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Study of the Structural and Electrical Properties of Cadmium Selenide Doped with Zinc in Different Proportions

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Abstract— Three samples of pure CdSe doped with zinc (4% and 8%) were prepared by the slow cooling method at 325°C and pressed into discs. The structural properties of the prepared samples were studied using XRD. It was found that the structure was cubic and polycrystalline, as the crystallization phase did not change as a result of doping with zinc. Using a Senko fluorescence spectrometer, the fluorescence spectrum of the prepared samples was studied, and it was observed that the intensity of fluorescence increases with zinc doping ratio due to the appearance of two peaks at 631.8nm and 704.9nm. By studying the electrical properties (I-V) of the prepared samples, it was observed that there is an improvement in the electrical conductivity of the compound (CdSe) after doping it with zinc, and from calculating the activation energy (Ea) of the samples, it was found that it decreases with increasing zinc doping ratio in order to form impurity levels above the energy gap.

Keywords— CdSe, Zinc doping, Slow cooling, XRD, Optical properties, Fluorescence.

I. INTRODUCTION

Semiconductors are among the most important compounds that have attracted the attention of researchers since their discovery because of their importance in advanced technology. They are used in electronic and optical applications because of their unique and useful properties, starting from their use in manufacturing electronic components such as switches, transistors, and integrated circuits, all the way to economic lighting and power generation with solar cells.[1]. In recent years, new focus has been placed on cadmium chalcogens, such as cadmium selenide, cadmium telluride, and cadmium sulfide, due to their diverse applications such as optical carriers, transistors, gamma detectors, sensors, and solar cells [2]. Cadmium selenide is considered one of the most famous compounds of the semiconductor group. Its elements belong to the second and sixth columns (II-IV) of the Mendeleev table. It is a chemical compound with the formula CdSe and is in the form of a brown crystalline powder [3]. Cadmium selenide is transparent in the infrared spectrum with its sensitivity to light in the same range of vision for the human eye, that is, the nanocrystals are CdSe (emits light within the visible range 450-650 nm) and therefore all Colors from blue to red can be available using CdSe, and it crystallizes CdSe compound (according to the cubic or hexagonal crystal structure, as shown in Figure (1)[4].

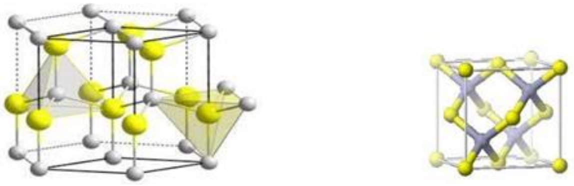

Fig. (1): Crystallization of CdSe–according to the hexagonal or cubic structure.

CdSe is an important material because of its applications in the field of photoconductors, where it is characterized by its high sensitivity to light, making it suitable for solar cells and photoelectrochemical cells in the visible area [2]. Doping the compound (CdSe) with zinc improvse the cell efficiency. The results demonstrated that CdSe/CdS doped with zinc is a promising material for cell development. High-performance solar [5]. In 2012, a group of researchers studied the fluorescence properties of samples ZnS/CdSe to produce white light, as the fluorescence spectrum showed two peaks at the wavelengths 550 nm and 682 nm [6]. Many scientific studies have confirmed the improvement of structural and optical properties. Although the method of preparing samples differs when doping the CdSe compound with zinc [7].

II. EXPERIMENTAL PART

In this work, samples of CdSe powder were prepared using slow cooling. To benefit from it, impregnate it with zinc. Mineral powders (cadmium and selenium) were used. The materials were weighed using the molar mass method and placed in a porcelain bowl in an ashtray inside a convection heating oven at 325 °C for two hours, then left to cool using slow cooling. The samples were divided into three: The first was pure (CdSe) the second was doped with 4% of zinc (CdSe: 4%Zn) , and the third was doped with 8% zinc (CdSe: 8%Zn). The samples were then

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compressed using a press into a mold with a force of 3ton/cm^2.To form metal discs from samples to study their structural properties , optical and electrical, to determine the extent to which they can be used in optical applications.

III. RESULTS AND DISCUSSION

A. *Structural Properties*

X-ray diffraction was studied for the three samples. The results showed the presence of a sharp peak at 2θ = 25° in addition to the presence of two broad peaks, at 42° and 50° corresponding to the crystallographic directions (111), (220) and (311) , as shown in the figure (2) due to the presence of small particles could be the reason for the expansion of the scattered peaks.

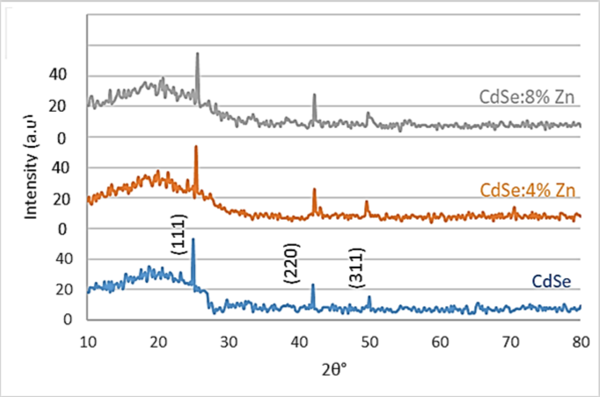

Fig. (2): The X-ray diffraction of the three pure and doped zinc samples.

The X-ray diffraction pattern shows a match with the cubic phase of CdSe (with a card). (JCPDS data card No.03-065-2891). Depending on the angle 2θ and the values of d , after adding zinc, as shown in Figure (2), it was noted that the location of the peak (CdSe) shifted slightly on the 2θ axis, because of the effective ionic radius of cadmium (Cd^{+2}) and Zinc (Zn^{+2}). It is respectively 0.95A^0 and 0.74A^0. Therefore, the radius of the added ion is smaller than the radius of the host ion , and accordingly, the distance between the crystal planes decreases due to crystal deformation. The distance between the crystal planes (d_{hkl}) was calculated according to the direction (hkl) of the observed phases using the Bragg equation, from the following the relationship [9]

$n\lambda = 2d_{hkl} \sin\Theta$ …….(1)

where Θ is the angle of deflection, n is the degree of deflection, and λ is the wavelength of the X-rays. The constants of the crystal lattice were also calculated from the relationship [10].

$$\frac{1}{d_{hkl}} = \left(\frac{h^2+k^2+l^2}{a^2}\right) \dots\dots (2)$$

Which gives the distance between parallel planes in terms of the crystallographic constants of the cubic structure [2], and the relationship

$V = a^3$ ………. (3)

to find the size of the crystal lattice, as shown in Table (1).

Table (1): The crystal lattice factors for the crystal orientation (111)

Sample	**$2\theta^{\circ}$**	**θ°**	**Sinθ**	hkl	**d(Å)**	**a(Å)**	**V(Å)^3**
CdSe	25	12.5	0.2164	111	3.5617	6.1691	234.78
CdSe:4%Zn	25.4	12.7	0.2199	111	3.5065	6.0735	224.03
CdSe:8%Zn	25.6	12.8	0.2216	111	3.4796	6.0268	218.91

Doping cadmium selenide with Zinc leads to a decrease in the crystal constant (a) the size of the crystal lattice (V) , and the distance between the crystal planes (d). As for the crystallite size D, it can be determined according to the Debye-Sherrer equation using the relationship

$$D = \frac{K\lambda}{\beta\ cos\theta} \dots\dots\dots\dots (4)[11][13]$$

Where k is a constant (0.9), β is the full width at half maximum (FWHM) of the diffraction peak, λ is the wavelength of the X-ray , and θ is the diffraction angle. The crystal lattice strain (ε) and the dislocation density (δ) in the crystal lattice were calculated using the two relationships. [9] [13].

$\varepsilon = \frac{\beta\ cos\theta}{4}$ ………(5) , $\delta = \frac{n}{D^2}$ ………(6), where (n=1) , this is to obtain the lowest value for the density of dislocations

Table (2) : The crystallite size (D), dislocation density (δ), and crystal lattice strain (ε) of the prepared samples.

Sample	**CosΘ**	**β (RAD)**	**D (nm)**	**δ (lines.m^{-2})**	**ε *1000**
CdSe	0.9763	0.00349	42.52722	0.0006	0.85198
CdSe:4%Zn	0.9755	0.00611	24.32024	0.0017	1.48980
CdSe:8%Zn	0.9751	0.00873	17.03089	0.0034	2.12745

Table (2) shows that the width of the middle of the peak of the diffraction intensity increases with zinc, therefore, the crystallization size of the zinc- doped samples is smaller than that of the non-zinc-doped sample. meaning that the crystalline size of the zinc doped samples decreases due to the difference between the ionic radii of the host and added atoms , resulting from crystal deformation

B. *Optical Properties*

Figure (3) compares the fluorescence spectrum of pure samples of (CdSe) doped with zinc using an excitation wavelength of 420nm. We notice from the resulting spectrum that the intensity of fluorescence increases significantly in the doped sample (CdSe: 8%Zn). It is also noted that emission peaks appear at wavelengths of 631.8 nm and 704.9 nm, in addition to the appearance of several other peaks. This is due to the formation of trap levels at the bottom of the conduction band as a result of doping, and therefore, the emission spectrum is related to an emission close to the energy band of the CdSe sample. Also, a shift of the fluorescence wavelength towards the red color was observed, and this is consistent with scientific research [2].

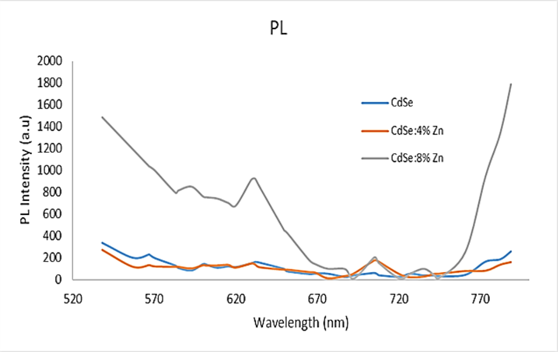

Fig. (3): The emission peaks for pure and zinc-doped with CdSe samples

C. Electrical Measurements

(I-V) was studied for the prepared samples by applying a field voltage of (0-2V) and taking the current values, and Figure (4) shows the feature for all samples. It is noted that with increasing the voltage applied to the sample, the sample current increases, and the current also increases with increasing the ratio of zinc doping and rising temperatures.

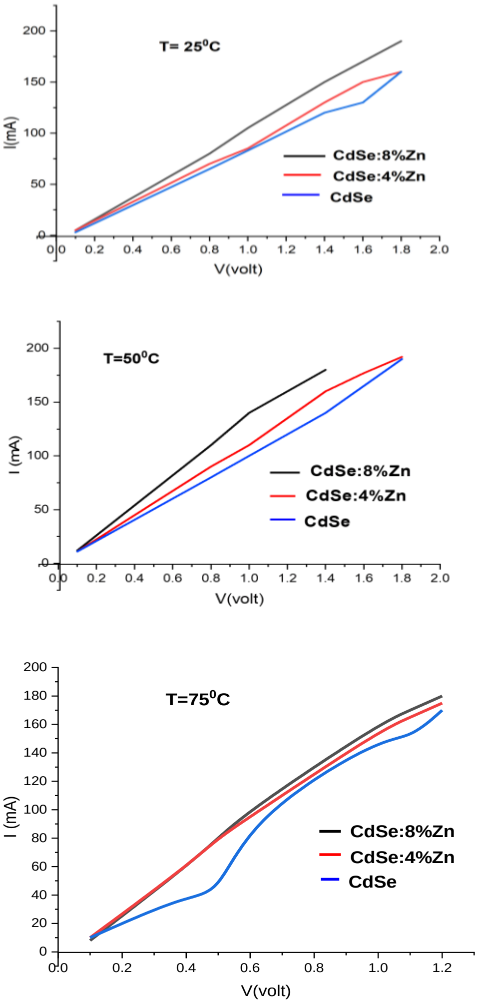

Fig. (4): The I-V for pure and Zinc-doped with CdSe at different temperatures.

The electrical resistance values of the prepared samples were found by calculating the reciprocal of the slope of the previous graphs, R=1/m

Table (4) : The change in electrical resistance with a change in temperature for the three samples.

$R(\Omega)*10^{3}$			
$T(C^{0})$	25	50	75
CdSe	10.56856	9.41426	7.10693
CdSe: 4%Zn	10.18960	8.97754	7.12920
CdSe: 8%Zn	9.33904	7.25643	6.81189

Table (4) shows the decreases in electrical resistance with increasing temperature and the increase in the percentage of doping which is due to the increased concentration of charge carriers generated by increasing temperature. The increase in the percentage of doping is a result of the formation of trap levels near the transport area , and therefore, the conductivity of the samples is good. The specific resistance and electrical conductivity were found through the following relationship (7) [8].

$$\rho = R*S/L \quad ....(7)$$

where R is the electrical resistance , S is the sample's area, and L is the sample's thickness . The electrical conductivity was calculated by finding the reciprocal of the specific resistance.

$$\sigma = 1/\rho \qquad (8).$$

Table (5) : The change in specific resistance (ρ) and electrical conductivity (σ) with change in sample temperature of the pure sample CdSe.

$T(C^{\circ})$	25	50	75
$T(k^{\circ})$	298	323	348
$1/T(k^{\circ})^{-1}$	0.003355705	0.003095975	0.002873563
$\rho\,(\Omega.m)*10^{-3}$	0.337	0.3	0.226
$\sigma\,(\Omega.m)^{-1}*10^{3}$	2.96	3.33	4.41
ln σ	1.08518	1.20297	1.48387

Table 6 : The change in specific resistance (ρ) and electrical conductivity (σ) with a change in sample temperature (CdSe: 4%Zn).

$T(C^{\circ})$	25	50	75
$T(k^{\circ})$	298	323	348
$1/T(k^{\circ})^{-1}$	0.003355705	0.003095975	0.002873563
$\rho\,(\Omega.m)*10^{-3}$	0.335	0.295	0.234
$\sigma\,(\Omega.m)^{-1}*10^{3}$	2.98	3.38	4.26
ln σ	1.09192	1.21787	1.44926

Table (7) : The-change in specific resistance (ρ) and electrical conductivity (σ) with a change in sample temperature (CdSe: 8%Zn).

T(C°)	25	50	75
T(k°)	298	323	348
$1/T(k^{\circ})^{-1}$	0.003355705	0.003095975	0.002873563
$\rho\ (\Omega.m)*10^{-3}$	0.330	0.259	0.243
$\sigma\ (\Omega.m)^{-1}*10^{3}$	3	3.85	4.11
ln σ	1.09861	1.34807	1.41342

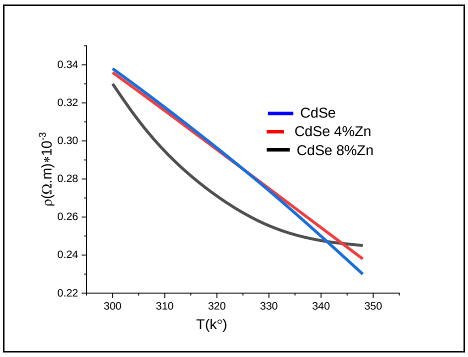

Fig. (5): The change of ρ with T change for the samples.

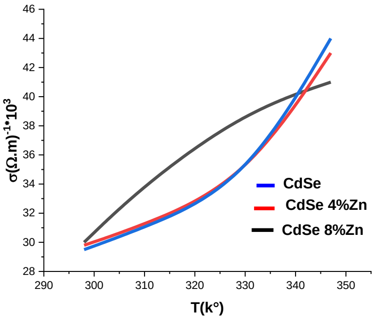

Fig. (6): The change of σ with T change for the samples.

Tables 5, 6, and 7 and Figures 5and 6 show that when the temperature increases, the specific resistance decreases and the electrical conductivity increases for pure and zinc-doped samples. The activation energy (Ea) was calculated based on the following relationship:

$$\sigma = \sigma_{\circ}\, e^{-Ea/kT} \ldots\ldots\ldots(9)\ [12].$$

Taking the logarithm of relation (9) we get:

$$\ln \sigma = \ln \sigma_{\circ} - Ea/kT \ldots\ldots\ldots(10)$$

The activation energy can be obtained by drawing the graphical relationship between lnσ and 1/T, where the activation energy can be calculated from the slope of the straight line of the previous relationship [8] as shown in Figure (7).

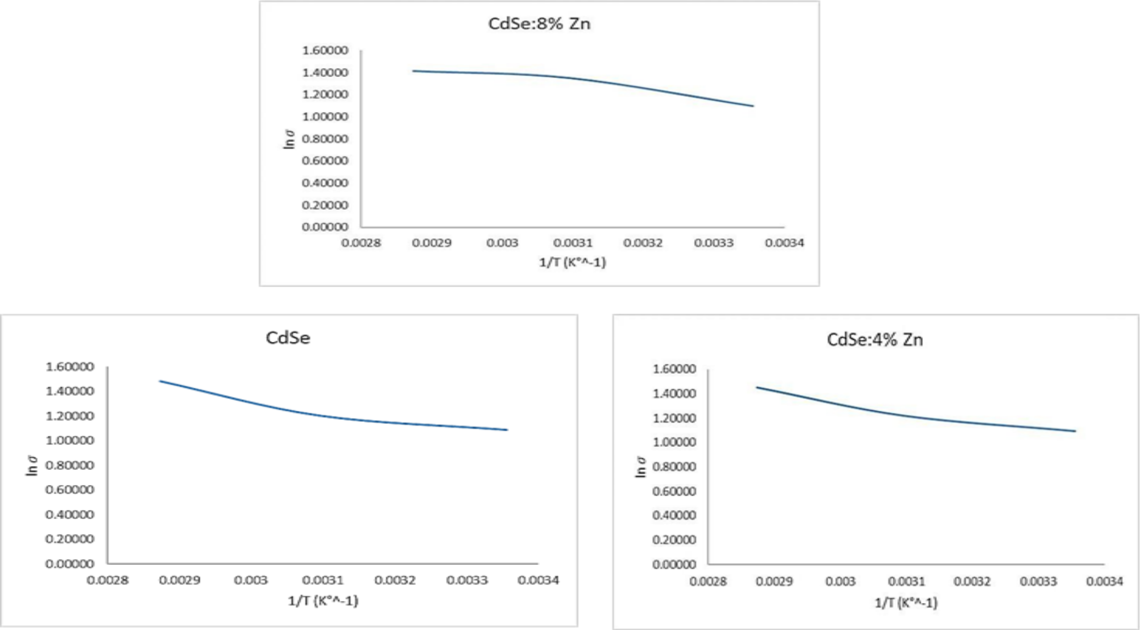

Figure (7): The change of ln σ and 1/T for pure and Zinc-doped with CdSe.

Table (8) : The activation energy (Ea) for pure and zinc doped (CdSe).

Samples	CdSe	CdSe: 4% Zn	CdSe: 8% Zn
Ea(eV)	0.069878809	0.063104235	0.057038414

Figure (7) and Table (8) show that there is a decrease in the activation energy of the samples after doping them with zinc due to the increase in the concentration of charge carriers upon doping and the formation of trap levels above the energy gap.

IV. CONCLUSION

The structural, optical , and electrical properties of the samples prepared from pure and zinc-doped (CdSe) were studied. It was found that the crystal structure of the samples is cubic, as both the crystal constant and the crystallization size of the doped samples decreased compared to the pure sample. It was noted from the fluorescence spectrum of the samples the appearance of several emission peaks and the fluorescence intensity was the highest possible for the sample (CdSe: 8% Zn) where two peaks were noted at the wavelength 631.8 nm and 704.9 nm, in addition to the appearance of several levels resulting from the trap levels formed upon doping. From the study of the feature (I-V), it was noted that there is an improvement in the electrical conductivity of the samples with an increase in the doping ratio and a decrease in the activation energy of the samples with an increase in the doping ratio.

CONFLICT OF INTEREST

The author declares that there is no conflict of interest.

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