

Effect of using Different Techniques on Structure and Optical properties of Prepared Nanoparticles CdS

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ABSTRACT: Nanoparticles CdS were prepared by using three techniques, firstly super cooling, and the second the liquid – liquid interface reaction and the third capping agent technique. The crystalline size was analyzed by x-ray diffraction data using Scherer method to be about 10 nm obtained from super-cooling and less to about 4nm by using capping agent. The amount of residual strain depends on the method of preparation .The band gap showed a blue shift from the bulk. The main reason for the blue shift are the quantum dimensional effect of the nanoparticles size according to the method used.

KEYWORDS: CBD, Supercooling, Liquid-Liquid Interface

I. INTRODUCTION

Nanoparticles semiconductor has a special optical and electronic properties that make it very differ from the bulk properties and this give it a great interest in the currently research [1]. When the structure of the semiconductor has a dimension enter in the nanoscale, the optical properties has a new distinguish proper than the bulk especially when the dimension comparable with Bohr radius then the properties show the quantum- size effect (quantum confinement) [2-6], this led to increase the optical band gap and the relation between the optical band gap and the size of nanostructure (size confinement) led to a great application in band gap engineering [7-10]. One of the important application of CdS is in the solar cells, it has a suitable properties that can be used to build a solar cell devices, it has a high photoconductivity gain and its spectral response is in the uv-visible range which make it useful to build visible radiation sensor[11,12] . The nanoparticles CdS has a great interest in the currently research because it can be used in fabrication of a single electron transistor and UV light emitting diode [13, 14, 15].

The main problem to prepare nanoparticles is that to prevent the accumulation and aggregation of the particles. There are many methods to prevent this aggregation such as using a super cooling, complex agent, super saturation. In this paper, nanoparticles CdS are prepared using super cooling, liquid –liquid interface reaction and capping agent methods and study its structure and optical properties using X-ray diffraction and UV-visible absorption spectrum.

II. EXPERIMENTAL DETAILS

A.PREPARATIO OF NANOPARTICLES CdS BY SUPERCOOLING

Nanoparticles CdS was prepared from aqueous solution of CdCl₂.H₂O (0.02 M) as a source of Cadmium, Na₂S.9H₂O (0.02 M) as a source of Sulphur. The chemical bath is prepared from the solution of CdCl₂.H₂O and Na₂S.9H₂O. At the first we dissolve 4.03 gm from CdCl₂.H₂O in 800 ml of deionized water by using magnetic stirrer till the read of PH-meter stable which indicate that we have homogenous solution. In another beaker we dissolve 5 gm from Na₂S.9H₂O in 200 ml of deionized water using magnetic stirrer till the read of PH-meter stable which indicate that we have a homogenous solution. Then we cooling the CdCl₂.H₂O solution using water bath tell the temperature reach to 5⁰C then we added drop by drop Na₂S.9H₂O solution by using burette to the CdCl₂.H₂O solution till the last drop is falling then leave the solution under high stirrer and that ow temperature for two hour then filtered and cleaned by deionized water and leave it to dry in oven under 60⁰C for twelve hour.



B.PREPARATION OF NANOPARTICLES CdS USING LIQUID –LIQUID INTERFACE REACTION

In this method we need to prepare the precursor at the first then the prepare of nanoparticle CdS, first step is to prepare the precursor which act as the source of the Cadmium and the second step the reaction at the interface between two immiscible liquid to get a nanoparticle CdS. So in the first step to get the precursor cadmiumdiethyldithiocarbamate, we applied the procedure that describe by O'Brien and R.Nomura [16]. In this procedure we dissolve (11 mM) from Sodium hydroxide in 50 ml methanol using a magnetic stirrer.then we added (1.128 ml) diethylamine and (0.65 ml) Carbon disulfide . We note that solution has a pale yellow.and after that and by using the ice bath we cooled the solution to 4°C for eight hour then we added by dropping wisely 50 ml of the methanol which dissolve in it (5.5 mM) from Cadmium Chloride and take it under stirrer for one hour and then we note that we have a yellow solid which represent to produse the precursor the we filtered and wished by methanol then water and at the last with methanol then dry it by oven in the temperature (65⁰-70⁰ c) for 12 hour. And in the Second step we work to prepare the nanoparticles CdS by apply the following steps at the first dissolve Na₂S in deionized water (11.46 mg .0.147 mmol) which consider as the source of sulfide .then added above it 50 ml of toluene containing 30 mg (0.073 mmol.) of cadmium diethyldithiocarbamate.now we noticed that we have two immiscible liquid one above each other and separated by interface layer as shown in the fig (1) then we put The beaker into an oven held at 65⁰ C and left undisturbed for 24 hour .at end of this time, a yellow thin film was found adhered to the interface of the two liquids. The procedure of the previous step can be explain in the following equation: at the first we reacted Sodium hydroxide with diethylamine and Carbon disulfide as shown in the following equation:

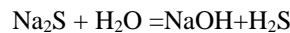


After cooling we added Cadmium Chloride and we get the following reaction:

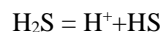


In this step we get the precursor Cd (S₂CNET₂)₂ which can be used in the following step to produce nanoparticle CdS as shown in the following equation:

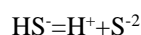
At the first we dissolved Na₂S in deionized water as shown in the following equation:



Then H₂S dissociated according to the following equation:



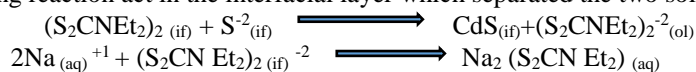
And at last HS dissociated as in the equation



All these done in aqueous solution for Na₂S, so the last result is the H⁺ and S⁻²

So when we layering the toluene above the aqueous solution which contain the Cd (S₂CNET₂)₂

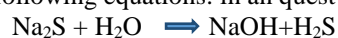
The following reaction act in the interfacial layer which separated the two solution



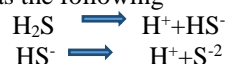
C.PREPARATION OF NANOPARTICLES CdS BY USING CAPPING AGENT

Dissolve 280 mg (3.6 mmol) in 50 ml methanol using ultrasonic and added to solution 130 ml from deionized water. At the same time and in another beaker ,Dissolve 110 mg (3.6 mmol) from Cd (NO₃)₂.4H₂O in 50 ml methanol then added 300 mg from polyvinylpyrrolidone (PVP) using magnetic stirrer for fifteen minuet then Added the solution which contain Na₂S drop by drop to the solution which contain Cd (NO₃)₂.4H₂O and using very high speed for stirrer for two hour then put in oven for 60°C for 12 hour then filtered and wished by deionized water three times and at the end washed by methanol then put the powder in oven to dry under 60°C for twelve hour.

We can ultrasited the reactions through the following equations: in an quest solution we have the following reaction:



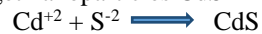
And because H₂S is a weak acid so it dissociate as the following



The Cd (NO₃)₂.4H₂O dissociate according to the following equation



At the last the following reaction happened to get nanoparticles CdS



And for characterization the structural and optical properties we use X-ray diffraction pattern, a Philips Xpert diffractometer utilizing monochromated CuK α radiation ($\lambda=0.15406$ nm) and UV-visible spectroscopy were recorded using PerkinElmer / lambda 35 double beam UV-vis-NIR spectrophotometer.

III. RESULT AND DISCUSSION

A. X-RAY DIFFRACTION RESULT

Figures 1, 2 and 3 show the x-ray diffraction pattern of CdS nanoparticles that are prepared using supercooling , liquid –liquid interface reaction and capping agent respectively . XRD peaks were found at 2θ values around 26° , 44° and 52° , referring to diffraction from (002), (110) and (112) planes reflections of the hexagonal modification or (111), (220) and (311) reflection of the cubical zinc blend CdS. Also there were shoulders around 25° corresponding to the hexagonal phase in the XRD spectrum. Therefore the samples are mixture of cubical and hexagonal structure. Tables (1, 2, 3) provide us the essential information about X-ray diffraction analysis for supercooling , interface reaction and capping samples respectively .

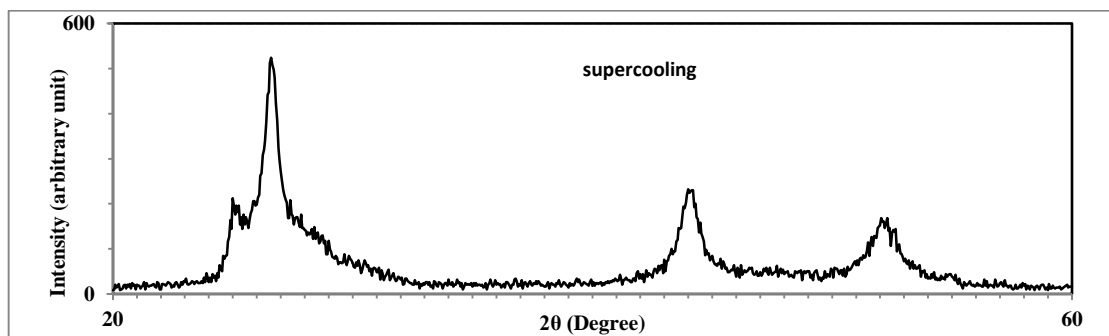


Fig. 1 x-ray diffraction pattern for nanoparticles using supercooling

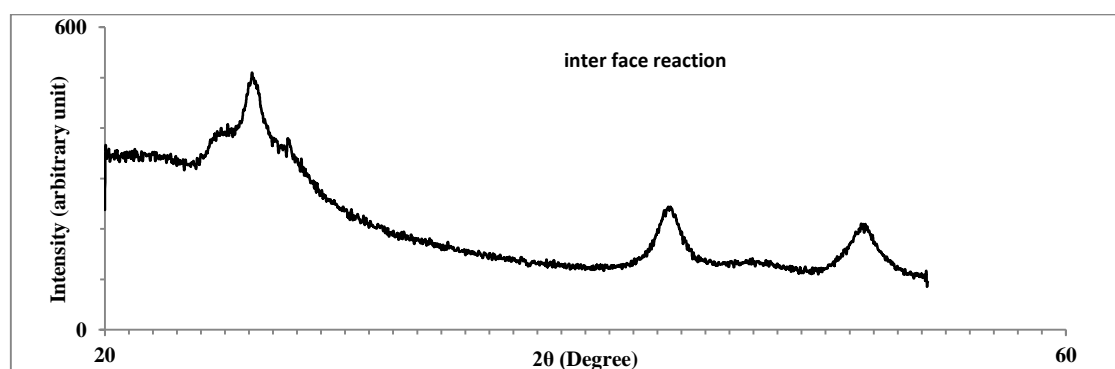


Fig. 2 x-ray diffraction pattern for nanoparticles using liquid –liquid interface reaction

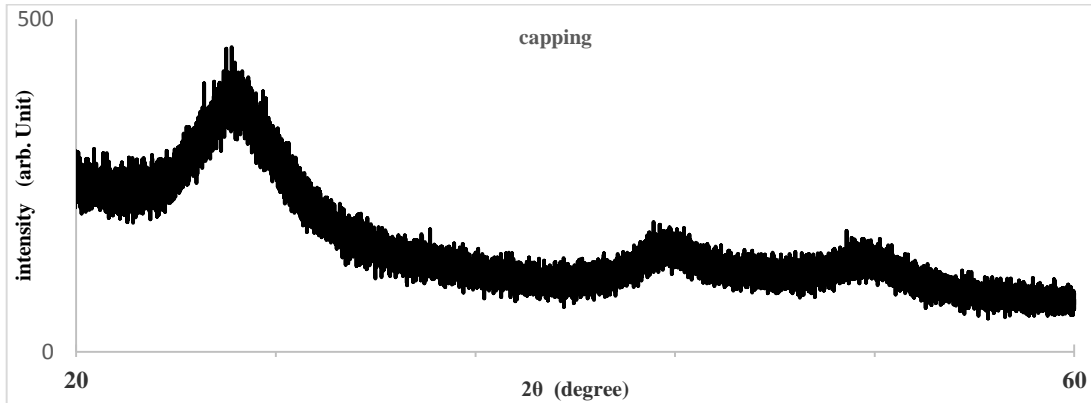


Fig. 3 x-ray diffraction pattern for nanoparticles using capping agent

Table 1 parameter from –ray diffraction analysis for super cooling

2θ (Deg.)	d _{hkl} Exp.(Å)	d _{hkl} Std.(Å)	phase	hkl	card No.
25.06	3.5506	3.5808	Hex.	(100)	96-900-8863
26.60	3.3484	3.3745	Hex.	(002)	96-900-8863
		3.3544	Cubic	(111)	96-101-1252
44.10	2.0519	2.0674	Hex.	(110)	96-900-8863
		2.0541	Cubic	(220)	96-101-1252
52.05	1.7556	1.7629	Hex.	(112)	96-900-8863
		1.7518	Cubic	(311)	96-101-1252

Table 2 parameter from –ray diffraction analysis for interface reaction

2θ (Deg.)	d _{hkl} Exp.(Å)	d _{hkl} Std.(Å)	phase	hkl	card No.
24.93	3.5688	3.5808	Hex.	(100)	96-900-8863
25.59	3.4782	3.3745	Hex.	(002)	96-900-8863
		3.3544	Cubic	(111)	96-101-1252
42.50	2.1253	2.0674	Hex.	(110)	96-900-8863
		2.0541	Cubic	(220)	96-101-1252
52.13	1.7531	1.7629	Hex.	(112)	96-900-8863
		1.7518	Cubic	(311)	96-101-1252

Table 3 parameter from –ray diffraction analysis for capping

2θ (Deg.)	d _{hkl} Exp.(Å)	d _{hkl} Std.(Å)	phase	hkl	card No.
25.06	3.5506	3.5808	Hex.	(100)	96-900-8863
26.44	3.3683	3.3745	Hex.	(002)	96-900-8863
		3.3544	Cubic	(111)	96-101-1252
43.78	2.0661	2.0674	Hex.	(110)	96-900-8863
		2.0541	Cubic	(220)	96-101-1252
51.86	1.7616	1.7629	Hex.	(112)	96-900-8863
		1.7518	Cubic	(311)	96-101-1252

International Journal of Advanced Research in Science, Engineering and Technology

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The broadening of diffraction peak provides information about average particle size was calculated using Debby Scherer's formula

$$d = 0.9 \lambda / \beta \cos \theta \quad (1)$$

Where d is main average of particles size, λ is the wave length of the X-ray diffraction ($\lambda = 0.15406 \text{ nm}$), β is full width at half maximum (FWHM), θ is the Bragg diffraction angle. Corresponding to the maximum intensity peak ($2\theta \approx 26.0^\circ$) particle size was 12.6 nm for nanoparticles CdS prepared using supercooling, 7.9 nm for nanoparticles CdS prepared using liquid –liquid interface and 6.1nm for nanoparticles using capping agent reaction.

Table (4, 5, 6) give us the calculation for grains size using Debby Scherer relation for supercooling, interface reaction and capping agent samples

Table 4 calculation grain size using Debby-Scherer relation for CdS nanoparticles using supercooling.

2θ (degree)	Observed FWHM (degree)	Corrected k_{a2} (degree)	After K_{a2} and Instrumental Broadening Corrections (degree)	Uncorrected G.S (nm)	corrected G.S (nm)	Integral breadth (degree)	Shape factor
26.60	0.7724	0.7674	0.7225	11.7	12.6	1.175	0.658
44.10	1.0130	1.0032	0.9537	9.4	10.0	1.227	0.825
52.05	1.1805	1.1685	1.1163	8.3	8.8	0.862	1.370

Table 5 calculation grain size using Debby-Scherer relation for CdS nanoparticles using Interface reaction

2θ (degree)	Observed FWHM (degree)	Corrected k_{a2} (degree)	After K_{a2} and Instrumental Broadening Corrections (degree)	Uncorrected G.S (nm)	corrected G.S (nm)	Integral breadth (degree)	Shape factor
25.89	1.1949	1.1907	1.1459	7.6	7.9	1.631	0.733
42.50	1.0584	1.0494	1.0306	8.9	9.2	1.279	0.828
50.13	1.6482	1.6387	1.5872	5.9	6.1	1.989	0.829

Table 6 calculation grain size using Debby-Scherer relation for CdS nanoparticles using Capping agent

2θ (degree)	Observed FWHM (degree)	Corrected k_{a2} (degree)	After K_{a2} and Instrumental Broadening Corrections (degree)	Uncorrected G.S (nm)	corrected G.S (nm)	Integral breadth (degree)	Shape factor
26.44	1.5477	1.5435	1.4986	5.9	6.1	1.808	0.856
43.78	1.1802	1.1713	1.1219	8.1	8.5	1.587	0.744
51.86	1.8420	1.8323	1.7802	5.3	5.5	1.930	0.954

We can attributed the result for the size in the following tables (7, 8,9,10), from these table we can note that the grain size is mainly depend on the method of preparation and we notice that the grain size for nanoparticles prepare using the capping agent has a smallest value , so we can consider the effect of capping agent play a great role to prevent the aggregation of particle than the other parameter that which be include in the other method , but this capping agent may help us to get a smallest size but in the other hand it also prevent the another material to reacted with nanoparticles which may be effect on the study the exist of these nanoparticle in the biological medium or to study the effect of doping material

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Table 7 the grain size with respect to the theta angle diffraction using Debby-Scherer equation for nanoparticles CdS prepared by supercooling

supercooling				
2θ°	26.60	44.10	52.05	
d nm	12.6	10.0	8.8	Average = 10.46

Table 8 the grain size with respect to the theta angle diffraction using Debby-Scherer equation for nanoparticles CdS prepared by liquid –liquid interface reaction

Interface reaction				
2θ°	25.89	42.50	50.13	
d nm	7.9	9.2	6.1	Average = 7.73

Table 9 the grain size with respect to the theta angle diffraction using Debby-Scherer equation for nanoparticles CdS prepare by capping agent

Capping				
2θ°	26.44	43.78	51.86	
d nm	6.1	8.5	5.5	Average = 6.7

Table 10 the average grain size with respect to method of preparation compare with bohr radius

Method for preparation	Average d nm	Bohr radius nm	Size confinement
supercooling	10.46	3	weak
liquid –liquid interface reaction	7.73	3	strong
capping agent	6.7	3	strong

Scherer's equation may give us the result that are different from actual size [17] the grain size and the residual stresses play a great role on the broadening the peaks. There some change in planar spacing and there is a shifting in the peaks due to the stresses which cause from the strain.. We adopted the Williamson –Hall method [18], to calculate the average crystallite size including strain, where the strain (ϵ) and crystallite size (L) are related to the measured β following the equation:

$$\beta \cos \theta / \lambda = 1/L + \epsilon \sin \theta / \lambda \quad (2)$$

Where β , λ and θ are the full-width at half maximum (FWHM) of the diffraction peaks, wavelength of the x-ray source and Bragg's angle, respectively. For this calculation, the most prominent peaks as shown in the Figs. (1, 2, 3) were analyzed. Figs. (4, 5, 6) represent the plots of $(\beta \cos \theta / \lambda)$ versus $\sin \theta / \lambda$ which is a straight line. The slope of the plot gives the amount of residual strain, whereas reciprocal of intercept on the y-axis give the average particle size.

Table 11 the calculation of $\beta \cos \theta / \lambda$ and $\sin \theta / \lambda$ from x-ray diffraction pattern of Nanoparticles CdS prepare using supercooling

supercooling									
θ2	θ	hkl	deg) (β	rad) (β	sin θ	θ Cos	λ nm	sin θ / λ	β cos θ / λ
26.5°	13.25	002	0.7225	0.0126	0.23	0.97	0.15406	1.5	0.07935547
43.6°	21.8	110	0.9537	0.0166	0.375	0.927	0.15406	2.53	0.1001051
51.9°	25.95	112	1.1163	0.0195	0.438	0.899	0.15406	2.85	0.1136336

**International Journal of Advanced Research in Science,
Engineering and Technology**

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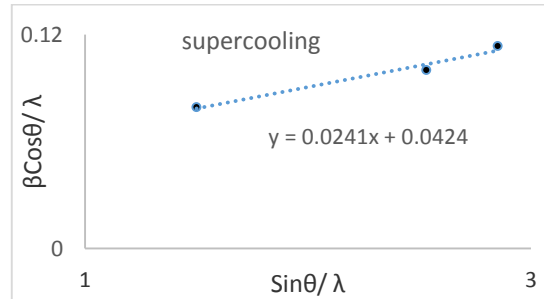


Fig. 4 Williamson –Hall plot to determine the particle size and strain of nanoparticles CdS Prepared using the supercooling

The slope of the plot gives the amount of residual strain, whereas reciprocal of intercept on the y-axis give the average particle size. Values $2.41 \cdot 10^{-2}$ and 23.6 nm are obtained for strain and average grain size, respectively.

Table 12 the calculation of $\beta \cos \theta / \lambda$ and $\sin \theta / \lambda$ from x-ray diffraction pattern of Nanoparticles CdS prepare liquid-liquid interface reaction

Liquid-liquid interface reaction									
θ_2	θ	hkl	deg) (β	rad) (β	$\sin \theta$	θ Cos	λ nm	$\sin \theta / \lambda$	$\beta \cos \theta / \lambda$
26.5^0	13.25	002	1.1459	0.01998	0.23	0.97	0.15406	1.5	0.1258
43.6^0	21.8	110	1.0306	0.01797	0.375	0.927	0.15406	2.53	0.1081
51.9^0	25.95	112	1.5872	.02768	0.438	0.899	0.15406	2.85	0.1616

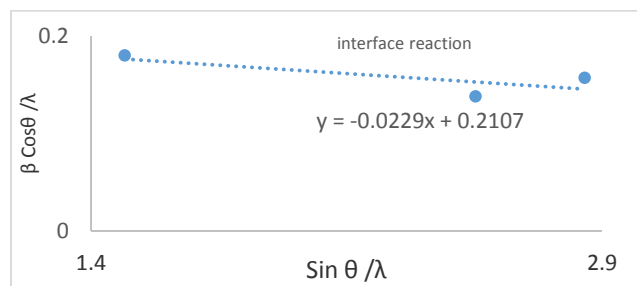


Fig. 5 Williamson –Hall plot to determine the particle size and strain of nanoparticles CdS prepared By liquid-liquid interface reaction

The slope of the plot gives the amount of residual strain, whereas reciprocal of intercept on the y-axis give the average particle size. Values $2.29 \cdot 10^{-2}$, 4.74 nm are obtained for strain and average grain size, respectively.

Table 13 the calculation of $\beta \cos \theta / \lambda$ and $\sin \theta / \lambda$ From x-ray diffraction pattern of nanoparticles CdS prepare using capping agent

Capping	θ	hkl	rad) (β	$\sin \theta$	θ Cos	λ nm	$\sin \theta / \lambda$	$\beta \cos \theta / \lambda$
26.5^0	13.25	002	0.0348	0.23	0.97	0.15406	1.5	0.252
43.6^0	21.8	110	0.0314	0.375	0.927	0.15406	2.53	0.21
51.9^0	25.95	112	0.0314	0.438	0.899	0.15406	2.85	0.233

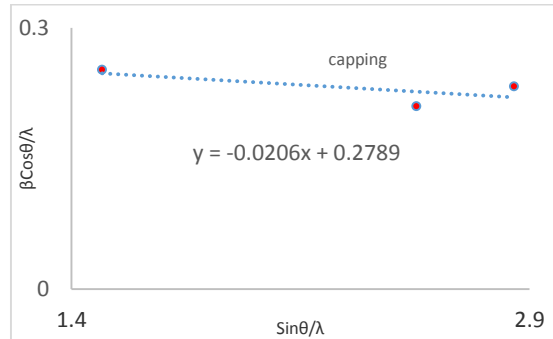


Fig. 6 Williamson –Hall plot to determine the particle size and strain of nanoparticles CdS prepared by capping agent

The slope of the plot gives the amount of residual strain, whereas reciprocal of intercept on the y-axis give the average particle size. Values 2.0×10^{-2} and 3.58nm are obtained for strain and average grain size, respectively.

Table 14 the variation of grain size using deby scherer and Williamson –hall equation with Respect to method of preparation

	d(nm) Deby Scherer's	d (nm) Williamson –Hall	residual strain
supercooling	10.46	23.6	2.41×10^{-2}
Interface reaction	7.73	4.74	2.29×10^{-2}
capping	6.7	3.58	2×10^{-2}

From these methods we note that the capping agent gives us a small radius for nanoparticles and these indicate to the effect of capping agent is big effect than the other factor that use in the other method. From previous result we note that the method that use the capping agent is the produce nanoparticles with smallest diameter and this indicate that the capping was succesfull to prevent the particles to aggregation and stabilizer these particles where super cooling produce nano-size but it is weak in quantum confinement and these indicate that the energy of atoms not reduce to value that cannot accumulation and aggregation. Although the capping agent it is a good method to prepare the nanoparticle but the capping is surrounding the atoms and this prevent the doping when we need to study the effect of the doping on the properties of nanoparticles CdS.

IV. UV-VISIBLE SPECTRUM ANALYSIS

Figure (7, 8, 9) explain the absorption spectrum on CdS nanoparticle prepared by three methods, supercooling, liquid – liquid interface reaction and capping agent. We observed from the following Table a blue shift in band edge for nanoparticles CdS prepared by these method as a compared to bulk CdS absorption edge.

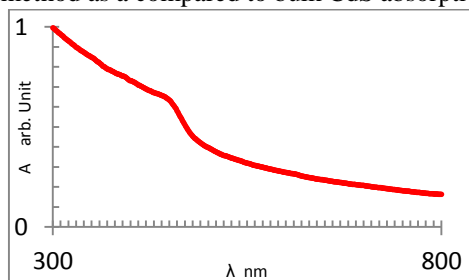


Fig 7 optical absorbe spectrum of CdS nanoparticles prepared by supercooling

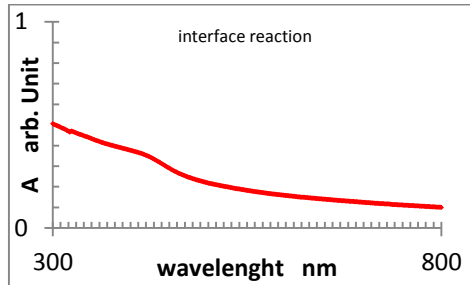


Fig 8 optical absorbtion spectrum of CdS nanoparticles prepared using liquid – liquid interface reaction

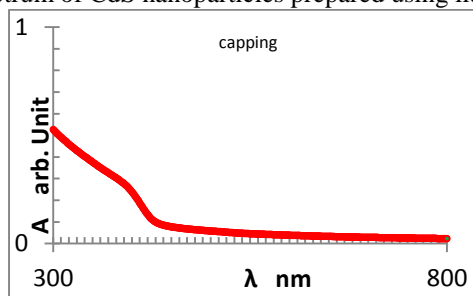


Fig 9 optical absorbce spectrum of CdS nanoparticles prepared using capping agent

Table 15 the blue shift amount with respect to the method of preparation for nanoparticles CdS prepare using supercooling, liquid –liquid interface reaction and capping agent.

	cuttoff nmλ	Shift in band edge nm
Bulk CdS	512	0
Supercooling	468	44
Liquid – liquid interface reaction	443	69
capping	413	99

The main reason for the blue shift are the quantum dimensional effect of the nanoparticles , which induce the wider band gap and the blue shift of absorption band due to the decrease of particle size , and surface effect of the nanoparticles , because the large surface force will cause crystal lattice aberration and a small crystal constant .at the same time , the short band length will induce the increase of the bond intrinsic oscillation frequency of nanoparticles , leading the blue shift of the absorption band . Therefore, the nanoparticles size is smaller and the blue shift is more obvious [19]. The Estimeated the nano size from the absorb spectrum using Gaussian fitting model

Proposed by Viswanatha and sarma was followed in order to obtain estimates of mean diameter of nanoparticles using absorption spectra [20-25]. This method provide accurate estimates of experimental diameters for different families of semiconductor nanoparticles such as CdS.To apply this method, the position of peak (E_0), as well as its full width at half maximum (FWHM) are obtained using the first derivative of the curve as shown in Fig. 10

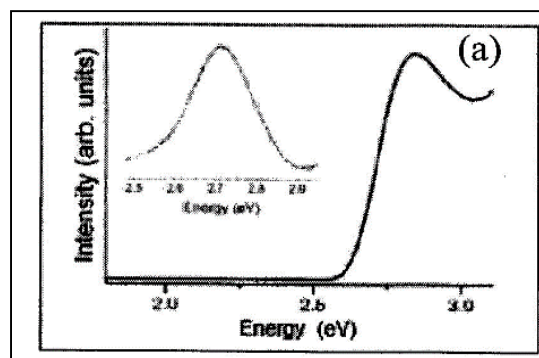


Fig. 10 Exhibits: (a) Electronic absorption spectrum of CdS nanocrystalline thin film, (b) Gaussian fitting of the spectra the CdS nanocrystalline thin film [23]

The UV absorption spectrum for CdS is shown in Figure (10a) Differentiation of this absorption spectrum yields the curve shown in Figure 10b. In order to obtain the position of absorption maxima, Gaussian function fitting of absorption spectra was performed, as shown in Figure 10b. To apply this method, the position of the peak energy E_0 is obtained using the first derivation of the curve. The E_0 is translated as d (average) [21-24] by the use of the formula

$$\Delta E_g = 1/ad^2 + bd + c$$

Where a , b and c are constants that depend on the identity of the semiconductor; for CdS their values are 0.1278, 0.1018 and 0.1821 respectively. Here, ΔE_g is the observed shift in the band gap (E_g) given by $E_0 - E_g$ Similarly, E_1 and E_2 can be translated to sizes (d_1 , d_2). Which, E_1 is ($E_0 - FWHM/2$) and E_2 is ($E_0 + FWHM/2$) The main diameter (d), is obtained by solving equation Then we can define the apparent and real relative percentage distribution according to these equations

$$\Delta D_{app}\% = (d_1 - d_2)/d_{av} \times 100$$

$$\Delta D_{real}\% = A \times (\Delta D_{app})^2 + B \times \Delta D_{app} + C$$

Where: $A = -0.0025$, $B = 0.524$, and $C = -1.41$

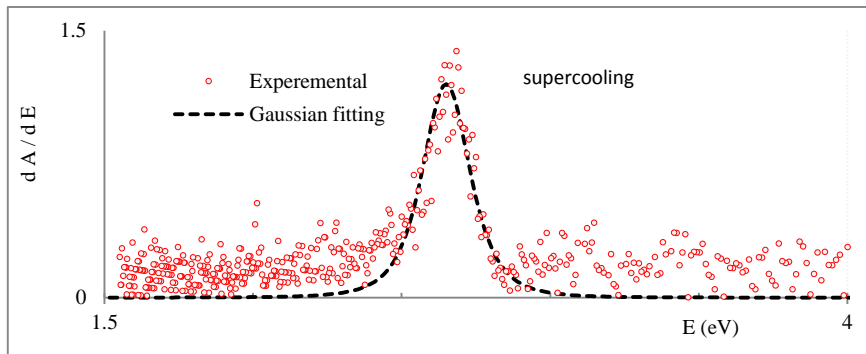


Fig. 11 first derivative for adsorbe with respect to energy as a function for energy for CdS nanoparticles prepared by supercooling

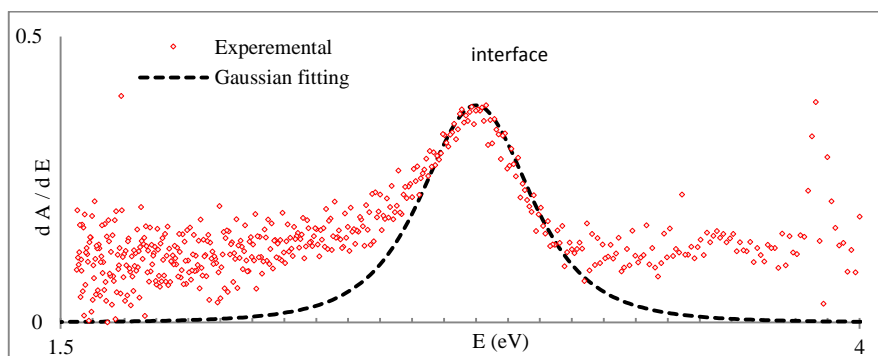


Fig. 12 first derivative for adsorbe with respect to energy as a function for energy for CdS nanoparticles prepared by interface reaction

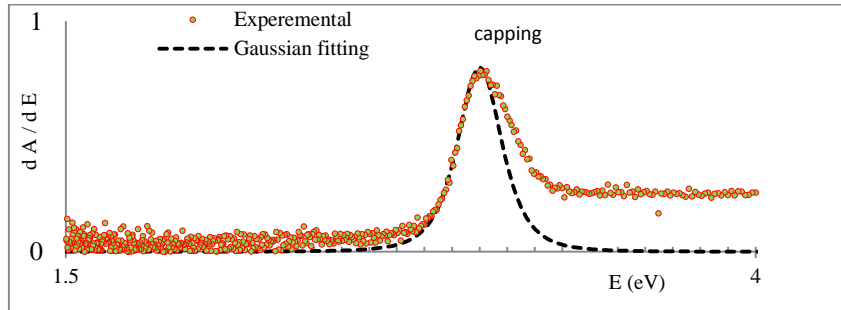


Fig. 13 first derivative for adsorbe with respect to energy as a function for energy for CdS nanoparticles prepared by capping agent

From Table 14, 15, 16, we note that the technique that use capping agent give us a small nanoparticles size with small deviation in size, from this we can consider that the capping agent has a strong effective to prevent the aggregation of the size, but the liquid –liquid interface reaction give us a nanoparticles without sourroding material and this usefull when we need to study the reacted of nanoparticles with other material. From the previous table we note that the radius of particles is in the range of nanoscale (less than 100 nm) and is Compatible with Bohr radius which give us quantum confinement (size – effect) which give a nanoparticle the Special properties that distinguished from bulk

Table 16 grain size corresponding to the method of preparation of nanoparticle CdS using supercooling , liquid –liquid interface reaction and capping agent

Eg bulk eV	Method to prepare nanoparticles	Eg nanoparticles eV	ΔE_g eV	d nm	Bohr radius nm	Quantum confinement
2.42	Supercooling	2.65	0.23	5	3	Strong
2.42	Liquid –liquid interface reaction	2.8	0.28	3.9	3	Strong
2.42	Capping agent	3	0.58	3	3	Strong

Table 17 distribution of nanoparticles size with respect the method of preparation the nanoparticles CdS using supercooling , liquid-liquid interface reaction and capping agent

Method to prepare nanoparticles	E_0 eV	β	E_1 eV	E_2 eV	d_0 nm	d_1 nm	d_2 nm	$D_{app}\Delta\%$ $= (d_1 - d_2)/d_{av} \times 100$	$\Delta D_{real}\%$ $= A \times (\Delta D_{app})^2 + B \times \Delta D_{app} + C$ A= -0.0025, B= 0.524, C= -1.41
Supercooling	2.65	0.2	2.75	2.55	5.1	6.7	4.2	49	18
Liquid –liquid interface reaction	2.8	0.4	2.6	3	3.9	5.7	3	70	23
Capping agent	3	0.2	2.9	3.1	3	3.4	2.8	20	8

Table 18 the grain size of nanoparticles CdS with respect to the method of preparation supercooling , liquid – liquid interface reaction and capping agent

Technique of preparation	d (nm) Debby-Scherer formula	d (nm) Williamson –Hall	d (nm) Gaussian fitting
Supercooling	10.46	23.6	5.1
Liquid –liquid interface reaction	7.73	4.74	3.9
Capping agent	6.7	3.58	3

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V. CONCLUSIONS

In this work, we use three techniques to prepare nanoparticles of CdS, supercooling, liquid-liquid interface reaction and capping agent. The aim is to prevent the particles from aggregation and give us a particle with nanosize, we find that the capping agent gives us a particle with the smallest size and very comparable with Bohr radius. We estimated the nanosize (diameter) from XRD –diffraction using the Debye – Scherrer and Williamson –Hall, and from UV-Visible spectrum using the tight –binding model that is derived by Samara et al. All these models give us the same behavior of the size according to the method of preparation and we consider that the tight –binding model is much more accurate between them because it estimates the size with any reduction parameter such as the little shift in angle of diffraction due to the nanosize.

REFERENCES

- [1] R.Banerjee,R.Jayakrishnan,P.Ayyub, "Effect of the size-induced structural transformation on the band gap in CdS nanoparticles" , "J. Physics Condens Matter" VOL.12 , NO.50 , PP. 10647 , 2000.
- [2] A.P.Alivisatos, "Perspectives on the Physical Chemistry of Semiconductor Nanocrystals", "J. Phys. Chem.", VOL. 100, NO.31, pp. 13226-13239, 1996
- [3] Y.K.ayanuma, " Quantum-size effects of interacting electrons and holes in semiconductor microcrystals with spherical shape", "Phys.Rev.B" , VOL.38, ISS.14,9797 ,1988.
- [4] G.Ledoux, O.Guillois,D.Porterat,C.Reynaud,F.Huisken,B.Kohn,andV.Paillard," Photoluminescence properties of siliconnanocrystals as a function of their size", *Phys.Rev.B* ,VOL.62,ISS.23, 15942, 2000.
- [5] C.C.Yang and S.Li, "Size, dimensionality, and constituent stoichiometry dependence of bandgap energies in semiconductorquantum dots and wires" *Phys.Chem.C.*, VOL.112, 2851(2008).
- [6] S.Sapra and D.D.Sarma, "Evolution of the electronic structure with size in II-VI semiconductor nanocrystals" *Phys.Rev.B* VOL.69, ISS.12, PP.125304 , 2004 .
- [7] J.Li and L.-W.Wang,*Phys.Rev.B* "Band-structure-corrected local density approximation study of semiconductor quantum dots and wires" VOL. 72, ISS. 12 , PP.125325, 2005.
- [8] P.Nandakumar, C. Vijayan, andY.V.G.S.Murti, "*Absorption and photoluminescence studies on CdS quantum dots in Nafion*",*J.Appl.Phys.*"VOL.91, NO.3, PP.1509-1514,2002.
- [9] A.Milekhin,M.Friedrich,D.R.T.Zahn,L.Sveshnikova,and S.Repinsky,*Appl "Phys.A:Mater.Sci. Process."* , VOL.69, PP.97,1999.
- [10] K.Murakoshi, H.Hosokawa, andS.Yanagide, *jpn.J.Appl.Phys, Part1*,VOL. 38, PP.522 , (1999)
- [11] R. H . Bube "*Photoconductivity of Solids*" (John Wiley and Sons, New York), 1960, p391.
- [12] Gayakwad Rama Kanta,A naloge and digital Control System (Prentic-Hall Interational Edition , London), 1988, p46.
- [12] Gayakwad Rama Kanta,A naloge and digital Control System (Prentic-Hall Interational Edition , London), 1988, p46.
- [13] R.K. Duchaniya , "Optical Studies Of Chemically Synthesis CdS Nanoparticles" , "International Journal of Mining, Metallurgy & Mechanical Engineering (IJMME) Volume 2, Issue 2 (2014) ISSN 2320–4060 (Online) "
- [14] K.K. Nanda, S.N. arangi, S. N. Sahu , " Measurement of surface roughness by atomic force microscopy and rutherford back scattering spectrometry ofCdS nanocrystalline films", "*Nanostructure Mater*", VOL10, NO.8, PP. 1401-1410, (1998).
- [15] M. Maleki, M. Sasani Ghamsari, Sh. Mirdamadi, R. Ghasemzadeh , " A facile route for preparation of CdS nanoparticles", "*Semiconductor Physics, Quantum Electronics & Optoelectronics.*" VOL. 10, NO. 1, P. 30-32.,2007
- [16] P.O'Brien and R. Nomura, "Single-molecule precursor chemistry for the deposition of chalcogenide(S or Se)-containing compound semiconductors by MOCVD and related methods" "*J.Mater.Chem.*"VOL. 5,ISS.11,PP. 1761-1773, 1995
- [17] G.Cao,"*Nanostructure and Nanomaterials*",1st ed ., Imperial College Press,London,2004.
- [18] G.K.Williamson , W.H.Hall , " X-ray line broadening from field Al and W " , "*Acta Metall .1*" , pp.22-31 , 1953
- [19] Z.Jinxin ,Z.Gaoling , and H.Gaorong , " Preparation of CdS nanoparticles by hydrothermal method in microemulsion " , "*Front .Chem.China.*"VOL.2,NO.1,PP.98 ,2007
- [20] C.N.R.Rao,P.J.Thomas., G.U.Kulkarni,"*Nanocrystals:Synthesis,Properties , and A plications* " , first ed ., material science , 95 . 2007 , springer
- [21] R.Viswanatha, et al., "Synthesis and Characterization of Mn-Doped ZnO Nanocrystals *The Journal of Physical Chemistry B*", VOL.108,NO.20, PP. 6303-6310, 2004.
- [22] S.Sapra, and D.D. Sarma, "Evolution of the electronic structure with size in II-VI semiconductor nanocrystals". "*Physical Review B*",VOL. 69,NO.12,PP. 125304 , 2004
- [23] R.Viswanatha, et al., " Electronic structure of and quantum size effect in III-V and II-VI semiconducting nanocrystals using a realistic tight binding approach." , " *Physical Review B*" , . VOL.72,NO.4, PP. 045333, 2005
- [24] S.Sapra,N. Shanthi, and D.D. Sarma,"Realistic tight-binding model for the electronic structure of II-VI semiconductors.", "*Physical Review B*", VOL.66 , NO.20 , PP. 205202 , 2002.
- [25] D.Fan, and P.J. Thomas, "Easy synthesis of luminescent CdS nanocrystals using a biphasic oil–water system." , "*Materials Chemistry and Physics*",VOL. 129 , ISS. (1–2): PP. 564, 2011.



ISSN: 2350-0328

International Journal of Advanced Research in Science, Engineering and Technology

Vol. 2, Issue 4 , April 2015

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