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DESIGN AND SIMULATION OF THIN-FILM SILICON QUANTUM WELL PHOTOVOLTAIC CELL

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A new thin-film silicon photovoltaic cell could be designed by inserting quantum well layers in the intrinsic region. Calculations show the improvement in spectral absorption due to the quantum well layer insertion. This article reports the design parameters and enhanced spectral absorption for a newly designed thin-film silicon quantum well photovoltaic cell.

Keywords: SILICON, QUANTUM WELL, PHOTOVOLTAIC CELL, DESIGN, SIMULATION.

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1. INTRODUCTION

Quantum well photovoltaic cells (QWPVC) are hetero-structure devices intended to achieve higher efficiencies than conventional cells. Generally this concept is used in well defined III-V & II-VI material systems. First, in 1990s Barnham group at Imperial College has demonstrated experimentally that the conversion efficiency of p-i-n photodiodes illuminated by broadband radiation could be enhanced simply by inserting quantum wells in the intrinsic region of the device [1, 2]. In context with the material of interest for terrestrial photovoltaic cell i.e. silicon, R. Sircar et al. first showed enhancement in amorphous silicon (a-Si) photovoltaic cell by inserting crystalline silicon (c-Si) quantum well layers [3]. Further, the effect of inserting quantum wells on electrical parameters of microcrystalline silicon photovoltaic cell was reported by B. Tripathi et al. [4]. In this paper, enhanced spectral absorption because of inserting quantum well structures inside the intrinsic layer of conventional microcrystalline silicon photovoltaic cell is reported and design parameters are discussed.

2. OPTICAL ABSORPTION OF A-Si AND C-Si

2.1 Reference spectrum

The AM1.5 reference solar spectrum is shown in Fig. 1 to highlight the absorption bands of amorphous silicon (a-Si) and crystalline silicon (c-Si), because in this article authors would show that how one can significantly improve the spectral absorption in thin-film silicon based photovoltaic cells by inserting silicon layers of higher crystallinity in the intrinsic region. It is

observed in the Fig. 1 that significant solar radiation is available in higher wavelength side i.e. beyond the absorption zone of a-Si (optical band gap ~ 1.75 eV, which corresponds to a wavelength of ~ 750 nm) which remains unabsorbed in the a-Si based thin-film photovoltaic cells. It could be found that if thin silicon layers of higher crystallinity are inserted in the intrinsic region of p-i-n or n-i-p type amorphous silicon photovoltaic cell then that absorbs the solar radiation beyond the absorption zone of a-Si. It is shown in this article that because of intersubband absorption there would be enhancement in the spectral absorption in the device structure.

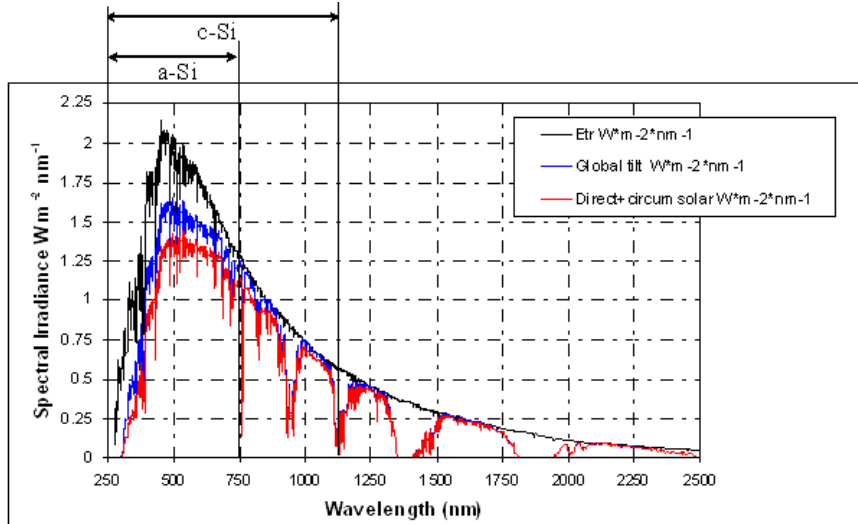


Fig. 1 – Absorption band of amorphous silicon (a-Si) and of crystalline silicon (c-Si) shown in the ASTM G173-03 reference spectra showing spectral irradiance versus wavelength consisting of AM1.5 solar spectrum (Source: <http://rredc.nrel.gov/solar/spectra/am1.5/> [Downloaded on Feb 1, 2009]).

2.2 Absorption coefficient

The reason for amorphous silicon (a-Si) being material of choice and being preferred over crystalline silicon (c-Si) for thin film photovoltaic application can be explained on the basis of difference in their absorption coefficient. It is shown in Fig. 2, that a-Si has high absorption coefficient by one order of magnitude in the energy band from 1.8 to 3.3 eV compared to crystalline silicon (c-Si). The information which may be extrapolated from Fig. 2 is that the absorption coefficient of hydrogenated microcrystalline silicon ($\mu\text{c-Si:H}$) may lie near to that of c-Si based on the order of crystallinity in the thin-film of $\mu\text{c-Si:H}$. Also from Fig. 1, one may observe that the peak of incident solar spectrum lies in this energy band (1.8 to 3.3 eV). So it becomes important to use a-Si as thin-film photovoltaic cell material. But till now the commercial single-junction a-Si photovoltaic cell efficiency have not been reported more than 8 %. While using a-Si as a suitable material for thin-film photovoltaic application it may be useful to sandwich the lower effective bandgap material ($\mu\text{c-Si:H}$) in the intrinsic region of the device to have extra spectral absorption in order to have improved power output per unit area.

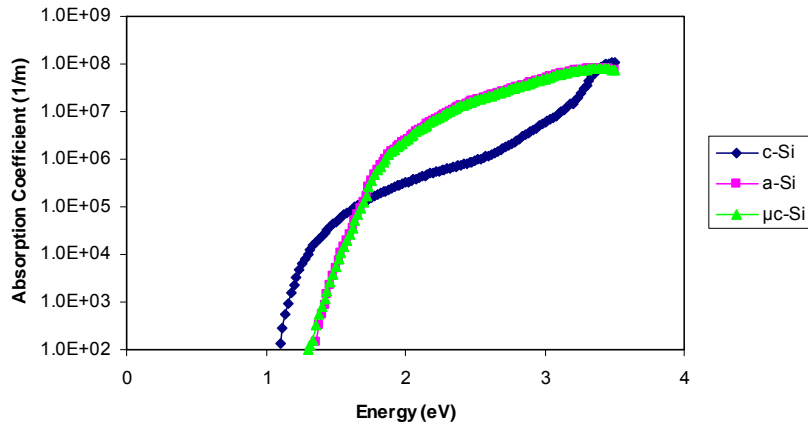


Fig. 2 – Absorption coefficient of crystalline silicon (*c-Si*) and amorphous silicon (*a-Si*) in the energy band of maximum spectral irradiance.

3. QUANTUM CONFINEMENT

Although the concept of quantum confinement is already known to the scientific community but it is necessary to explain the same in context of the work reported in this article. The concept of quantum confinement may be explained in terms of a square quantum well shown in the Fig. 3 (a), (b), & (c). When a smaller band gap semiconductor material (say “B”) thin layer is sandwiched between two broader band gap semiconductor material (say “A”) layers then it creates an offset in the band structure, which is called a quantum well (Fig. 3 (c)). Discrete energy levels inside the quantum well are schematically shown in the Fig. 3 (c). This concept of quantum wells has been theoretically studied, experimentally demonstrated, and has been widely used via III-V, II-VI material systems for various applications e.g., Lasers, Detectors, Solar cells etc.

Similarly, a $\mu\text{c-Si:H}$ thin film which has a smaller band gap than the hydrogenated amorphous silicon (a-Si:H) can be sandwiched between two a-Si:H thin layers so as to give rise to quantum mechanical effects. The quantum mechanical effect, giving rise to quantized energy levels in the sandwiched structure, could lead to extra absorption of incident radiation in such structure. To observe the effect of $\mu\text{c-Si:H}$ layer insertion in the intrinsic region of a-Si:H p-i-n or n-i-p photovoltaic cell one needs to calculate intersubband absorption coefficient for such band structure.

4. INTERSUBBAND ABSORPTION COEFFICIENT CALCULATION

Since micro-crystalline silicon material has indirect band gap so it is fair to assume the existence of ellipsoidal quantum wells due to insertion of $\mu\text{c-Si:H}$ layers between the a-Si layers. We refer to Brown & Eglash [5] for the calculation of the quantum-well intersubband absorption by electrons in ellipsoidal valleys. An experimentally measurable quantity is the fractional absorption per quantum well, ζ , as a function of frequency ω , expressed as:

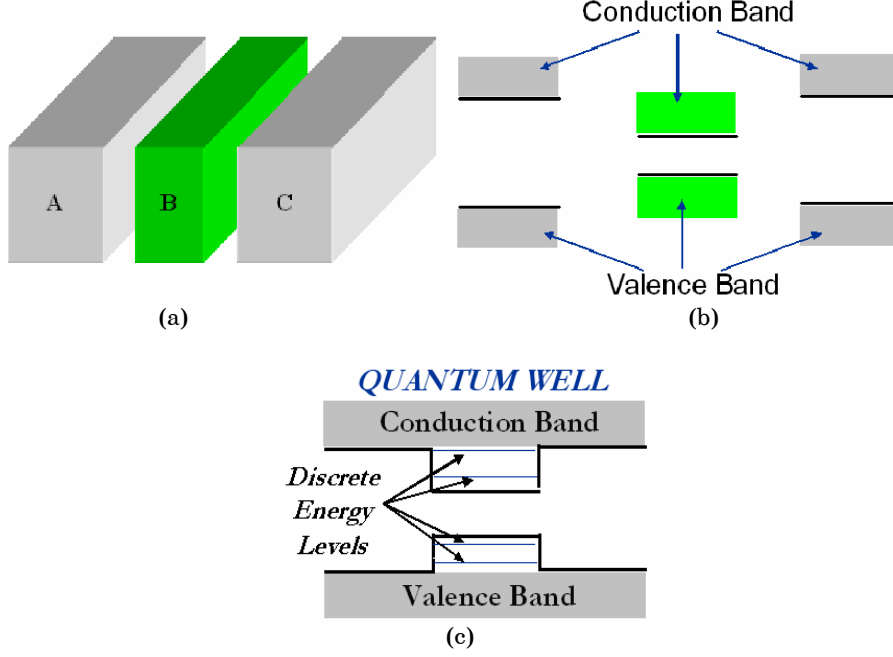


Fig. 3 – Bulk semiconductors A & B with a difference in the band gap (a); schematic diagram of conduction band and valence band of the bulk materials in sequence (b); schematic diagram of a quantum well created in both the bands i.e. valence band and conduction band due to the band offset of the materials A & B.

$$\zeta(\omega) = \frac{256\hbar e^2 \omega_0 \sigma_T}{27\pi n c \omega M_C w_{zz}} \frac{\Gamma_s}{(\hbar\omega_0 - \hbar\omega)^2 + \Gamma_s^2 / 4} \sum_{\eta=1}^{M_C} \frac{(A_x w_{xz}^{(\eta)} + A_y w_{yz}^{(\eta)} + A_z w_{zz}^{(\eta)})^2}{|\bar{A}|^2} \quad (1)$$

where e represents the electronic charge, ω_0 represents cut-off frequency, σ_T is the total sheet charge density in the first state, n represents refractive index of the material, c represents velocity of light, Γ_s is the energy broadening parameter, \bar{A} represents vector potential, M_C represents the number of ellipsoids contributing to the absorption of frequency ω and w_{mn} represents effective mass tensor component which is equal to $\hbar^{-2} \partial^2 E(\vec{k}_0) / \partial k_m \partial k_n$.

4.1 Absorption Coefficient

The absorption coefficient for a quantum well of width L_z , for which the fractional absorption is given by Eq. (1), can be calculated for following two cases:

- when the radiation is incident normal to the plane of quantum well;
- when the radiation is incident at an angle θ with respect to normal.

From geometrical considerations, the absorption will occur over a length L_z in the former case, and over a length $L_z \sec\theta$ in the latter case. Now

taking the length of absorption as $L_z \sec\theta$, one can define a direction dependent absorption coefficient as:

$$\exp[-\alpha(\omega)L_z \sec\theta] = 1 - \zeta(\omega) \quad (2)$$

It is assumed implicitly that the magnitude of vector potential decays negligibly across the width of the quantum well (i.e., between $z = 0$ and $z = L_z$). This is equivalent to $\zeta(\omega) \ll 1$, which leads to the approximate expression for the absorption coefficient, $\alpha(\omega) = \zeta(\omega)/L_z \sec\theta$. From the infinite barrier approximation, $L_z = (3\hbar\pi^2 w_{zz} / 2\omega_0)^{1/2}$. These relation and Eq. (1) lead to the following expression for the absorption coefficient at $\omega = \omega_0$:

$$\alpha(\omega_0) = \frac{\hbar\sigma_T}{\Gamma_s} \left[\frac{1024\xi(2\hbar\omega_0 w_{zz} / 3)^{1/2}}{27\pi^2 n} \cos\theta G(\theta, \varphi) \right] \quad (3)$$

where $\xi = e^2/\hbar c \cong 1/137$ is the fine-structure constant, $G(\theta, \varphi)$ is called as crystallographic factor and is given by the dimensionless expression

$$G(\theta, \varphi) = \frac{w_{zz}^{-2}}{M_C} \frac{\sum_{\eta=1}^{M_C} (A_x w_{xz}^{(\eta)} + A_y w_{yz}^{(\eta)} + A_z w_{zz}^{(\eta)})^2}{|\bar{A}|^2} \quad (4)$$

Since a real beam of light impinging on the quantum well at $\theta = 90^\circ$ is, in the sense of Fourier optics, a distribution of plane waves of different spatial frequencies. Each spatial frequency (except the dc component) corresponds to a plane wave incident at a θ different than 90° , so that absorption of the beam as a whole is nonzero.

5. DESIGN OF A MICRO-CRYSTALLINE SILICON QWPVC

The design of silicon QWPVC consists of a sequence of thin layers over a TCO coated glass substrate. The p-layer and n-layer thickness is taken as 20 nm as per general modeling criterion. The intrinsic region of designed photovoltaic cell consists of a group of thin barrier and well layers. Barrier layer has to be sufficiently thick in order to avoid tunneling and dark current so thickness of this layer is taken as 30 nm. The selection of well layer thickness is based on the quantum efficiency calculations with respect to wavelength. The intersubband absorption coefficient could be calculated for $\mu\text{-Si:H/a-Si}$ hetero-structure (as per the design shown in Fig. 4) using the theory referred in section 4 and assuming that most of the crystallites in the thin-film have (111) orientation or alternatively the thin film is (111) oriented silicon thin-film sandwiched between two amorphous thin films.

5.1 Quantum efficiency calculation

The external quantum efficiency is an important parameter for assessment of the performance of photovoltaic cell, which defines the number of electron-hole pair generated per incident photon in the device structure. For calculating quantum efficiency we refer to Nelson [6], where the quantum efficiency is defined as:

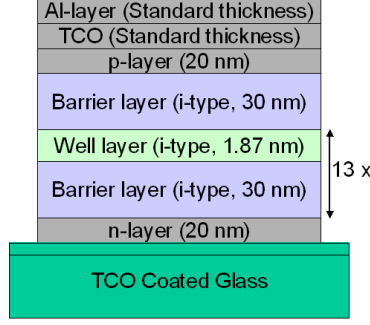


Fig. 4 – Design of a quantum well photovoltaic cell.

$$EQE(E) = \frac{-j_n(E) - j_p(E) - j_{dr}(E)}{qb_s(E)} \quad (5)$$

where, q represents electronic charge, $b_s(E)$ represents incident photon flux, $j_n(E)/qb_s(E)$, $j_p(E)/qb_s(E)$ and $j_{dr}(E)/qb_s(E)$ represent contributions of n , p and depletion layers respectively to external quantum efficiency.

In this article the enhanced spectral absorption is shown due to the band gap engineering being done in the depletion region (which includes intrinsic region). So it is important to precisely calculate the contribution of depletion region to the external quantum efficiency, which is expressed as following [7]:

$$\frac{j_{dr}(E)}{qb_s(E)} = (1 - R(E)) \exp(-\sum \alpha_i z_i) [1 - \exp(-\alpha_B W - N_W \alpha_W L_z)] \quad (6)$$

where, $R(E)$ represents reflection coefficient, α_i represents absorption coefficient of i^{th} layer from front side, z_i represents thickness of the i^{th} layer, α_B represents absorption coefficient of base material, W represents thickness of intrinsic layer, N_W represents number of well layers, α_W represents intersubband absorption coefficient, L_z represents thickness of the well layer. One may optimize the well layer width by substituting the calculated value of intersubband absorption coefficient using Eq. (6). This theory is used to plot quantum efficiency against energy associated with incident radiation.

5.2 Well layer width optimization

An optimized value of well layer width could be obtained at a fixed wavelength value of 1000 nm where the peak lies in the incident solar spectrum as shown in the Fig. 1. For optimizing the well layer width the values of quantum efficiency at various well widths were plotted as shown in Fig. 5. For a wavelength of 1000 nm the optimized width of the well layer is calculated to be 1.87 nm.

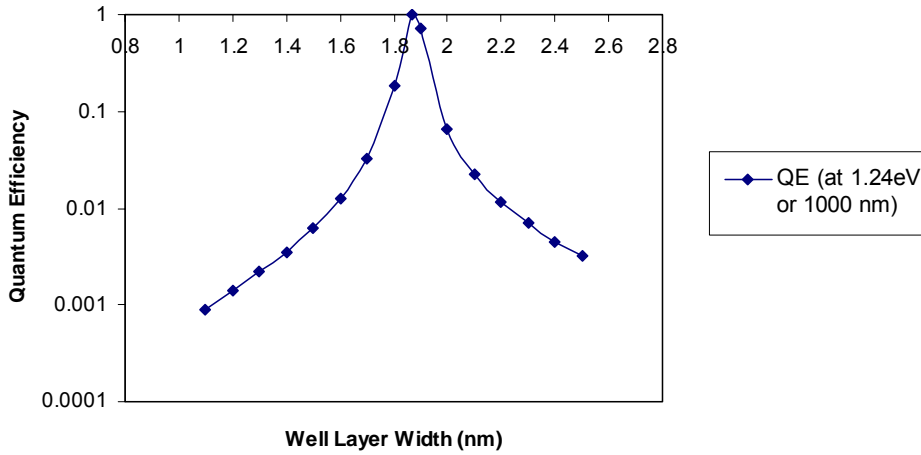


Fig. 5 – Quantum efficiency versus well layer width at a wavelength of 1000 nm.

The insertion of this well layer is justified because for a wavelength of 1000 nm, which corresponds to 1.24 eV, there was no absorption in conventional thin-film Si n-i-p photovoltaic cell as shown in Fig. 5. By introducing quantum well layer of calculated thickness in the intrinsic region of μ -Si photovoltaic cell (either in n-i-p or p-i-n configuration) it is expected that a significant portion of the solar spectrum would be absorbed efficiently.

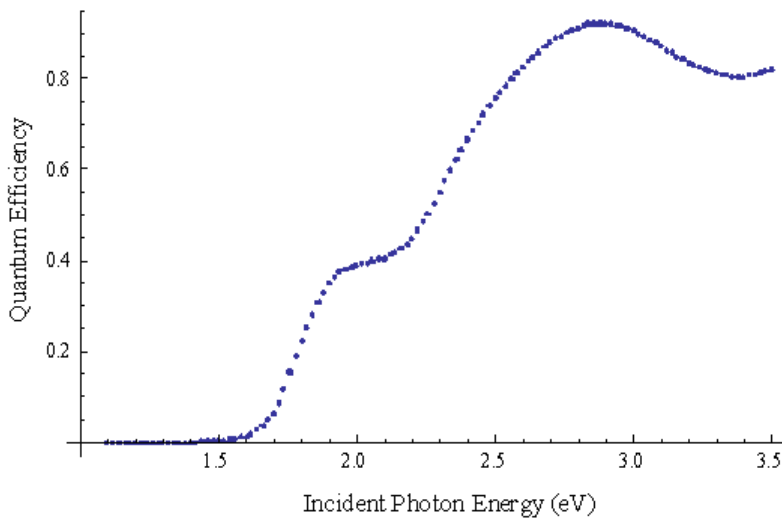


Fig. 6 – Quantum Efficiency versus Incident Photon Energy for p-i-n microcrystalline silicon photovoltaic cell

The outlined theory is used to calculate quantum efficiency values against energy associated with the radiation incident over a photovoltaic cell with quantum wells. The quantum efficiency data is plotted against incident photon energy as shown in Fig. 6. It is observed that there is enhanced spectral absorption due to insertion of quantum well layers in the intrinsic region of amorphous/microcrystalline silicon photovoltaic cell, because there is an extra

peak at an energy value of 1.24 eV, when compared with Fig. 5. The enhancement in the spectral absorption could be easily observed by comparing Fig. 5 (photon energy versus quantum efficiency before inserting quantum well layers) and Fig. 7 (photon energy versus quantum efficiency after inserting quantum well layers) at incident photon energy of around 1.24 eV.

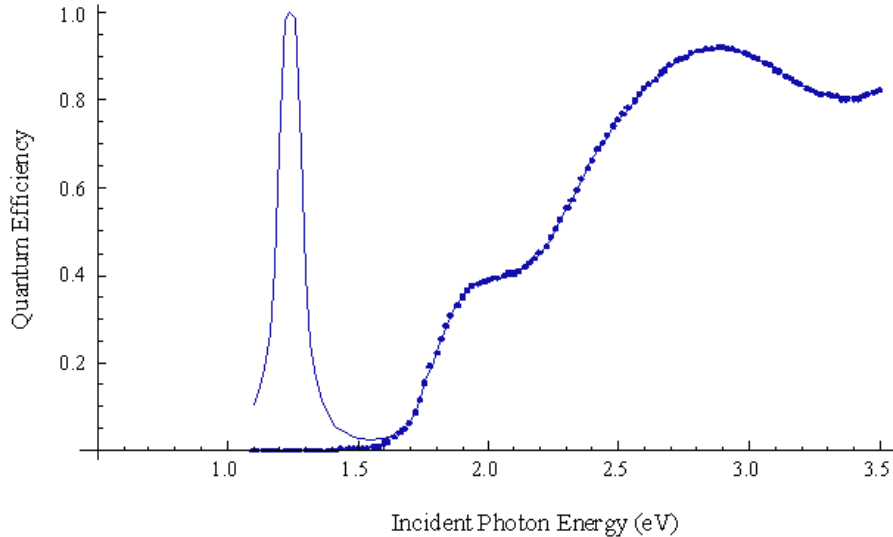


Fig. 7 – Quantum Efficiency versus Incident Photon Energy for QWPVC (solid curve) and microcrystalline silicon photovoltaic cell without quantum wells (dotted curve)

6. CONCLUSION

It is concluded that enhanced spectral absorption is recorded due to insertion of quantum well layers in the intrinsic region of microcrystalline silicon photovoltaic cell. A theory for modeling device structure of a microcrystalline QWPVC and calculating quantum efficiency of the same is established. It is shown that the well layer width plays a critical role for absorption of specific wavelengths. For efficient absorption of a band of wavelength centered around 1000 nm (1.24 eV) the optimized width of the well layer is calculated to be 1.87 nm.

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