Adjustable Mechanisms Of Quantum Efficiency In Cds/Mgzno Heterostructures Quantum Dot Solar Cells

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Abstract

The quantum efficiency QE and absorption spectrum of CdS/MgZnOheterostructuresquantum dot (QD) solar cells areestimatedfordifferent QD sizes and junction depths. Several mechanisms have beencarried outafter that to investigate QE. Among them is study the heterostructuressolar cells using one layer of the QD that found to be effective and give high QEsolar cells.Another mechanism isstudyingthe effect of changing QD size, and it is found to be efficient in tuning QE and its spectrum. Thestructural studies are carried out by using spectrum ranges within the range of 250-500 nm that is essential in solar cells applications to cover UV and visible spectrum.

Keywords: Nanomaterial, Quantum Dot, Quantum Efficiency, Solar Cells.

1. Introductions

The growing world demands to clean and renewable energy to replace the fossil fuel energy as well as the needs for developing effectivesolutions for environmental pollution have been among the mostimportantglobal issues in the past few years[1]. At the present time, solar cells (SCs) have been identifiedas an alternative source of energy that can solve these issues which produces a clean and sufficient energy [2]. SCs have been very attracted due to their productive power conversion energy with stabilityfor long period of time inenergy generation[3]. A lot of studies for different new technologies to develop new kinds of solar cells have been carried out, such as Dye sensitive, solid state dye, bulk heterojunction, nanocrystalline, and hybrid organic inorganic SCs [4].Also,significant attention and many scientific efforts have focused in developing third generation solar cells. This includes developing nanostructured quantum dots (QDs) absorption mediumsthat have played an important role insolar cells efficiency[5]. These QDs structures are characterized by their unique size dependent optoelectronic properties[6, 7]. Their quantum behaviors are very close to natural atoms or small molecules properties with discrete energy levels[8, 9]. They show unpredictedphysical characteristics due to their Nano-size with theirquantum mechanical properties [10]. Semiconductor QDs have recentlyattracted significant attention in the field of light harvesting in photovoltaic devices because of their high absorption coefficient, size-dependent bandgap and quantum size effects [11].Among them are II-VI semiconductorsthat have effective optoelectronic properties, such as high performance of radioactive recombination and high absorption coefficient in the most regions of the solar spectrum. CdS has been used as QDs due to its narrow bandgap of (2.4eV) in the II-VI group. It has been a promising photovoltaic material used in high efficiency solar cells [12-16]. Further, another interesting semiconductor material is MgZnOthat identified to be used in photovoltaic applications due to their wide bandgap, excellent carrier mobility, and easyfabrication. Its bandgap alloys can be modified from 3.34 eV (ZnO) to 7.8 eV (MgO), which covers the ultra-violate solar spectrum vary from 4.42 eV (280 nm) to 5.6 eV (220 nm). Beside its effective optical properties, MgZnO haslattice constants close to that of ZnO with large exciton binding energy [18, 24]. It has been succeeding for applications in SCs [17-19].Also, MgZnO has a changeable and controllable bandgap that has been exploiting as a barrier layer in then-CdS/ p-MgZnO. It is a promising candidate for optoelectronic devices thatcovers a broad portion of the UV spectrum and most part of visible spectrum.

Quantum efficiency (QE) plays a significant role in photovoltaic devicesperformance. It is particularly adopted to investigate the efficiency of incident optical energy in output electrical power production. Its importance can be attributed to its qualitative information about theratio of collected light spectral to current generationsthat convert to electrical power of the solar cell[20, 21].In this work, the QE and the absorption coefficient for theCdS/MgZnO QD SCs are calculated. The CdS QD layer is used asn-type while MgZnO bulk layer is p-type. QDs structures supposed to be tiny disks and the effect of changing their height and radius values on QE profile were analyzed. It was also detected that the bandwidth is increased and QE is decreased by increasing thedisk height, while both QE and bandwidth are decreased by increasingdisk radius. Improved QE can be acquired for n-CdS/p-MgZnO structure at long junction depth of the SC structure.

2. QE IN QD SOLAR CELLS

The minority carrier continuity equation when the injection very low levels for the holes in p-type side and electrons in the n-type side, respectively, can be written as follows [22]:

$$D_p \frac{\partial^2 \delta p_n}{\partial x^2} - \frac{\delta p_n}{\tau_p} + G_L = 0 \qquad (1)$$

$$D_n \frac{\partial^2 \delta n_p}{\partial x^2} - \frac{\delta n_p}{\tau_n} + G_n = 0 \qquad (2)$$

where electron concentration which created due to external source of excitations is expressed as $\delta p_n = p_n - p_{n0}$ $(\delta n_p = n_p - n_{p0})$with $p_n(n_p)$is the total hole concentration in the n-region (p-region), and $p_{n0}(n_{p0})$is the hole concentration without any injection. $\tau_p(\tau_n)$is the hole (electron) life time. $D_p(D_n)$is the diffusion coefficient of the hole. The electron-holegeneration rate as a function of the distance is given by $G(x)=G_L$ [21], that:

$$G_n = (1-R)\alpha_n \Phi \times \exp\{-(\alpha_n x_j + \alpha_d W + \alpha_p[x - x_j - W])\} (3)$$

where, R is the optical reflectivity between the air and semiconductor, $\alpha(x)$ is the absorption coefficient (as a function of the distance x) of the optical intensity, and Φ is the illuminated photon number. Note that the $\alpha_p, \alpha_n, \alpha_d$ are the absorption coefficients of p-, n-, and depletion layers respectively. (x_j) is the depletion depth, and W is the depletion width. Eqs. (1) and (2) are solved by summing the homogeneous and particular solutions.

The relation of the hole density is given by [16],Thesolution of Eq. (1) can be written as follows:

$$\delta p_n = \frac{\alpha_n \phi(1-R)\tau_p}{(\alpha_n^2 L_p^2 - 1)} \left\{ \frac{\cosh(x/L_p)}{\sinh(x_j/L_p)} [-\frac{(D_p\alpha_n^2 - S_p)}{(D_p/L_p^2 - S_p)} e^{(x_j/L_p)} + e^{-\alpha_n x_j}] + \frac{(D_p\alpha_n^2 - S_p)}{(D_p/L_p^2 - S_p)} e^{(x/L_p)} - e^{-\alpha_n x} \right\} \quad (4)$$

S_p is the surface recombination velocity at the p-layer. The holediffusion photocurrent in the n side, which is dominated by the diffusion, is given byequation,

$$J_n = qD_n \frac{\partial}{\partial x} \delta p \quad (5)$$

By the same way, one can write for electron current density,

$$J_n = q \frac{\phi \alpha_p L_n (1-R)}{(\alpha_p^2 L_n - 1)} e^{-(\alpha_n x_j + \alpha_d W)} \times \left\{ \frac{(\alpha_p^2 - S_n) L_n^2}{(D_n - S_n L_n^2)} e^{-\alpha_p H'} - 2e^{-\frac{H'}{L_n}} + \alpha_p L_n e^{-\alpha_p H'} \right\} \quad (6)$$

Then, the relation for the electron diffusion photocurrent in the p-region is by [22],

$$J_{dr} = q\phi(1-R) e^{-\alpha_n x_j} (1 - e^{-\alpha_d W}) \quad (7)$$

Note that the QE of QD SC is given by[22],

$$QE = \frac{(J_p + J_n + J_{dr})}{q\phi(1-R)} \quad (8)$$

3. Narrative of the QD Solar Cell Structure

This work focuses on studying the QE in CdS QDs grown on MgZnO barriers. QDs are implicit in the form of quantumdisks. The sizes studied were (1-2 nm in height and 12-14nm in radius). Aschematic diagram of different regions in the structure was shown in Fig. 1.Material parameters of CdS and MgZnO QDs are listed in Table 1.

Additionally, we calculated the QE and the absorption coefficient for the CdS/MgZnO, where the MgZnO bulk layer.High efficiency was obtained for the structure, and wide bandwidth was obtained. It is found, also,that increasing the disk height increases the bandwidth and reduces QE , while increasing the disk radius reduces both QE and bandwidth. High QE can be obtained for structure with CdS QD at long depth of the junction of the SC structure.

4. Absorption Coefficients of QD Structures

QDs absorb high density of photons with wide spectrum of energies due to randomly distributed and imperfections in shape on the substrate,which results in an inhomogeneous broadening .Thus,the absorption can be written as [23].

$$\alpha(\hbar\omega) = \frac{\pi e^2}{n_b c \varepsilon_0 m_0^2 \omega} \sum_i \int_{-\infty}^{\infty} dE' \left|M_{env}\right|^2 \left|e^\wedge . p_{cv}\right|^2 \times D(E') L_g(E', \hbar\omega)$$
$$[f_v(E', F_v) - f_c(E', f_c)] \qquad (9)$$

where m_0 is the free electron mass, ε_0 is the permittivity of free space, c is the speed of light in free space, n_b is the background refractive index of the material, ω is the angular frequency of the injected optical signal and E' is the optical transition energy, M_{env} is the envelope function overlap between the QD electron and hole states. The term $\left|\hat{e}.P_{cv}\right|^2 = \frac{3}{2}(m_0/6)E_p$ is the momentum matrix element for electron-heavy hole transition energy in TE polarization, E_p is the optical matrix energy parameter. $D(E')$ is the inhomogeneous density of states of self-assembled QDs and it is expressed as [23]

$$D(E') = \frac{s^i}{V_{dot}^{eff}} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(E' - E_{max}^i)^2}{2\sigma^2}\right) \qquad (10)$$

where s^i is the degeneracy number at each state of a QD, $s^i = 2$ for the ground state and $s^i = 4$ in the excited state. V_{dot}^{eff} is the effective volume of the QDs, σ is the spectral variance of the QD distribution, and E_{max}^i is the transition energy at the maximum of QD distribution of the i^{th} optical transition. The terms f_c and f_v are the respective quasi-Fermi distribution function for the conduction and valence bands, respectively. The global state has been used to describe the global quasi-Fermi levels of the conduction F_c and valence band F_v where the contributions to the Fermi-levels from the barrier layer and WL are included in addition to that from QDs. They can determine from the surface carrier density per QD layer as follows [23]

$$p_{2D} = n_{2D} + N_A^-$$

$$n_{2D} = N_D \sum_i \frac{s^i}{\sqrt{2\pi\sigma_e^2}} \int dE_c' e^{-(E_c'-E_{ci})/2\sigma_e^2} f_c(E_c', F_c) + \sum_l \frac{m_e^* K_B T}{\pi \hbar^2} \ln(1+e^{(F_c-E_{cl})/K_B T}) + \tau_b \frac{1}{2\pi^2}\left(\frac{2K_B T m_{eb}^*}{\hbar^2}\right)^{\frac{3}{2}} e^{\left(\frac{F_c-E_{cb}}{K_B T}\right)} \quad (11)$$

$$p_{2D} = N_D \sum_i \frac{s^i}{\sqrt{2\pi\sigma_h^2}} \int dE_h' e^{-(E_h'-E_{hi})/2\sigma_h^2} f_v(E_h', F_v) + \sum_m \frac{m_{hh}^* K_B T}{\pi \hbar^2} \ln(1+e^{(F_v-E_{vm})/K_B T}) + \tau_b \frac{1}{2\pi^2}\left(\frac{2K_B T m_{hhb}^*}{\hbar^2}\right)^{\frac{3}{2}} e^{\left(\frac{F_v-E_{hhb}}{K_B T}\right)} \quad (12)$$

where n_{2D} and p_{2D} are the surface densities of the electrons and holes per QD layer, respectively. The terms E'_c and E'_h are the energy in the conduction band andthe energy in the valence bandrespectively. While the terms E_{ci} and E_{hi} are representing the respective confined QD state in the conduction and valence bands. σ_e and σ_h are the spectral variance of QD electron and heavy hole distributions respectively. The terms $m_e^*(m_{hh}^*)$ and $E_{cl}(E_{vm})$ are the effective electron (hole) mass and the sub-band edge energy of the conduction (valence) band of WL. The term τ_b is the thickness of SCH barrier. The terms $m_{eb}^*(m_{hhb}^*)$ and $E_{cb}(E_{hhb})$ are the effective electron (hole) mass and the conduction (valence) band edge energy of the barrier layer. The Lorentzian line shape function $L_g(E', \hbar\omega)$ for the absorption coefficient is given by [22]

$$L_g(E', \hbar\omega) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(E'-\hbar\omega)^2}{2\sigma^2}\right) \quad (13)$$

5. Describing of the QD Solar Cell structure:

This work is devoted for studying the QE in CdS QDs grown on MgZnO barriers and. QDs are assumed to be in the form of quantum disks. The sizes studied were 1–3 nm in height and 12–14 nm in radius. A schematic diagram of different regions in the structure is shown in Fig. 1.Material parameters of CdS QDs and MgZnO barriers are listed in Table 1.

Results and Discussion

The absorption coefficient is first calculated using Eq. (9), then QE, using Eq. (8), for CdS/MgZnO, SC structures at the sizes referred to in the above section.

Calculation of Absorption Coefficient of CdS/MgZnO

1-Effect of disk height: h = 2 nm, ρ =14 nm: Fig.2(a) shows the absorption spectrum of the CdS/MgZnO QD system when the disk height is 2 nm and the disk radius is 14 nm. The spectrum covers the range of 210–255 nm. There are two absorption peaks wavelength were at 218 nm, second one at 230 nm, the first peck comes from the second sub-band transition,and the second peak comes from third sub-band transitions. The second peak has absorption intensity bigger than the first one.

2. Effect of disk height: h= 1, ρ = 12: Fig.2(b) shows the absorption spectrum of the p-doping CdS/MgZnO QD system when the disk height decreases by 1 nm and radius by 2 nm. The spectrum becomes wider where it covers the range of 200–270 nm. It splits into three separate peaks. The first one lies at 210 nm wavelength and comes from the seventh, eighth, and ninth sub-band transitions. Thesecond peak which is the highest peak lies at 335 nm wavelength, which comes from the second sub-band transition, and the third oneat 255 nm which is come from the third sub-band transition and the spectrum width increasesby 25 nm.

And intensity for the peaksare 4600 cm^{-1}, 6300 cm^{-1},and 2000 cm^{-1} respectively. The Nanoparticles which have dimensions h=2 nm and radius 14 nm represent worst result where degreasing of the absorption peak and reduces the coverage area of the spectrum from 210 nm to 255 nm ,and the absorption peak intensity from 6300 $cm^{-1}$to 1700 cm^{-1}.

QE as function of size

Fig.3 shows the QE for the CdS/MgZnOstructure when h=1nm and ρ =12nm. The contribution of the MgZnO bulk p-doped region appears here as a QE for the p-doped region QE_p. It has the lowest contribution due to low absorption of the bulk region compared with CdS QD region. QE of CdS/MgZnOhas a wide bandwidth where it can absorb wavelength within range of $200-260nm$. Another important feature that can be seen is the wide peak along all of these wavelengths which has not obtained in any other solar cell structure. QE was found to be around 0.75 which is perfect value of the structure solar cells due to high absorption of CdS QD region.

Fig.4 shows the QE for the CdS/MgZnOstructure when h=2nm and ρ =14nm. The QE at this dimension become lower than that previous one due to the increasing the QD particles size as result for tuning physical properties,where the QE of the structures reduce to 0.57 which reduce by 0.18 while the bandwidth it can absorb new wavelength to be start from 170 nm to 207 nm which is shift to the short wave length to start from 170 nm instead of 200 nm and end to 207 nm instead of 270 nm byreduce range to be 33nm.

Another important feature is that for CdS/MgZnO QD structure,Figs. 5 the QE curves increase incrementally at small values of junction depths. One must remember that the quantum efficiency of CdS/MgZnOFig. 3 which is representgreat results at each value of diffusion length (Ln), and then it becomes high at small junction depth.This is also the reasonthe Quantum efficiency is high value for the small value of junction depth to gives a good bias between curves.

Conclusions

This work is focused on the study of QE of CdS/MgZnO QD SCs in which the band structure has been calculated for the QDs assuming that they are in the quantum disk shape. Their absorption spectra were calculated, and then QEs were studied at different QD sizes and junction depths. While, it is shown that doping the barrier layer gives high QE at a wide bandwidth, it is also found that increasing both the disk height and radius degreases the bandwidth and reduces QE (less). Further, degreasing disk radius and disk highincreases both QE and bandwidth. High QE can be obtained for CdS at long depth of thejunction of SC structure.

Table 1: Parameters Used to Calculate QE of CdS/MgZnO QD SCs.

Parameter	Symbol (Unit)	CdS Value	MgZnO Value
Electron diffusion length	Ln (μm)	0.12	0.06
Hole diffusion length	Lp (μm)	0.01	0.04
Electron carrier lifetime	τn ns	0.048	0.082
Hole carrier lifetime	τp ns	0.06	0.061
Depletion width	W (μm)	0.99	0.99
Junction depth	xj (μm)	0.1	0.1 .10-6
Super lattice thickness	H (μm)	0.81	0.99
Front surface power reflectivity	R	0.99	0.99
Illumination photon number	ϕ Photon/s	10^8	10^8

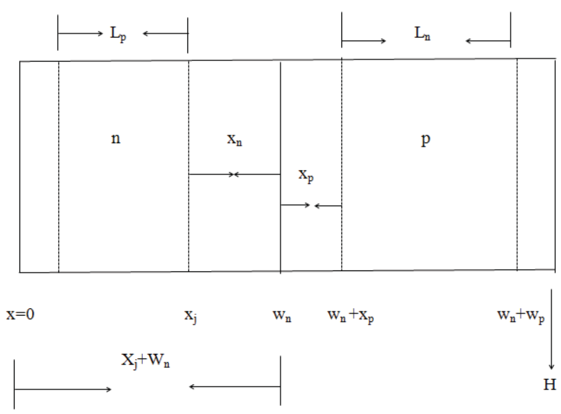
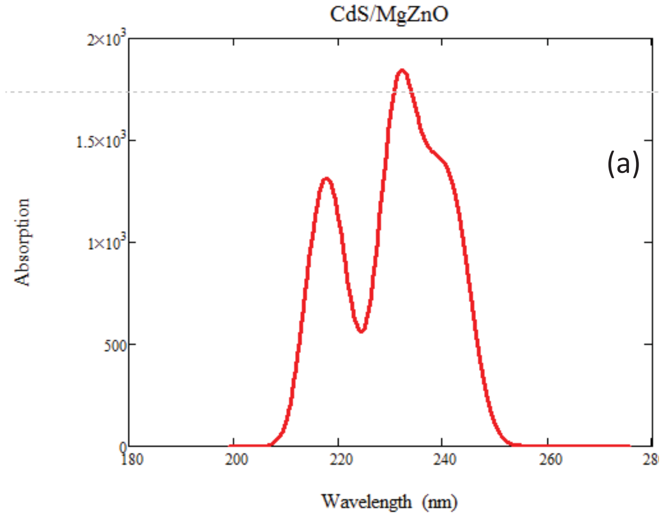


Fig. 1: Schematic representation of the QD solar cell layers structure.



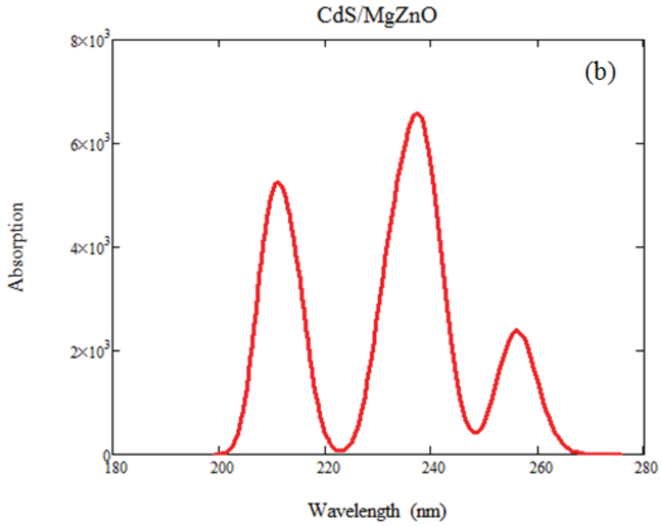


Fig. 2: Shows the QE for the CdS/MgZnO structure when a) h=2nm and ρ =14nm, b) h=1 nm and ρ =12nm.

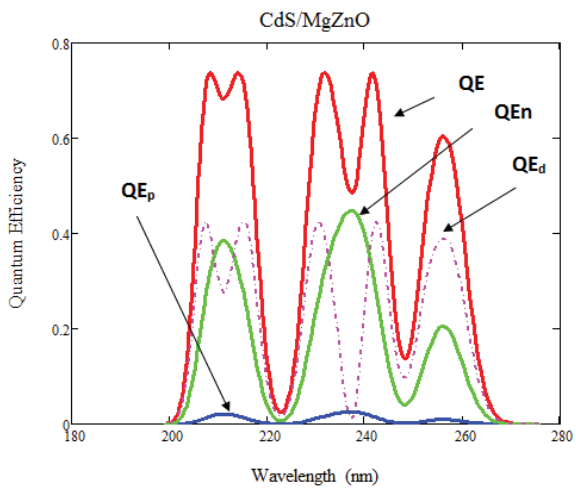


Fig. 3: Quantum efficiency CdS⁄MgZnO QD structure (h = 1 nm, ρ= 12 nm).

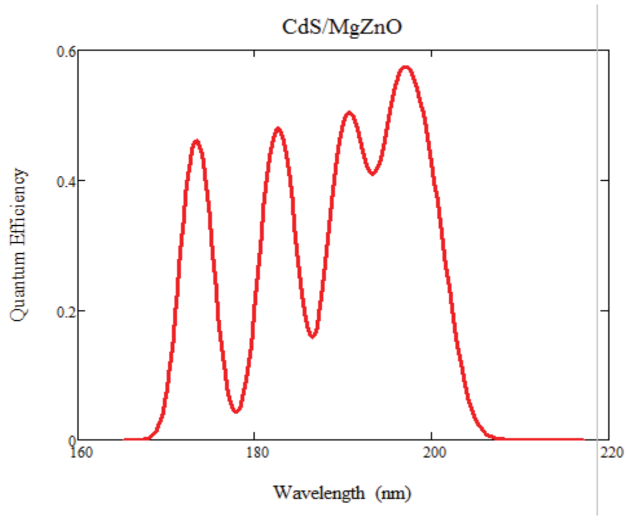


Fig. 4: Quantum efficiency CdS⁄MgZnO QD structure (h = 2 nm, ρ= 14 nm).

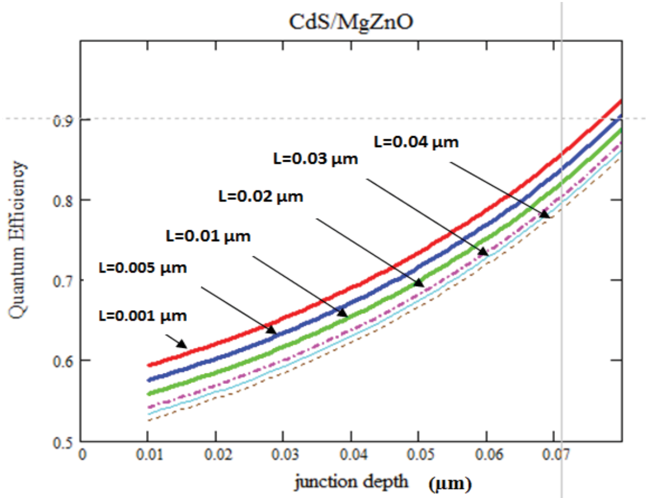


Fig. 5: QE of CdS/MgZnO QD structure at different values of hole diffusion length L_p

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