray diffraction pattern of CdSe: 1% Ag films for different annealing temperatures

Table 1. X-ray diffraction data for CdSe: 1%Ag films.

Sample	T_a (K)	(hkl)	2θ (degree) Observed	d(A) Observed
CdSe	**RT**	002 103	25.357 45.807	3.515 1.987
CdSe: 1% Ag	**RT**	002 103	25.361 45.801	3.517 1.998
	423	002	25.339	3.503
	473	002	25.348	3.513
	523	002	25.342	3.496

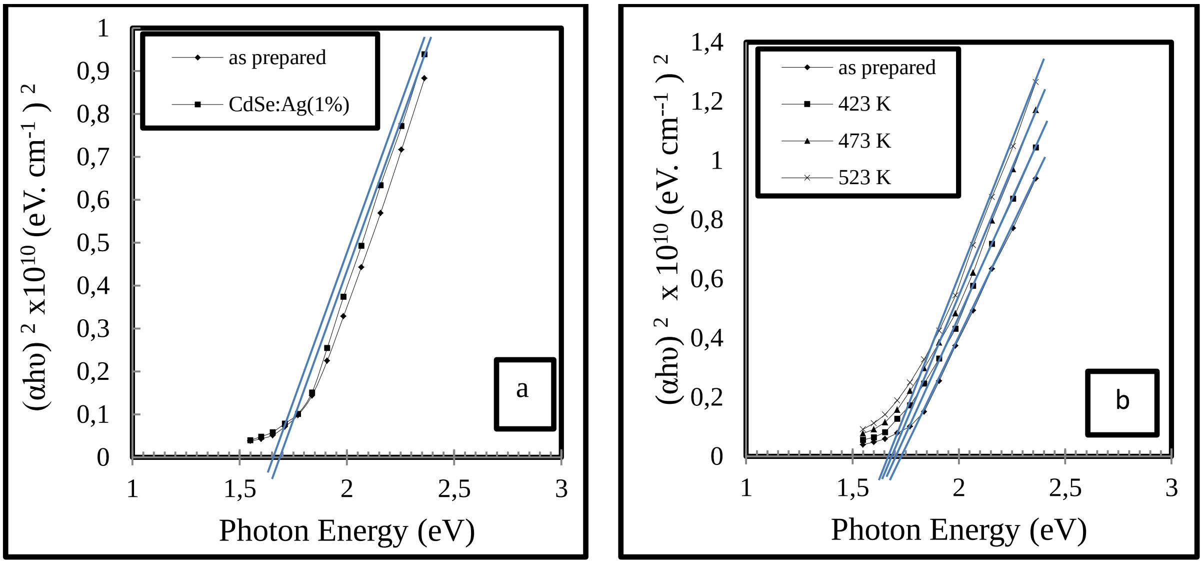


Figure 2. $(\alpha h\nu)^2$ as a function of hν for (a): CdSe and CdSe: 1% Ag films, (b): CdSe: 1% Ag films at different annealing temperatures.

The absorbance spectrum for CdSe and CdSe: 1% Ag films shows in Figures (3: a and b). The absorbance spectrum shifts to longer wavelengths with increasing of Ta for all the samples and the absorbance decreases with increasing of annealing temperature and this may be due to improving the crystallite size and increasing the transmittance [16], but the absorbance increases after doped CdSe films with silver as show in Figure (3: a), which agree with result obtained by Abbas [15].

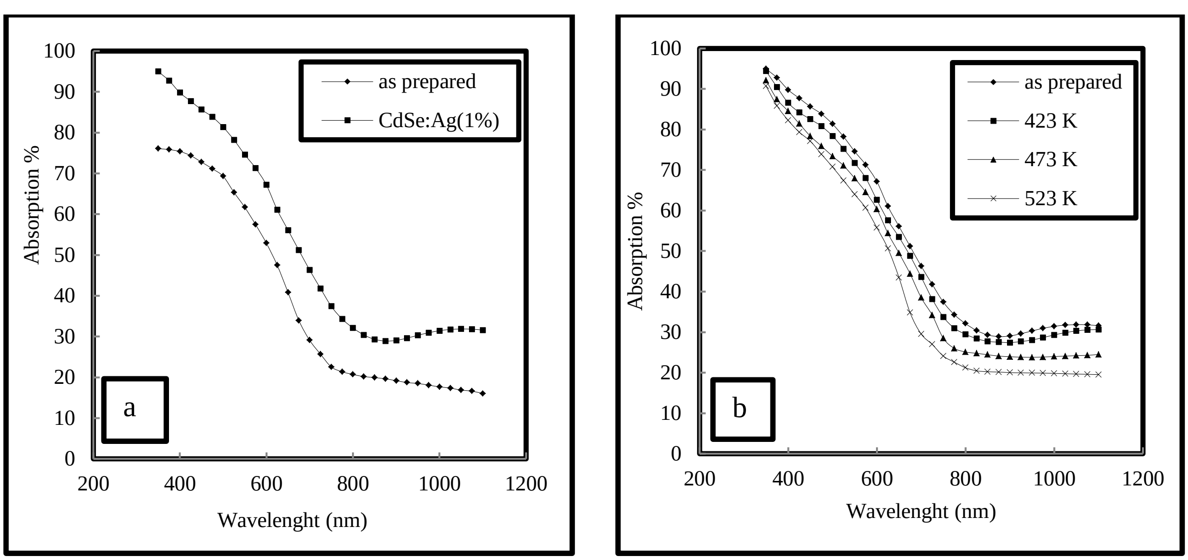


Figure 3. Absorbance spectrum as a function of wavelength for (a):CdSe and CdSe:1%Ag films,(b): CdSe:1%Ag films at different annealing temperatures

The transmission in variations as function of wavelength for CdSe and CdSe: 1% Ag films shows in Figures (4: a and b). The shifts of transmittance spectrum to shorter wavelengths with increasing of Ta for all samples. We can observe that the transmission decreases after doped CdSe films with silver because of the effect of impurities atoms, which is working on the composition of localized levels in the energy gap. The transmission spectra refer to increases when the annealing temperature increasing which as show in Figure (4: b).

This result agrees approximately with the result reported by Abbas [15].

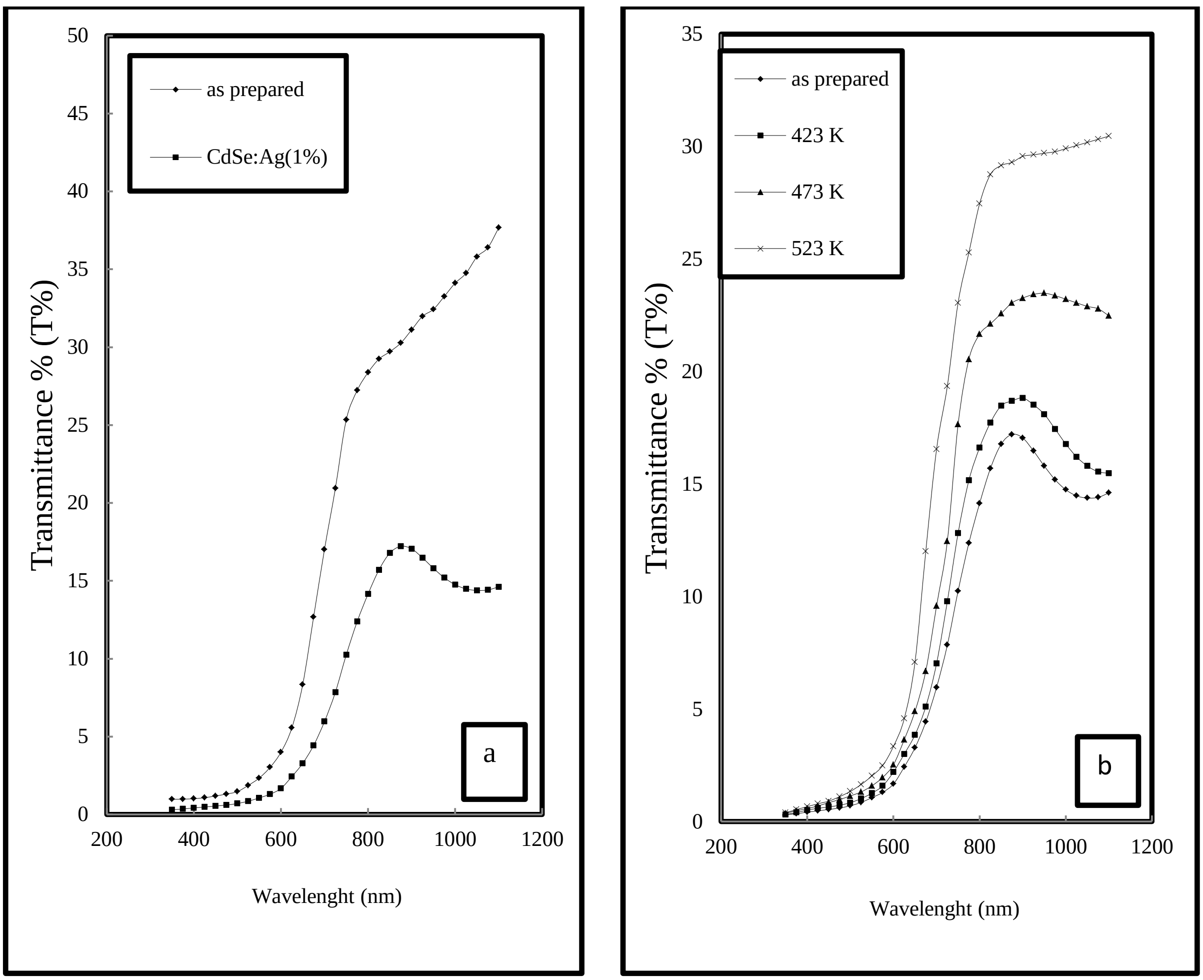


Figure 4. Transmission as a function of wavelength for (a): CdSe and CdSe: 1% Ag films, (b): CdSe: 1% Ag films at different annealing temperatures

We can notice that the absorption coefficient (α) in general decreases with increasing of annealing temperature due to the improvement in the structure by increasing T_a while the absorption coefficient increase after doping. This behavior is show in Figures (5: a and b) and this result agree with result obtained by Abbas [15] and Hider [16].

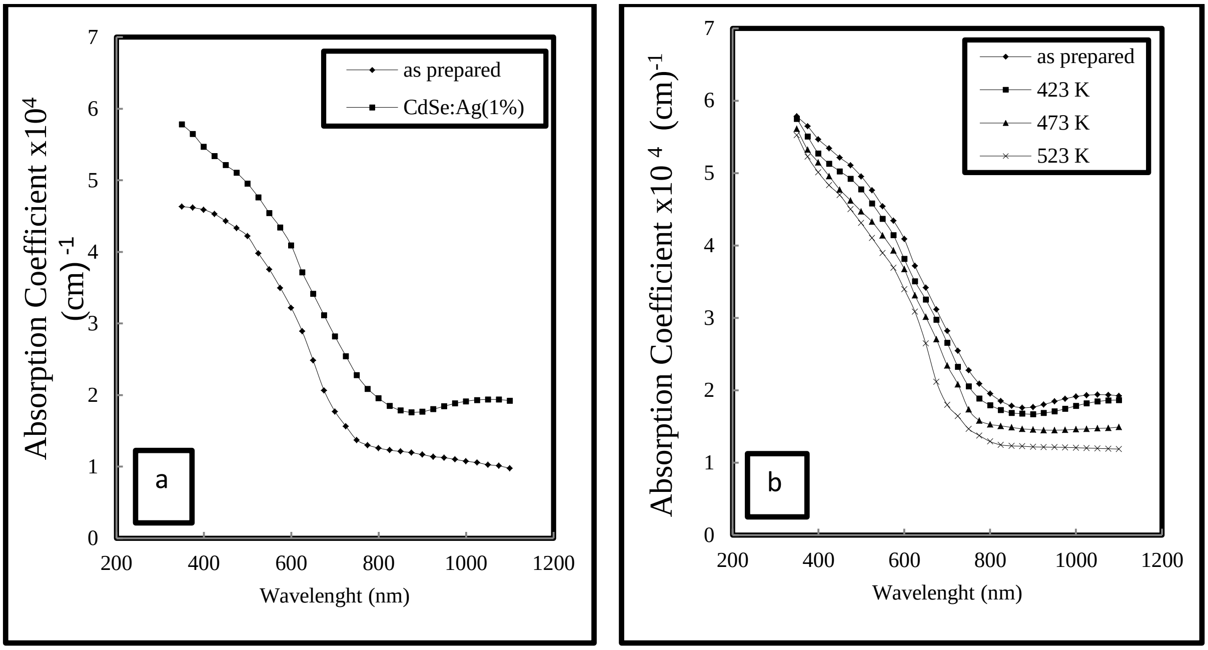


Figure 5. Absorbance Coefficient as a function of wavelength for (a): CdSe and CdSe: 1% Ag films, (b): CdSe: 1% Ag films at different annealing temperature.

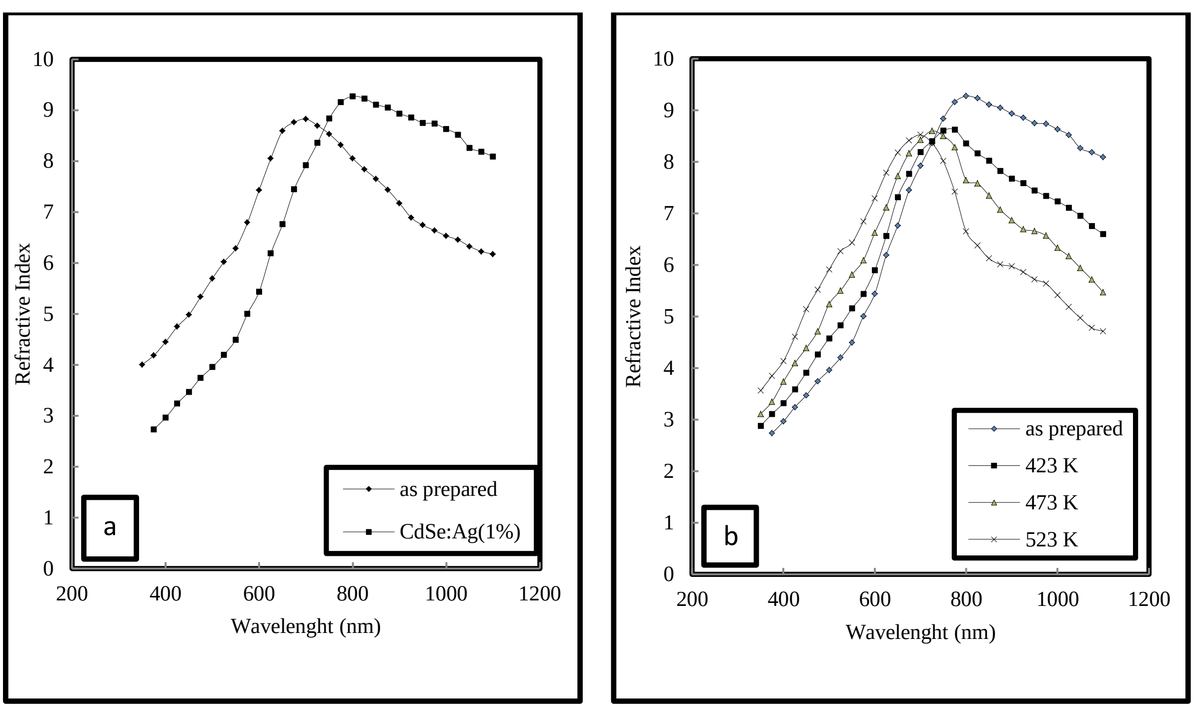
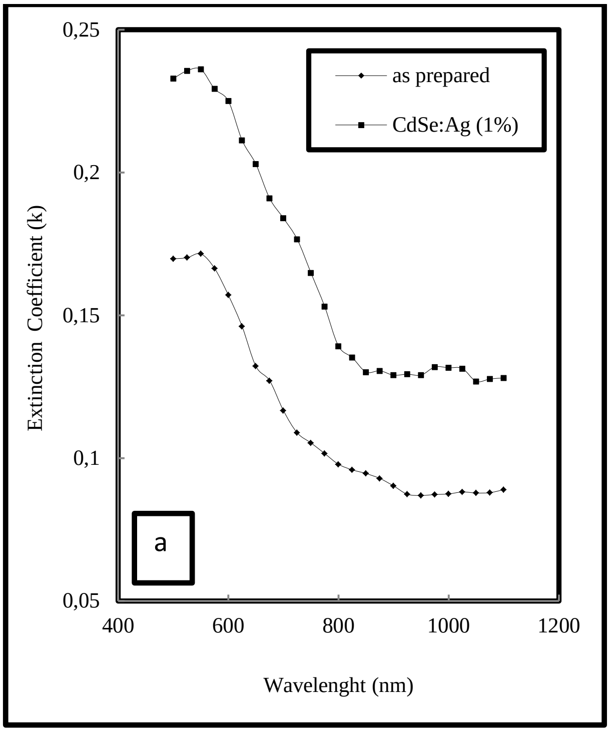


Figure 6. Refractive index as a function of wavelength for (a): CdSe and CdSe: 1% Ag films, (b): CdSe: 1% Ag films at different annealing temperature.



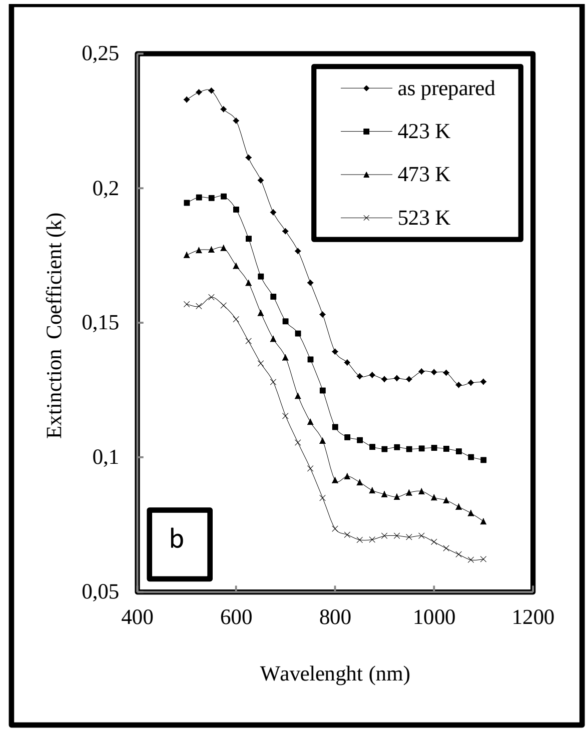
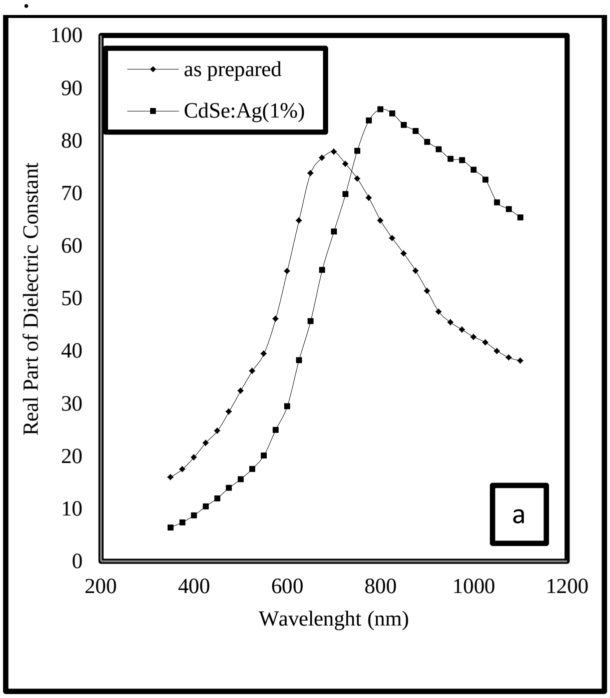


Figure 7. Extinction coefficient as a function of wavelength for (a): CdSe and CdSe: 1% Ag films, (b): CdSe: 1% Ag films at different annealing temperature



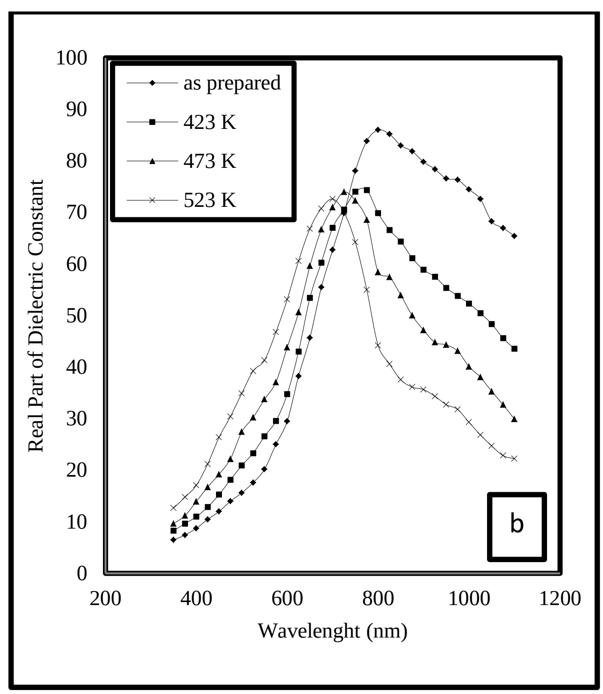


Figure 8. Real part of dielectric constant as a function of wavelength for (a): CdSe and CdSe: 1% Ag films, (b): CdSe: 1% Ag films at different annealing temperature.

The behaviors of the refractive index (n) as a relationship of the wavelength for CdSe: 1% Ag films at different annealing temperatures is shown in Figure (6: b), We can see from this figure that the value of (n) increases with increasing T_a due to the increases of the compactness of the films after the heat treatment simultaneously with the increasing of the crystallite size [1] , but the refractive index (n) increases after doped CdSe films with silver as show in Figure (6: a).

Figure (7: b) shows that the extinction coefficient (k) is decreased by increasing the value of annealing temperature and this may be due to increasing the absorption coefficient, while Figure (7: a) refers to the extinction coefficient (k) is increased after doping.

Figures (8 and 9: b) shows the variation of real and imaginary part of dielectric constant (ε_r and ε_i) respectively as a function of annealing temperatures It is found that ε_r and ε_i decreases with increasing annealing temperatures. Figure (8 and 9: a) shows the variation of real and imaginary part of dielectric constant (εr and εi) respectively as a function of doping which refers to increasing the real and imaginary part of dielectric constant (εr and εi) after doping. The behavior of ε_r is similar reasons mentioned previously for the refractive index, while ε_i depended of extinction coefficient.

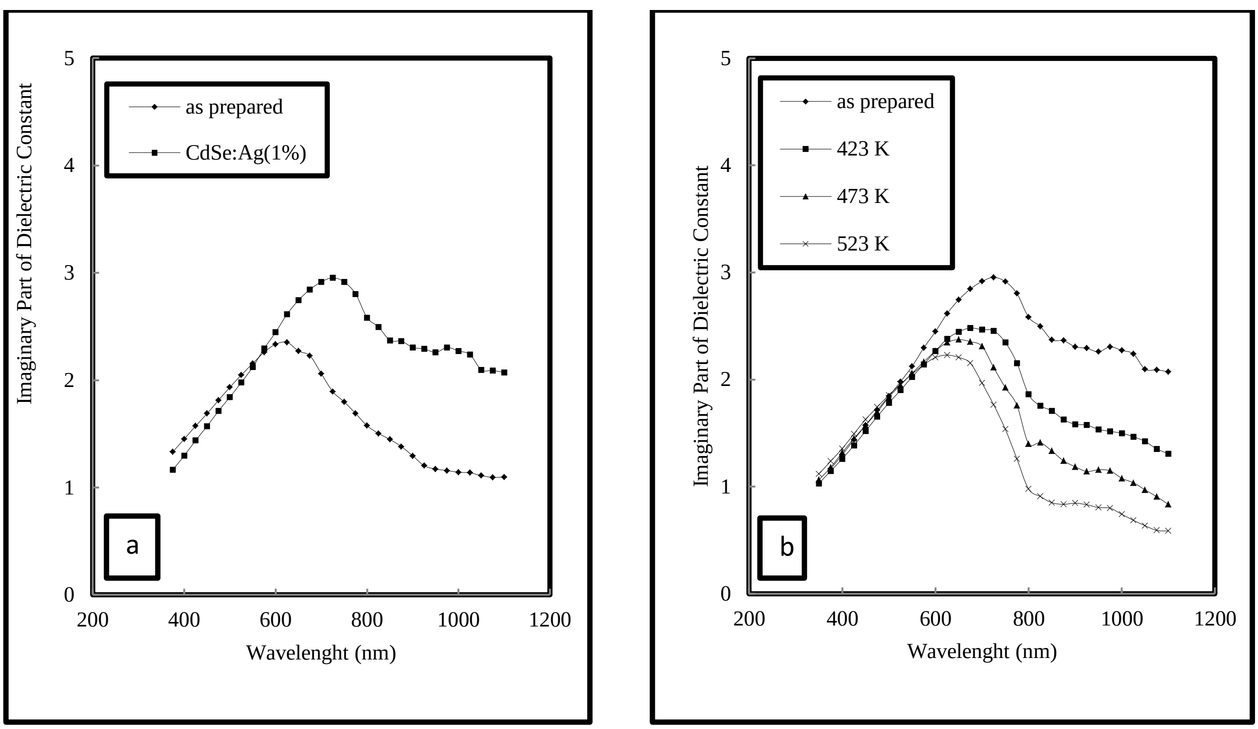


Figure 9. Imaginary part of dielectric constant a function of wavelength for (a): CdSe and CdSe: 1% Ag films, (b): CdSe: 1% Ag films at different annealing temperature

4. CONCLUSIONS

XRD analysis confirms that CdSe films are nearly single crystalline with a hexagonal structure and the preferred orientation is (002) after annealing temperatures and doping. Optical studies reveal that CdSe:1%Ag films has a direct band gap energy and the value of energy gaps (Eg) decreases with increasing of annealing temperatures and that the films has the highest transmission in the infrared region, so we can used CdSe:1%Ag films as IR window.

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