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Study of effect the particle size on CdS optical properties as solar cell

Cálculo de las variaciones de los elementos orbitales con diferentes perturbaciones para la órbita satelital retrógrada (LEO)

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ABSTRACT/ In this work, one can make theoretical studies to show the effect of the particle size on semiconductor properties. We chose Cadmium Sulphide CdS because it is a unique semiconductor material used in a wide range of modern applications [1]. An example of what can be applied by using CdS is the manufacture of solar cells because it has distinct electronic and optical properties. It is also known that solar cells have become an indispensable source of energy in the world. We design one layer of bulk CdS and one layer of Nano CdS within the visible region (300-800 nm) [Air\bulk CdS\Air] and [Air\ Nano CdS\Air]. The results show that the transmittance equal T= 53 at 550 nm for bulk CdS at normal incidence and for Nano CdS with particle size 3nm the transmittance is T= 75.4 and transverse-electric (S- Polarized) and transverse-magnetic (P- Polarized) transmittances are TE=71 and TM= 79 at non-normal incidence (θ=27º).
Keywords: transmittance, Nano particle size, CdS, refractive index.
RESUMEN/ En este trabajo, se pueden realizar estudios teóricos para mostrar el efecto del tamaño de partícula en las propiedades de los semiconductores. Elegimos Cadmium Sulphide CdS porque es un material semiconductor único utilizado en una amplia gama de aplicaciones modernas [1]. Un ejemplo de lo que puede aplicarse mediante el uso de CdS es la fabricación de células solares porque tiene propiedades electrónicas y ópticas distintas. También se sabe que las células solares se han convertido en una fuente indispensable de energía en el mundo. Diseñamos una capa de CdS a granel y una capa de Nano CdS dentro de la región visible (300-800 nm) [Air \ bulk CdS \ Air] y [Air \ Nano CdS \ Air]. Los resultados muestran que la transmitancia es igual a T = 53 a 550 nm para CdS a granel con incidencia normal y para Nano CdS con un tamaño de partícula de 3 nm, la transmitancia es T = 75.4 y transversa-eléctrica (S-polarizada) y transversa-magnética (P- polarizada) las transmisiones son TE = 71 y TM = 79 con incidencia no normal (θ = 27º).
Palabras clave: transmitancia, tamaño de partícula nano, CdS, índice de refracción.

1. Introduction

Solar cells started to bring vitality to urban and rural homes, as well as places of business. Solar cell electricity systems have become very important sources of energy in the world [1].
At the momentum, we cannot say that the use of photovoltaic (PV) systems is the best means of resolving the issues associated with energy consumption in the world. Employing renewable energy resources is, however, as an effective alternative option for maintaining and supporting a country's economy [2]. Solar cells generate electricity using p-n junction building blocks. They are made from different semiconductor materials, which absorb different portions of the sunlight spectrum [2].
In this work, we study the effect of the particles size on the properties of CdS Nano thin films.
"Cadmium Sulphide (CdS) is an important semiconductor appropriate for a wide scope of uses because of its unique electronic and

optical properties". CdS is a II-VI compound semiconductor group; CdS is one of the most important materials for applications to electro-optical devices such as solar cells, photo sensors, laser materials and optical waveguides [3]. CdS has proven to be an ideal material when used as window layer in thin-film solar cells of heterojunction with CdTe or Cu (In, Ga) Se2 [4, 5]

2. Theory

2-1 Transmittance and reflectance

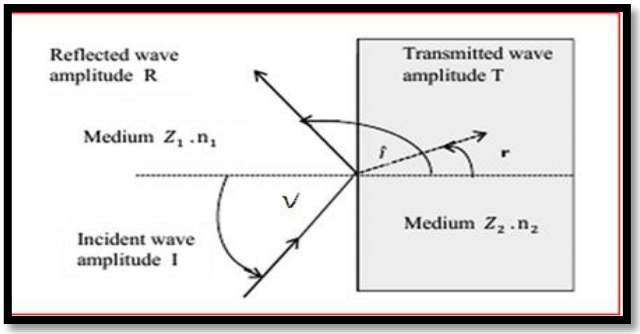


Figure 1 shows the geometry of a plane electromagnetic wave incident on a plane surface [7].

A plane electromagnetic wave is incident on a plane surface separating isotropic media, as shown in figure 1. The equation $r = (n_1 - n_2)/(n_1 + n_2)$ can be used to define the Fresnel amplitude reflection coefficient (r) for a point of interaction between two non–absorbing media at normal incidence. Here, n_1 and n_2 are the (real) directories of refraction of the two media [6]. The calculations are carried out for transparent media calculated using the following relation: [7]

$$R = \left(\frac{y_o - y_1}{y_o + y_1}\right)\left(\frac{y_o - y_1}{y_o + y_1}\right)^* \qquad (1)$$

Where y_ρ "is known as the characteristic optical admittance of the medium $(y_\rho = N_\rho \gamma)$ and γ is the admittance of free space "[7]:

$$T = \frac{y_2}{y_1}\tau^2 = \frac{4y_1y_1}{(y_1+y_2)^2} \qquad (2)$$

Where τ is transmission coefficients $\tau = 2y_o/[y_o + y_1]$ .For an oblique incidence the reflectively and the transmission are known as the relationship

$$R = \left(\frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\right)\left(\frac{\eta_0 - \eta_1}{\eta_0 + \eta_1}\right)^* \qquad (3)$$

$$T = \frac{4\eta_0 \mathrm{Re}(\eta_1)}{(\eta_0+\eta_1)(\eta_0-\eta_1)^*} \qquad (4)$$

Where $\eta_p = y_\rho / \cos\upsilon$ and $\eta_s = y_\rho \cos\upsilon$ and υ is angle of incidence [7]

2-2. Quantum size effects

Nanoscience and nanotechnology basically deal with structure, characterization, exploration, and utilization of nanostructured materials. Nanostructures establish an intermediate between the molecular scale and infinite bulk. Individual nanostructures comprise bunches, quantum dots, nanocrystals, nanowires, and nanotubes [8].

We can determine Urbach energy (Eu), optical energy gap (Eg), the absorption coefficient and the nature of the transition by calculating optical absorption spectra of thin films. One could use the thickness (t) to determine the optical absorption coefficient α_o by estimating the T (l) and R (l) as follows [9]:

$$\alpha_o = \frac{1}{t}\ln\frac{(1-R^2)}{T} \qquad (5)$$

The photon energy (hυ) and the absorption coefficient α_o are related by the equation [9].

$$\alpha_o hv = \beta(hv - Eg)^n \qquad (6)$$

Where β is the band tailing parameter (a constant), which depends on the effective mass of the electrons and holes and the optical middle density. The power exponent n depends on the nature of the transition.

The Effective Mass Approximation (EMA) or Brus model is the most popular to clarify how the value of the energy band gap depends on the semiconductor quantum-dot size. This model depends on the value of the effective mass m_e^* and m_h^* of electrons and holes, according to the Brus equation [10,11]:

$$\Delta E_g = \frac{\hbar^2\pi^2}{2\mathcal{R}^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right] - \frac{1.786e^2}{\varepsilon\mathcal{R}} - \frac{0.124e^4}{h^2\varepsilon^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right]^{-1} \qquad (7)$$

Where $\mathcal{R}$ is the radius of the quantum dot and ε is the dielectric constant [12, 11]

$$\Delta E_g = E_g^{nano}(\mathcal{R}) - E_g^{bulk} \qquad (8)$$

$E_g^{nano}(\mathcal{R})$ Is the energy gap for the marital in the quantum dot (effective band gap) , E_g^{bulk} is the bulk band gap of energy. Equation (8) becomes [10 ,12 and 13]:

$$E_g^{nano}(\mathcal{R}) = E_g^{bulk} + \frac{\hbar^2\pi^2}{2\mathcal{R}^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right] - \frac{1.786e^2}{\varepsilon\mathcal{R}} - \frac{0.124e^4}{h^2\varepsilon^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right]^{-1} \qquad (9)$$

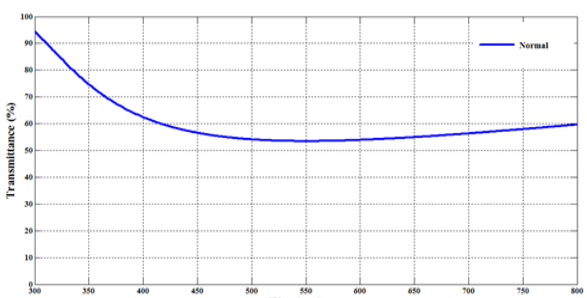
3. Results and Discussion

For this research we designed a computer program (MATLAB) to calculate transmittance for CdS at visible wavelength (300 -800 nm) and the effect nano particle sizes on transmittance and other properties such as the energy gap and refractive index. This program depends on the Effective Mass Approximation (EMA) equation, the radius of the quantum dot and the effective band gap. Table 1 shows the values of the physical properties that used in the program

Table 1 shows some physical properties of Cadmium Sulphide CdS

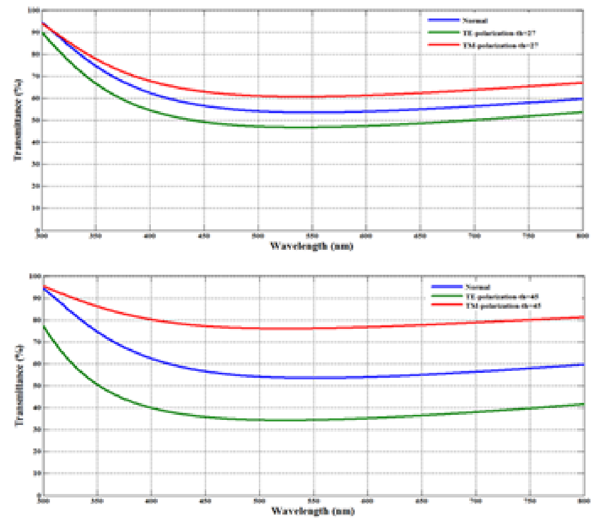
Parameters	**CdS**
Energy gap E_g (eV)	2.42
Type of energy gap	direct
Electron effective mass (m_e*)	0.153
Hole effective mass (m_h*)	0.7
Conductivity type	n
Refractive index	2.3

The coating consists of CdS and the substrate (Air) with the refractive index n=1, transmittance of wavelength at λ_o=550nm. Figure 2 shows the transmittance for the bulk CdS and we find T= 53. at 550 nm .
It was happening according to destructive and constructive interference occurs at CdS layer and determine the transmission depending on optical thicknesses of layer which was quartered-wavelength long and refractive index and angle of incidence light using equation (4) as shown in Figure 3 , the transmittance for bulk CdS and incidence angles 27°, 45° and 9°, and Table 2 gives the transmittance values of a 550 nm wavelength at oblique incidence.



Figer 2 shows the Transmittance as function of wavelength at normal incidence for bulk CdS.
Table 2. The values of bulk CdS transmittance for the air substrate for incidence angles 27 °, 45 ° and 90 °.

Incidence angle	27°	45°	90°
Transmittance -TE	46	34	0
Transmittance -TM	60	76	0



Figer 3(a,b,c) shows the transmittance as function of wavelength at the incidence angle 27°, 45° and 90° for bulk CdS.
One can be used CdS nano thin films and investigated the effect of the particles size on some physical properties. We took 20 different particle sizes ranging from 3nm to 22 nm in steps of 1 nm
Figure 4 and Table 3 shows the effect of the particle size on the effective energy band gap and refractive index of the nano particles. When the particle size decreases, the energy gap increases and that according to equation (8) and the refractive index of the nano particles decreases when the particle size decreases (particle size approaches Bohr exaction radius (αo=3 nm)) .

Table 3 .The effect of particle size on the energy gap and refractive index for nano CdS

Particle Size	refractive index(ng)	energy gap(Eg)
3	1.7223	3.7512
4	2.0833	3.1688
5	2.2505	2.8992
6	2.3413	2.7528
7	2.396	2.6645
8	2.4315	2.6072
9	2.4559	2.5679
10	2.4733	2.5398
11	2.4862	2.519
12	2.496	2.5032
13	2.5036	2.4909

14	2.5097	2.4811
15	2.5146	2.4732
16	2.5186	2.4668
17	2.5219	2.4615
18	2.5247	2.457
19	2.527	2.4532
20	2.529	2.45
21	2.5308	2.4472
22	2.5323	2.4448

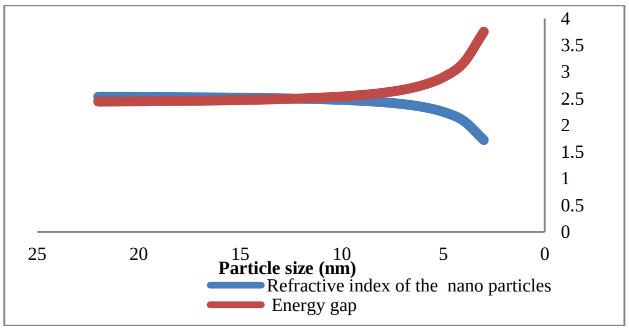


Figure 4 shows effect the particle size on the Nano enrgy gap and refractive index of the Nano particles .

According to the change in energy band gap and refractive index, because the particle size, the transmittance became better and clear as shown in Table (4) and figures 5 and 6, the transmittance at the normal incident at 550 nm for all 20 particle sizes,

Figure 4 Shows the transmittance as a function of wavelength at normal incidence for CdS at 550 nm and particle sizes from 3nm to 12nm .

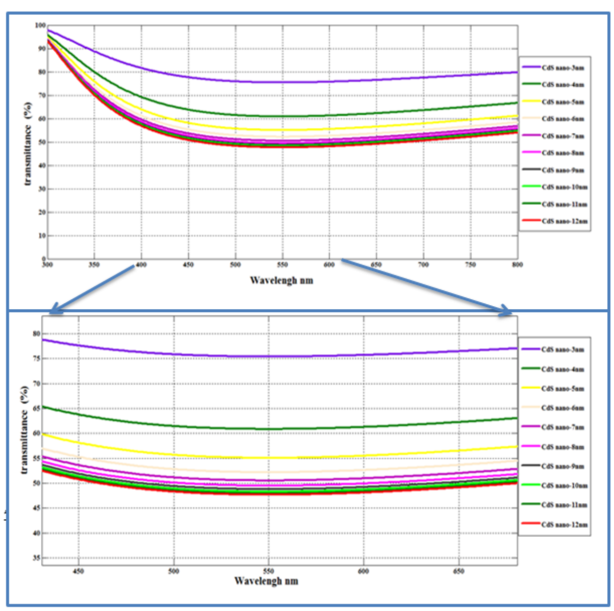


Figure 5 Shows the Transmittance as function of wavelength at normal angle for CdS at 550 nm and particle sizes from 3 nm to 12 nm.

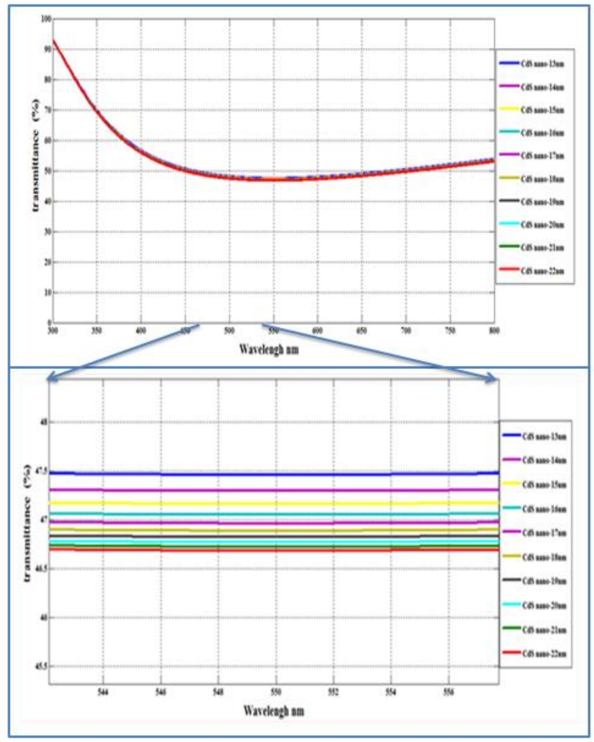


Figure 6 Shows the Transmittance as function of wavelength at normal angle for CdS at 550 nm and particle sizes from 13 nm to 22 nm.

Table 4 Transmittance at normal incidence for Nano CdS at 550 nm for 20 different particles sizes.

Partial size e nm	Transmittance at 550 nm	Partial size e nm	Transmittance at 550 nm
3	75	13	47
4	60	14	47
5	55	15	47
6	52	16	47
7	50	17	46
8	49	18	46
9	48	19	46
10	48	20	46
11	47	21	46
12	47	22	46

At oblique incident 27o, the TE and TM transmittance change as shown in figures 7. The transmittance increases when the particle size decreases at non-normal incident (27o) and Table 5 shows the results for the TE and TM transmittance.

The center wavelength of the transmittance will shifts toward the shorter wavelengths as the angle of incident increases; The equation $\lambda = \lambda_o\sqrt{1 - \sin^2\theta/\eta^2}$ can be used to describe this dependence[13].

Here λ_o is the central wavelength at normal incident, η is the effective refractive index inside the layer. When the incident angle increases, a split the transmission characteristics for the S-and P-polarized beams can exist, this was clearly shown in figures 5 and 6.

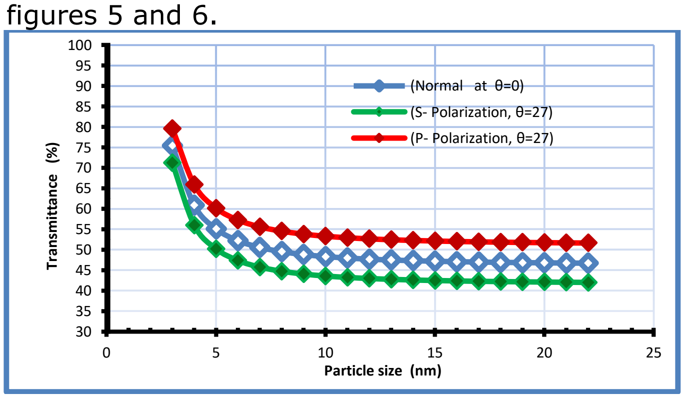


Figure 7 Transmittance as a function of particle size at non-normal incidence (θ=27o).

Table 5 Transmittance TE and TM at non-normal incidence θ=27 for Nano CdS at 550 nm for 20 different particles sizes.

Transmittance-TE at angel (27o) at 550 nm	Transmittance-TM at angel (27o) at 550 nm	Particle Size
71.1883	79.5957	3
56.0060	65.8706	4
50.2054	60.1567	5
47.3605	57.2608	6
45.7426	55.5866	7
44.7301	54.5287	8
44.0525	53.8165	9
43.5759	53.3135	10
43.2276	52.9447	11
42.9651	52.6662	12
42.7622	52.4507	13
42.6022	52.2804	14
42.4736	52.1434	15
42.3688	52.0317	16
42.2821	51.9392	17
42.2097	51.8619	18
42.1485	51.7966	19
42.0964	51.7409	20
42.0516	51.6931	21
42.0128	51.6516	22

Also the refractive index of the nano particles affects the transmittance. When the refractive index of the nano particles decrease the transmittance increases as show in Figure 7. Inversely, the transmittance increases when the energy gap of the effective band gap increases as shown in figure 8.

"The effect of quantum confinement appears" when particle size (Ps=2R) is equivalent or less than the Bohr exciton radius (ɑo=3nm) and "the effect of quantum confinement" increments drastically, resulting in increased transmittance of material

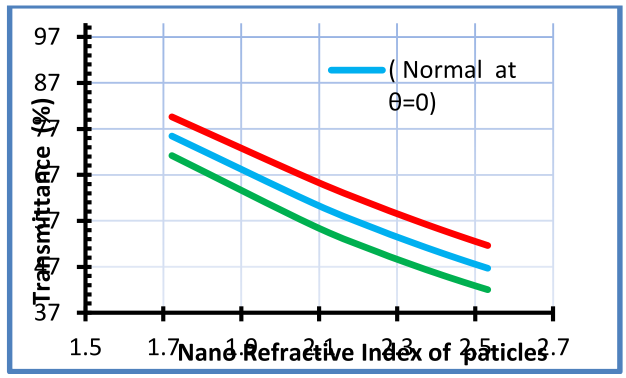


Figure 8 Shows the transmittance as a function of refractive index of nano particles at non-normal incidence (θ=27o).

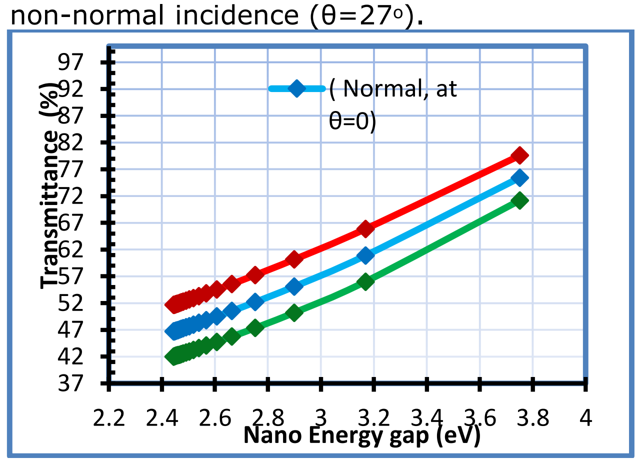


Figure 9 Transmittance as a function of the energy gap for effective band gap, at non-normal incidence (θ=27o).

4. CONCLUSION

Overall, we can see that the particle size has more significant effect on some physical properties of Cadmium Sulphide. When the radius of particles is equal or smaller than the Bohr radius of the exciton. The energy gap increase and the index of refraction decreases because of quantum confinement and this leads to higher transmittance when the particle size is smaller.

The particle size has an effect on the nano energy gap and refractive index of the nano particles as shown in figure 9. The nano energy gap increases when the particle size decreases and refractive index of the nano particles decreases when the particle size decreases. This change in properties affects the transmittance and that is clearly seen in figure 4. The best coating to use in solar cells' applications at wavelength 550 nm results in a transmittance of 75.4 for a particle size of 3 nm at the normal incidence, and TE=71, TM= 79 at non-normal incident θ=27° .one can be added another layer of different material with different nano thickness to the first layer to get higher transmittances as a future project.

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