

STUDY OF THE EFFECTS OF NANO-PARTICLE SIZES ON THE TRANSMITTANCE OF CdTe THIN FILM

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In this, we study the optical properties of CdTe thin film as a function of the nano particle sizes on them. We use a MATLAB software program ((version 7.6.0324) we developed, for applications in the spectrum range 400–700 nm. We study the effect of partial l size on both the energy gap and the refractive index of CdTe thin film . The refractive index decreases with the particle size while, the energy gap increases . As consequence, the transmittance increases when nano- particle size decreases . One can obtain a high transmittance $T=92.52\%$ at $\lambda_0=550\text{nm}$ when the nano- particle size is set to 2.6nm . For a nano- particle size of 2.4nm transmittance reaches $T=99.9965\%$.

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1. Introduction

Solar cells based on nanoparticles have high interesting because of the possibility of solution synthesis[1], the relatively inexpensive of manufacturing and large area flexibility. Compared with their counterparts of organic solar cells that have these advantages, Nano crystal thin-film solar cells offer easy tuning of the light response over a broad range by adjusting the quantum effect of the size of colloidal nanoparticles Up to now, high interesting has been paid to photovoltaic nanomaterial's which could be adopted in thin-film solar cells, such as PbS , CuInS₂ , and CdTe [1].

CdTe, a direct IIB–VIA semiconductor is a promising material for many optoelectrical applications Lately, there is interesting towards of the main physical properties CdTe's [2] ,the two attractive characteristics of CdTe are its high optical absorption coefficient up to $>5 \times 10^5 \text{ cm}^{-1}$ ("means that high quantum yield can be expected over a wide wavelength range, from the ultraviolet to the CdTe band gap $\lambda \sim 825 \text{ nm}$. Short-wavelength photons, with energy greater than E_g , are absorbed near the CdTe surface, making CdTe an attractive absorber-layer material for thin-film solar cells"[3].)) and its nearly ideal band gap of $\sim 1.5 \text{ eV}$ for single p-n junction photovoltaic[4] that is nearly ideally conformity to the solar spectrum for photovoltaic energy transformation[3]. Therefore, a thickness of $\sim 1 \mu\text{m}$ of CdTe can absorb almost 90% of the incident light[4]. Refractive index (2.69)[3], and an exciton Bohr radius of 7.3 nm.[5]. Presently, there is a big intention of interesting to optical and structural properties of nanometer-sized semiconductor particle or thin films[4].

2. Theory

2.1. The Transmittance and Reflectance

At a sharp limit between two media, there are basic connections that must be obeyed between the fields on the two sides. The parts of the fields E and H parallel to the surface are equivalent on the two sides, whereas the normal components of D and B should likewise be continuous. Full proof of these conditions, which we shall use extensively in what follows, is

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given in the texts on electromagnetic theory[6, 7]."Application of the boundary conditions allows us to derive reflection and transmission coefficients for electromagnetic waves. Suppose that a plane electromagnetic wave with wave-vector k and electric field amplitude E_0 is incident on a plane surface separating two isotropic media with refractive indices n_1 and n_2 . The angle of incidence is \hat{i} between the incident" [6], as shown in figure 1 "The plane containing the incident wave-vector k as well as the reflected and transmitted wave-vector and the normal \hat{n} is the (x, z) plane, and the z -direction is chosen along vector \hat{n} . One can be denoted the amplitudes (electric field magnitudes) of the incident, reflected and transmitted waves by I, R and T respectively".[6].

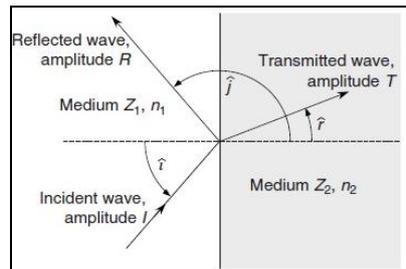


Fig. 1. shows incident ,transmitted and reflected waves at the interface between two isotropic media of respective indices n_1 and n_2 .[6]

Give us for straightforwardness a chance to center on the forces of the signs. It is a typical practice to characterize the transmittance T and reflectance R , of the example as the proportion of the intensity of the transmitted light (I_T) and that of the approaching light (I_E) and I_R is The reflected intensity[7] :

$$T = \frac{I_T}{I_E} \tag{1}$$

$$R = \frac{I_R}{I_E} \tag{2}$$

If we manage a sample that does neither diffusely dissipate nor assimilate the light, then the in this manner characterized transmittance and reflectance, must be summarized to the value one – merely because of the energy conservation law. Practically speaking, a specific part of the light intensity is diffusely scattered .That leads us to the meaning of the optical scatter S ,and As needs be, we characterize the absorptance (A) As in the following equations[7]:

$$S = \frac{I_S}{I_E} \tag{3}$$

$$A = \frac{I_A}{I_E} \tag{4}$$

Where (I_A) absorbed intensity and (I_S) is the intensities of the Scattered light, In the presence of scattering and absorption ,the energy conservation law might be composed as:

$$T + R + A + S = 1 \tag{5}$$

So that these four quantities are dependent on each other, and accurate information of three of them allows the fourth to be directly calculated. Nevertheless, all four quantities $T, R, S,$ and A may, on a fundamental level, be measured independently from each other. The algebraic sum of absorption and scatter is often called optical loss L [7]:

$$L \equiv S + A = 1 - T - R \tag{6}$$

In order to qualitatively understand the performance of thin-film optical devices, it is important to acknowledge a few basic explanations [8]." The amplitude reflectance of light at any boundary between two media is given by $(1 - \rho)/(1 + \rho)$, where ρ is the ratio of the optical admittances at the boundary, which, in the optical region, is also the ratio of the refractive indices. The reflectance (the ratio of irradiances) is the square of this quantity". We can find R and T by the following equation [8]:

$$R = \frac{I_R}{I_E} = \rho^2 = \left[\frac{n_0 - n_1}{n_0 + n_1} \right]^2 \quad (7)$$

$$T = \frac{I_T}{I_E} = \tau^2 = \left[\frac{n_0 + n_1}{n_0 + n_1} \right]^2 \quad (8)$$

where τ is transmission coefficients .

2.2. Quantum Size Effects

Crystals with considerable enhanced optical properties in terms of photostability, brightness, bleaching and blinking compared to traditional organic and protein fluorophores [9].

The most outstanding property of semiconductor Nano crystals is large changes in optical properties as a function of the particle size. As size is reduced, the electronic excitations levels move to higher energy, and there is focused on oscillator strength into only a few transitions. These essential physical phenomena of quantum confinement emerge because of the changes in the density of electronic states and can be understood by considering the relationship between position and momentum for limited particles[10]:

$$\Delta P \Delta x \geq \hbar/2 \quad (9)$$

In the extended case,"there is a relationship between momentum and energy, and to a first approximation, the change in energy as a function of the size can be estimated simply by realizing that the energy of the confined particle arises by superposition of bulk k states of differing energies". For a free particle, the dependence of energy on wave vector is quadratic[10]:

$$E = \hbar^2 k^2 / 2m \quad (10)$$

In the effective mass approximation, "this relationship is assumed to catch for hold for an electron or hole in the periodic potential of the semiconductor, with a reduced mass which is inversely proportional to the width of the band. Given the relationship between confinement in space and momentum superposition, this leads straightly to the approximate dependence of energy on size as $1/r^2$, as predicted for a simple particle in a box. For large sizes, the approximation is almost correct but it breaks down for even moderate sizes because energy does not depend quadratically on k in real crystallites"[10].

In a simple one-dimensional single band tight-binding model, the dependence of E on k is

$$E = \alpha + 2\beta \cos(ka) \quad (11)$$

where α , the energy of the linear combination of atomic orbitals inside the unit cell, determines the center location of the band in energy. β gives the half-width of the band and is directly related to the strength of nearest- expansion of the $\cos(ka)$ term for small k yields a quadratic as its leading term, so neighbor coupling and inversely proportional to the effective mass. So that one can see why the effective mass approximation only describes the band well near either its minimum or its maximum[10].

Optical absorption spectra of (CdTe) thin films have been calculated to determine the band tail width or Urbach energy (EU), the absorption coefficient, optical energy gap (Eg) and

the nature of the transition. Knowing the film thickness (t), the optical absorption coefficient (α_o) could be determined from the estimations of $T(l)$ and $R(l)$ by using the following equation [11]:

$$\alpha_o = \frac{1}{t} \ln \frac{(1-R^2)}{T} \quad (12)$$

the absorption coefficient (α_o) is identified with photon energy ($h\nu$) by the known equation as[11]:

$$\alpha_o h\nu = \beta(h\nu - E_g)^n \quad (13)$$

β is the band tailing parameter and it is a constant, depends on the effective mass for the electrons and holes and the optical middle density. E_g is the energy of the optical band gap and n as a power index determines the nature of the transition.

An absorption edge of semiconductors corresponds to the threshold of charge transition between the lowest nearly empty band and the highest nearly filled band. According to inter-band absorption theory, the films optical band can be calculated using the following relation [11]

$$(\alpha_o h\nu) = A(h\nu - E_g^{opt})^r \quad (14)$$

where A is the probability parameter for the transition and E_g^{opt} is the optical band gap of the material, $h\nu$ is the incident photon energy[11].

2.3. Nano Energy Band

There are many theories which can be used to explain how the value of energy band gap depends on the semiconductor quantum dot size, and the most popular is Brus model[12] or effective mass approximation (EMA), this model takes into consideration the value of each of the effective mass of the electron and hole which change from one material to another. According to this model, the value of the change in the energy gap for the quantum dots given according to the equation (Brus) as follows[12]:

$$\Delta E_g = \frac{\hbar^2 \pi^2}{2\mathcal{R}^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right] - \frac{1.786 e^2}{\epsilon \mathcal{R}} - \frac{0.124 e^4}{\hbar^2 \epsilon^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right]^{-1} \quad (15)$$

Where \mathcal{R} is the radius of the quantum dot, m_e^* , and m_h^* are the effective mass of the electron and hole respectively, ϵ is dielectric constant, and

$$\Delta E_g = E_g^{nano}(\mathcal{R}) - E_g^{bulk} \quad (16)$$

$E_g^{nano}(\mathcal{R})$ is the energy gap for the material in the quantum dot (Effective band gap), E_g^{bulk} is energy gap for the material in bulk band gap. Equation (15) becomes[13]:

$$E_g^{nano}(\mathcal{R}) = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2\mathcal{R}^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right] - \frac{1.786 e^2}{\epsilon \mathcal{R}} - \frac{0.124 e^4}{\hbar^2 \epsilon^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right]^{-1} \quad (17)$$

The second term on the right hand side shows that the effective band gap is an inverse relationship to \mathcal{R}^2 and increases as size decreases. The third term demonstrates that the band gap energy decreases with the decrease in \mathcal{R} because of the increase in Coulombic interaction force. However, given that the second term plainly prevails with small \mathcal{R} , the effective band gap is foreseeable to increase with the decrease in \mathcal{R} , especially when \mathcal{R} is small. The Coulombic interaction force is typically small compared with quantum confinement. The third term is much smaller than the first term. Therefore, these terms can be neglected. Thus, the equation may be expressed as[13]:

$$E_g^{nano}(\mathcal{R}) = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2\mathcal{R}^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right] \quad (18)$$

We note from the equation(18) the effective band gap shift inversely proportional to R^2 , and therefore we may expect an increase of the energy gap with decreasing R . At the point when the sizes (particle size P_{ζ}) of the nano-particles is equal to or smaller than the Bohr exciton radius (α_B), effects of quantitative confinement are expected to be important. In these materials, the electrons are confined in three directions control [13];[14];[15]; the optical properties of material depending on the particle size. Such a framework is known as a zero-dimensional framework, which is obvious in quantum dots. The Bohr radius is given by [15]:

$$\alpha_B = \frac{4\pi\epsilon\hbar^2}{e^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right] \quad (19)$$

where ϵ is the dielectric constant. m_e^* and m_h^* are the effective masses of electrons and holes, respectively.[13]. The exciton Bohr range gives an exceptionally valuable length scale to depict the spatial expansion of excitons in semiconductors, and ranges from ~2 to ~50 nm depending on the semiconductor, It is fascinating to note that the exciton Bohr radius α_o and the band gap of the semiconductor is connected. so that materials with wider band gaps possess smaller α_o .

The refractive index is firmly identified with the energy band structure of the material; many endeavors have been made to relate refractive index and energy gap (Eg) through basic simple relationships [12]. The linear form of the refractive index (n) as is presented as a function of energy gap(Eg)[16]:

$$n = \alpha + \beta E_g \quad (20)$$

Where ($\beta = -0.52 \text{ eV}^{-1}$), ($\alpha = 4.048$).

3. Results and discussion

In this work, we will present a description of the CdTe material properties in Nano scale sizes. We used MATLAB. the software program, for the spectrum range of 400–700 nm, where the program has been prepared using the Brus model or effective mass approximation (EMA). In this research, the study of the transmittance as a function of particle size for a thin film (CdTe). The particle size values were selected with the following optional values in nanometers (1.1,1.2,1.3,1.5,2,3,3.5,4,4.5,5,6,6.8,10,13,15).

Fig. (2) shows the change in energy gap as a function of particle size. The energy gap increases with decreasing particle size and that according to equation(18). The refractive index decreases when the particle size decreases (particle size approaches to the Bohr exaction radius ($\alpha_o = 7.3 \text{ nm}$) (figure 3)). It could distinguish change between the energy gap and refractive index as a function of particle size for nano CdTe as shown in figure (4) and Table 1.

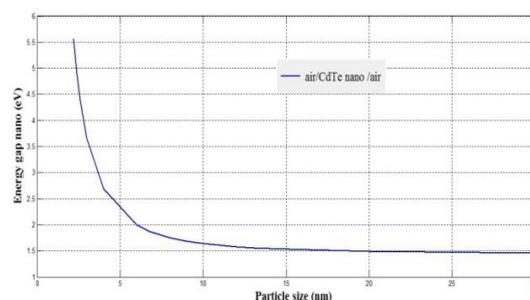


Fig. 2. Nano energy gap as a function of particle size of nano CdTe

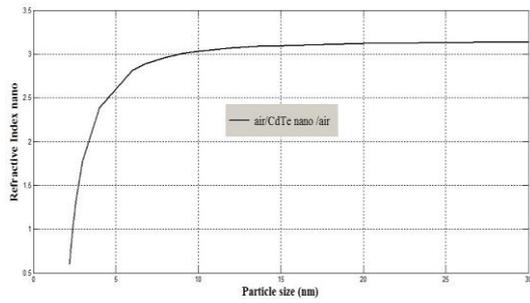


Fig. 3. Refractive index as a function of particle size of nano CdTe

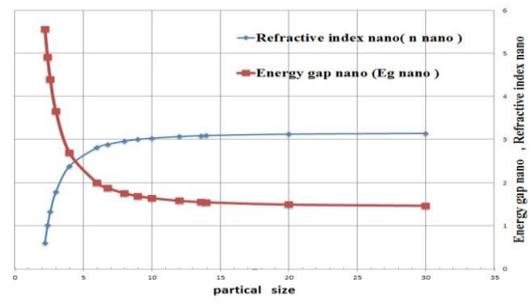


Fig. 4. Refractive index and energy gap as a function of particle size of nano CdTe.

Table . 1. The values of particle size ,Nano-energy gap , refractive index and the resulting transmittance for CdTe thin film at $\lambda_0= 550 \text{ nm}$

| Particle size | Nano energy gap | Refractive index | The Reflectivity at $\lambda_0 = 550 \text{ nm}$ | The transmittance at $\lambda_0 = 550 \text{ nm}$ |
|---------------|-----------------|------------------|--|---|
| 2.2000 | 5.5655 | 0.5974 | 22.4625 | 77.5375 |
| 2.4000 | 4.9065 | 1.0059 | 0.0035 | 99.9965 |
| 2.6000 | 4.3937 | 1.3239 | 7.4765 | 92.5235 |
| 3.0000 | 3.6586 | 1.7797 | 27.0470 | 72.953 |
| 4.0000 | 2.6880 | 2.3815 | 49.0297 | 50.9703 |
| 6.0000 | 1.9946 | 2.8113 | 60.1197 | 39.8803 |
| 6.8000 | 1.8718 | 2.8875 | 61.7497 | 38.2503 |
| 8.0000 | 1.7520 | 2.9618 | 63.2557 | 36.7443 |
| 9.0000 | 1.6865 | 3.0024 | 64.0453 | 35.9547 |
| 10.0000 | 1.6397 | 3.0314 | 64.5961 | 35.4039 |
| 12.0000 | 1.5787 | 3.0692 | 65.2968 | 34.7032 |
| 13.6000 | 1.5480 | 3.0883 | 65.6423 | 34.3577 |
| 20.0000 | 1.4899 | 3.1243 | 66.2828 | 33.7172 |
| 26.0000 | 1.4695 | 3.1369 | 66.5038 | 33.4962 |
| 30.0000 | 1.4622 | 3.1414 | 66.5831 | 33.4169 |

The transmittance of CdTe material is 42% at the wavelength 550 nm. Figures (5) shows the change in transmittance CdTe thin films as a function of the particle size. The transmittance of CdTe is affected by the decrease in particle size. Specifically, when particle size approaches the Bohr excition radius ($\alpha_0=7.3 \text{ nm}$). This is due to the effect of quantum confinement. At the point when particle size ($P_s=2R$) is equivalent or littler than the Bohr exciton radius , the effect of quantum confinement increments drastically, Resulting in increased transmittance of material as shown in and Table 1 .

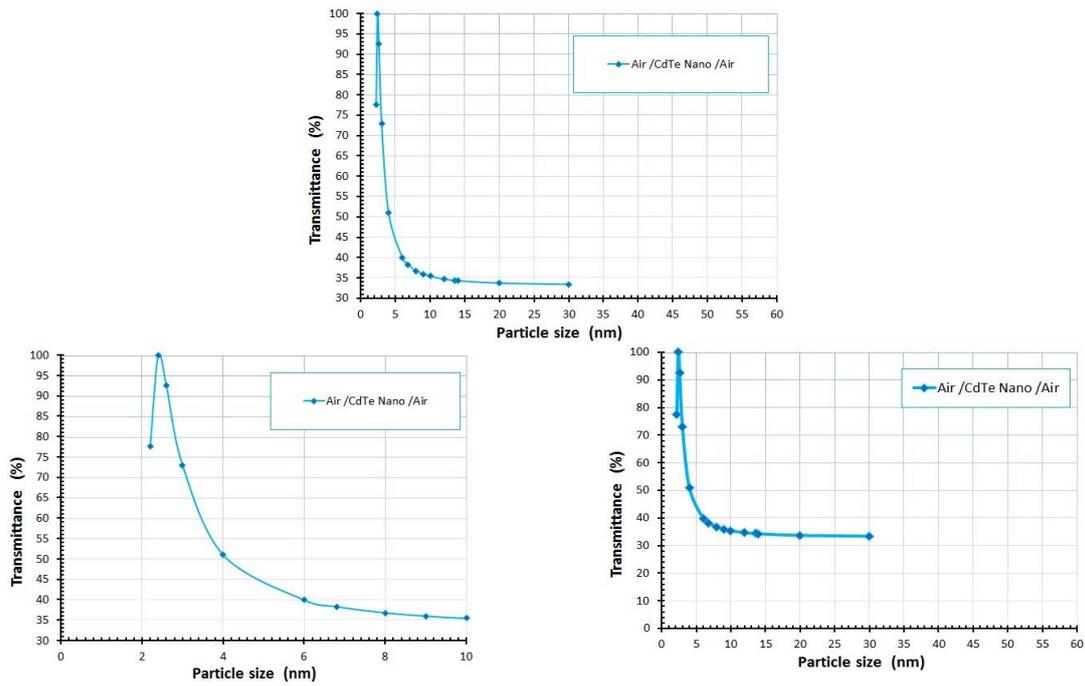


Fig. 5. Transmittance as a function of CdTe nano- particle size at $\lambda_0=550$ nm

Fig. 6 shows the effect the refractive index on transmittance, the transmittance increases with decreasing the refractive index (as in equation 8), also transmittance is affected by the particle size.

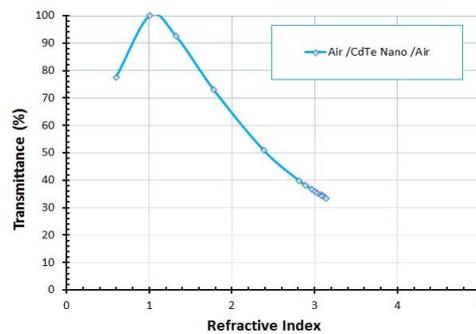


Fig. 6. Transmittance as a function of refractive index of nano CdTe at $\lambda_0=550$ nm.

Fig. 7 shows the transmittance increase when the energy gap is increased. This result can be explained through equation (20) because there is a linear relationship between the energy gap and the refractive index. The equation shows that the energy gap increases, leading to an increase in the negative value of the energy gap, then, the refractive index is reduced when (α) is Constant

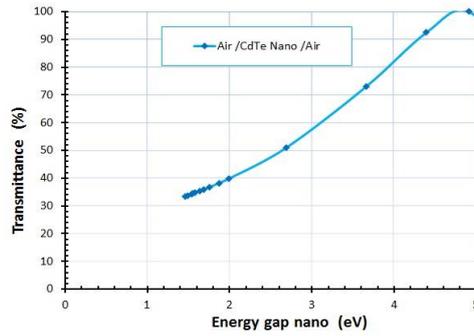


Fig. 7. Transmittance as a function of energy gap of nano CdTe at $\lambda_0=550\text{ nm}$

The result of various optical properties in function of particle size, led to obtain high transmittance of $T=92.52\%$ at $\lambda_0=550\text{nm}$ for the nano CdTe thin film with a particle size of 2.6nm and $T=99.9965\%$ for a particle size of 2.4nm as show in Figs. (8 and 9) and Table 1.

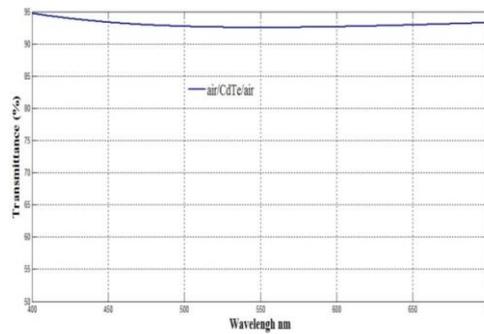


Fig. 8. shows the transmittance as a function of wavelength for the nano CdTe thin film $\lambda_0=550$ at ($ps=2.6$).

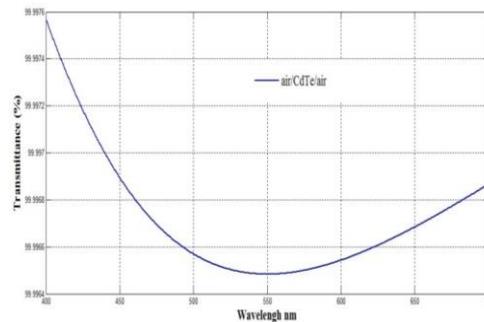


Fig. 9. Shows the transmittance as a function of wavelength for the nano CdTe thin film $\lambda_0=550$ at ($ps=2.4$).

When we used a glass substrate ($n=1.52$) with the interface design air /nano CdTe /glass, we obtained the transmittance shown in Table 2. This demonstrates, we can use nano CdTe thin film in solar cells applications, Specially with $Ps=2.4\text{nm}$ and $Ps=2.6\text{nm}$ for which the transmittances of 95.97% and 99.49% were respectively obtained.

Table 2. The values of particle size and the resulting transmittance for CdTe thin film at $\lambda_0 = 550$ nm at two designs.

| Particle size (Ps) | Transmittance [air / nano CdTe/air] | Transmittance [air / nano CdTe/glass] |
|--------------------|-------------------------------------|---------------------------------------|
| 2.2000 | 77.5375 | 61.5984 |
| 2.4000 | 99.9965 | 95.9734 |
| 2.6000 | 92.5235 | 99.4945 |
| 3.0000 | 72.953 | 87.6495 |
| 4.0000 | 50.9703 | 66.6757 |
| 6.0000 | 39.8803 | 54.1126 |
| 7.0000 | 38.2503 | 51.793 |
| 8.0000 | 36.7443 | 50.3502 |
| 9.0000 | 35.9547 | 49.3888 |
| 10.0000 | 35.4039 | 48.7148 |
| 12.0000 | 34.7032 | 47.8536 |
| 13.6000 | 34.3577 | 47.4273 |
| 20.0000 | 33.7172 | 46.6343 |
| 26.0000 | 33.4962 | 46.3597 |
| 30.0000 | 33.4169 | 46.2612 |

4. Conclusions

The optical properties of semiconductor materials are exceptionally connected with the particle size. When the radius of the material particle is equivalent to or smaller than the Bohr radius of the exciton, the quantum confinement causes the energy gap to increase and the index of refraction to decrease. This leads to a higher transmittance of materials when the particle size is smaller. The transmittance coating layer with the Visible region of (400-700) nm depends on refractive index, the Particle size effects on the refractive index and the value of refractive index can be controlled by particle size.

At normal incidence the transmittance for CdTe for an interface design air/nano CdTe /air for a particle size $ps=2.4$ nm is $T=99.99\%$ while for $ps=2.6$ nm, $T=92.52\%$ at a wavelength $\lambda_0=550$ nm. For interface design air/nano CdTe / glass, the transmittance at the same wavelength is $T=95.97\%$ for $Ps= 2.4$ nm and $T=99.49\%$ for $ps=2.6$ nm.

The particle size effect on both the refractive index and the energy gap, When the particle size decreases The refractive index decreases and When the particle size decreases the energy gap for thin film Increasing, therefore transmittance effect, it increasingly When the particle size decreases.

This shows that the optical properties of semiconducting materials are affected by the particle size. This is may be used for improving transmittance in applications such as solar cells.

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