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Computer simulation and modeling of solar energy based on photonic band gap materials

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In this paper, we have obtained theoretically a convenient way to improve the tandem solar cell efficiency by using one-dimensional binary photonic crystals in the anti-reflection coating and intermediate reflective layer. Also, we design and simulate our structure by using two different methods; MATLAB program based on a transfer matrix method and COMSOL Multiphysics software based on a finite element method. We have obtained the localization of the photons energy on the appropriate cell and then reduced the energy losses by controlling the photonic band gap. The present design is more convenient for cold countries.

Keywords: photovoltaic, thermal energy, renewable energy, photonic crystals, anti-reflection coating.

1. Introduction

Recently, many authors studied the solar energy by different methods to increase the efficiency. The way to enhance the efficiency of the solar cell is increasing the absorption probability for the solar photons impinging on the photovoltaic (PV) device and increasing the optical path length within the cell [1]. Firstly, we should estimate the energy losses within the cell to overcome it and then enhance the efficiency. To study the losses reasons, we divide the energy of the incident photons compare with the energy gap E_g. The first part is the incident photon with energy lower than energy gap E_g, these photons will be transmitted (non-absorbed) from the cell without any generation. The second part is the photons with energy higher than E_g of the absorber and will be generate electron–hole pairs. Since the electrons and holes tend to occupy the energy levels at the bottom of the conduction band and the top of the valence band, respectively. The excess in energy due to the electron–hole pairs created from the photon converted to thermal energy, and we have some other losses due to the total reflection, incomplete absorption resulting from the finite thickness, recombination, metal electrode coverage and shading losses [2].

Tandem solar cells are the main limitations for cost-efficient fabrication of the third generation solar cells. There are different types of tandem solar cells based on the kind

of materials [3]. In the present work, we will use two junctions tandem solar cell which consists of the hydrogenated amorphous silicon (a-Si:H) as a top cell and the microcrystalline silicon (μc-Si:H) as a bottom cell. Some authors suggested the introduction of an intermediate reflective layer (IRL) between the hydrogenated amorphous silicon as a top cell and the microcrystalline silicon as a bottom cell [4, 5] which have an important role in the cell. In the IRL layer, there is a high reflectance layer in the spectral region and a low absorption layer in the top cell. The high conductivity is to avoid Ohmic losses and the high transmission in the spectral region is to minimize the absorption of the top cell [1]. The reflection is about 35% [1] by the polished silicon solar cell without anti-reflection coating (ARC) at wavelength, $\lambda = 600$ nm due to the high refractive index of silicon. The reflection is increased to about 37% [6] by an average of the absorbed part of the solar spectrum (up to 1100 nm) and across all incident angles. Hence, to overcome this defect, we will insert ARC on the surface of the cell to reduce the power dissipation due to reflection. In the combination between ARC and IRL, we will observe some enhancement in the efficiency.

In the present work, we will try to reduce the power dissipations in the solar cell using photonic crystals or photonic band gap (PBG) materials [7]. Photonic crystals are artificial materials [8, 9]. Photonic crystals are artificial structures with periodically modulated refractive indices in one, two and three dimensions [10–13], and their lattice constants are in the order of a fraction of the optical wavelength. Photonic crystals have attracted a lot of attention in the recent years due to their unique features and the possibility to be used in several applications. The important feature is the PBG where the electromagnetic modes cannot propagate within these PBGs, regardless of the polarization and propagation direction of the refractive indices in the crystal interface.

2. Modeling

2.1. Anti-reflection coating

The simplest solar cell consists of an optically homogeneous slab with an optical thickness $d_{\text{opt}} = nd\cos^{-1}(\theta_2)$ where n and d are the refractive indexes and the thickness of the cell respectively, θ_2 is the refractive angle inside the cell [1]. Due to the contrast in the refractive index between a semiconductor material and air, the high amount of light energy did not reach to the active region but reflected on the surface. The ratio of reflection can be reduced by applying a planar ARC on the top of the cell which consists of a dielectric layer of thickness $\lambda/4$.

We will design a planar ARC which consists of silicon nitrite Si_3N_4 embedded between two layers of silicon dioxide SiO_2 [14] as shown in Fig. 1.

Figure 1**a** shows the schematic structure of ARC with meshing, where the size of meshing is ten times smaller than the lowest incident wavelength in the simulation procedure using a finite element method (FEM). Also, Fig. 1**b** represents the propagation of the incident electromagnetic wave through the considered structure of ARC. Sunlight is necessary to increase the temperature of the solar cell and the intensity of incident light [15]. We will study and simulate the effect of temperature on the structure

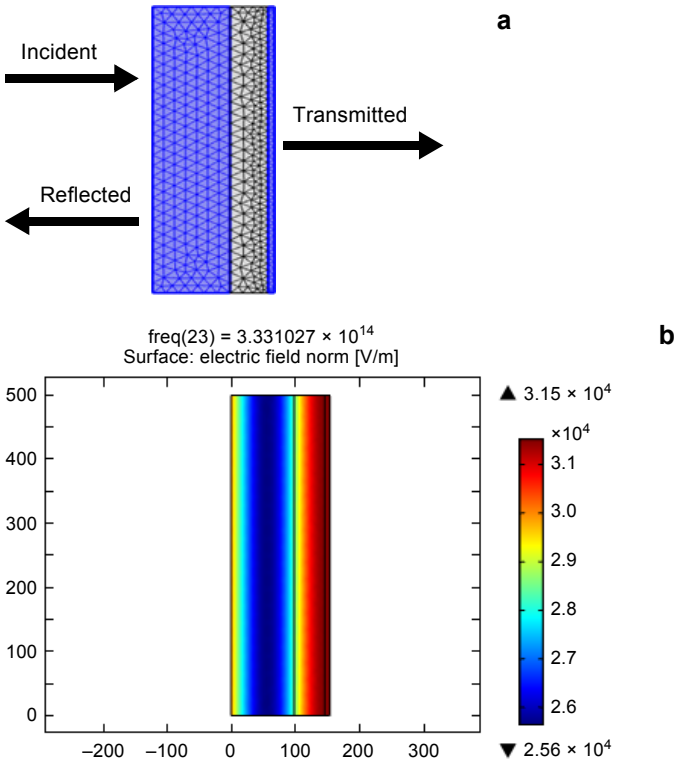

Fig. 1. Schematic structure of ARC with meshing (**a**), and electromagnetic waves distribution (**b**).

by using MATLAB based on transfer matrix method (TMM) [9], and by COMSOL Multiphysics based on FEM. Besides, the refractive index depends on the temperature due to a thermo-optical effect formula [16]

$$\Delta n = \gamma n(\Delta T) \tag{1}$$

where γ is the thermo-optic coefficient of the medium, n is the refractive index and ΔT is the variation in temperature. The thickness will be changed under the effect of a thermal expansion effect [16]

$$\Delta d = \alpha d(\Delta T) \tag{2}$$

where α represents the thermal expansion coefficient of the medium and d is the thickness of the material. This structure represents one-dimensional ternary photonic crystals for $N = 1$ in our analysis and simulation procedure.

2.2. Intermediate reflective layer

The IRL is employed between the hydrogenated amorphous silicon (top cell) with higher energy gap ($E_g \approx 1.7$ eV) and the microcrystalline silicon (bottom cell) with lower energy gap ($E_g \approx 1.1$ eV) to reflect a non-absorbed photon with the shorter wavelength

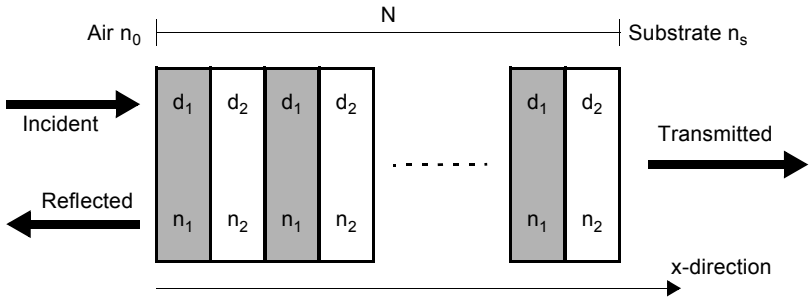

Fig. 2. Schematic diagram of one-dimensional binary structure; the thicknesses of the materials are denoted by d_1 and d_2, respectively, and the corresponding refractive indices are separately indicated by n_1 and n_2; n_0 is the index of the air, and n_s is the index of the substrate layer.

to the top cell. The IRL acts as a back reflector for the top cell and as a window for the bottom cell whereby the photons with longer wavelength are transmitted to the bottom cell. Therefore we use PBG materials to localize the photons on the favorable cell.

We design one-dimensional binary photonic crystals as shown in Fig. 2 with different periods of zinc oxide doped with aluminum (ZnO:Al) and μc-SiO_x:H with refractive indices 2 and 2.8, respectively [17]. PBG can be controlled by the dielectric contrast, the number of periods and the thicknesses of materials.

3. Result and discussion

3.1. Anti-reflection coating

Firstly, we studied the effect of the embedded material between the SiO_2 two layers. We obtained the optimal results for ARC thicknesses at 98 nm to the top SiO_2 layer and 48 nm to the Si_3N_4 layer with adding the third layer SiO_2 at 8 nm for one period to

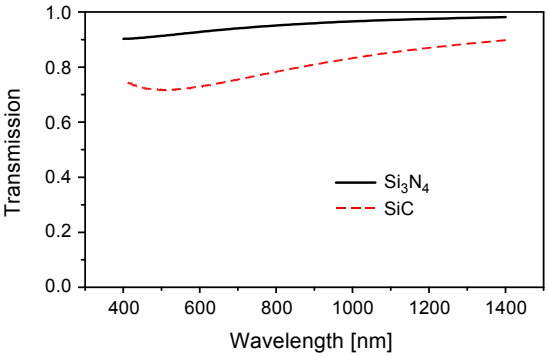

Fig. 3. Transmission of the structure with different embedded materials over the wavelength range of 400–1400 nm.

design one-dimensional ternary photonic crystal. By changing the embedded material as shown in Fig. 3, we found that the transmission increase in the case of Si_3N_4 with $n = 2.0167$ [15] relative to SiC with $n = 2.64$ [18], and this is suitable for ARC in the tandem solar cell because we observe the transmission approaching unity.

The results in Fig. 3 show the transmission which increased to 90% in the case of Si_3N_4 material and 80% in the case of SiC material. To achieve zero reflectance in the passband range, the quarter-wave stack must satisfy the following condition [18]:

$$\left(\frac{n_2}{n_1}\right)^2 = \frac{n_s}{n_0} \tag{3}$$

The effect of the interface between the dielectric ARC and the semiconductor material is due to the contrast in dielectric constants. We can optimize the thickness of the third layer (dielectric ARC) by coating the ARC on the surface of the hydrogenated amorphous silicon (a-Si:H) which is the top cell in the tandem solar cell as in Fig. 4**a**. The reflection in Fig. 4**b** decreases with increasing thickness of the SiO_2 third layer of ARC. Then we can consider the thickness of 8 nm which will be the optimum thickness in our design to reduce the reflection.

In Figure 5, we show the effect of temperature. It can be seen that the transmission increases when temperature decreases, due to a thermo-optical effect and thermal expansion effect. By this result, we can say that the cell is working well, especially in the winter season and is more suitable for cold countries. This is an advantage of the ARC

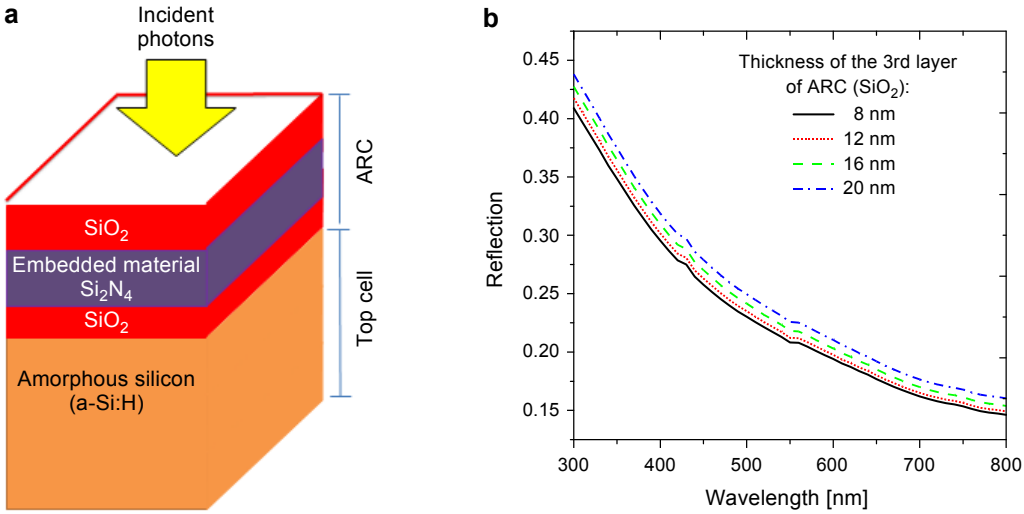

Fig. 4. Schematic diagram of the top cell with ARC (**a**). Reflection behavior in the structure at different thicknesses of the third layer of dielectric ARC; the thicknesses are 98 and 48 nm of the first and the second layer, respectively (**b**).

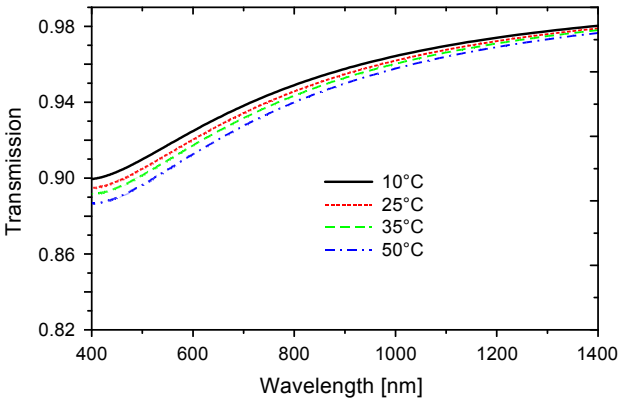

Fig. 5. Transmission curve at the ARC consists of the layer of Si_3N_4 embedded between two layers of SiO_2 at different temperatures. Results for ARC coating thicknesses of 98 nm for the top SiO_2 layer and 48 nm for the Si_3N_4 layer with the third SiO_2 layer fixed at 8 nm.

that works well in winter. In this case, all incident photons will be transmitted into the active region of the cell and generate the electron–hole pairs.

3.2. Intermediate reflective layer

As we mentioned before, in one-dimensional binary photonic crystals we designed two layers of ZnO:Al/μc-SiO_x:H [17] with thicknesses $d_1 = 62$ nm, and $d_2 = 40$ nm, respectively, and refractive indexes 2 and 2.8, respectively, with different periods. In Figure 6, we observed that by increasing the number of periods 5, 7 and 10, the reflection decreased to zero at 10 periods within PBG region. Maybe 10 periods is the op-

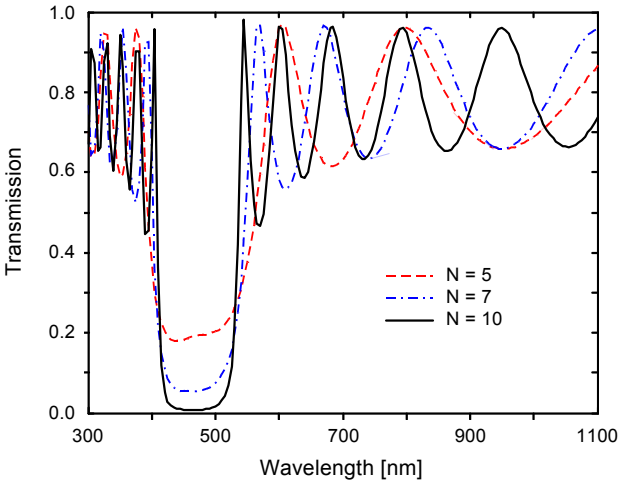

Fig. 6. One-dimensional binary photonic crystals of ZnO:Al and μc-SiO_x:H, the thicknesses of the materials are denoted by 60 and 40 nm, respectively, with different number of periods as shown.

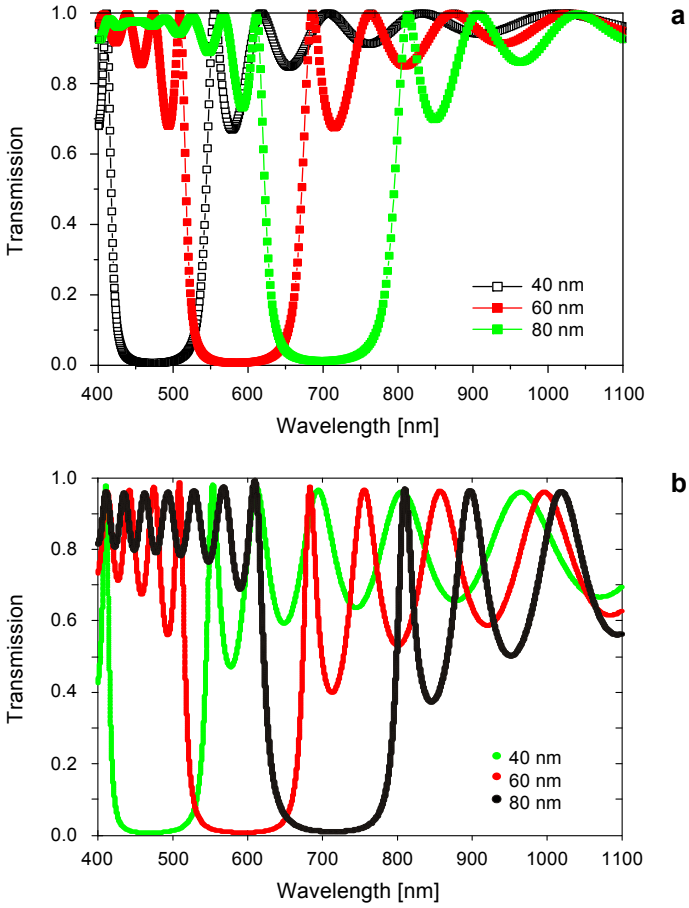

Fig. 7. One-dimensional binary photonic crystals of ZnO:Al with thickness 62 nm and μc-SiO_x:H with different thicknesses with ten periods: COMSOL Multiphysics (**a**), and MATLAB (**b**).

timum condition in our application as well as due to the unique properties of photonic crystals. Also, we found that the PBG shifted to the longer wavelength as shown in Figs. 7**a** and 7**b**. Three band gaps appear in the transmittance spectra (Fig. 7). From these figures, it is clear that as we increase the thickness, the band gaps shift slightly towards the longer wavelength region. The shifting of band gaps with the thickness is more pronounced than in Fig. 6, because the rate of change in the refractive index of the layers in Fig. 7 with thickness is more than the rate of change of refractive index of the layers in Fig. 6 with thickness. From this shift we can deduce why PBG depends on several parameters such as the dielectric contrast between the two layers and the thickness of each layer. Besides, we can confirm these results by two different methods; TMM in Fig. 7**b** and simulated procedure by FEM in Fig. 7**a**. These results explain how we can control and localize the electromagnetic waves by PBG and confirm the results by two methods: TMM and FEM.

We collected all the structures in a unique structure (Fig. 8**a**) which is considered as a quasi-one-dimensional photonic crystal to get wide PBG which is more suitable in solar cells.

In Figures 8**b** and 8**c**, the structure behaves like a back reflector to the top cell within the PBG from 400 to 775 nm and the reflection approximately reached 100%.

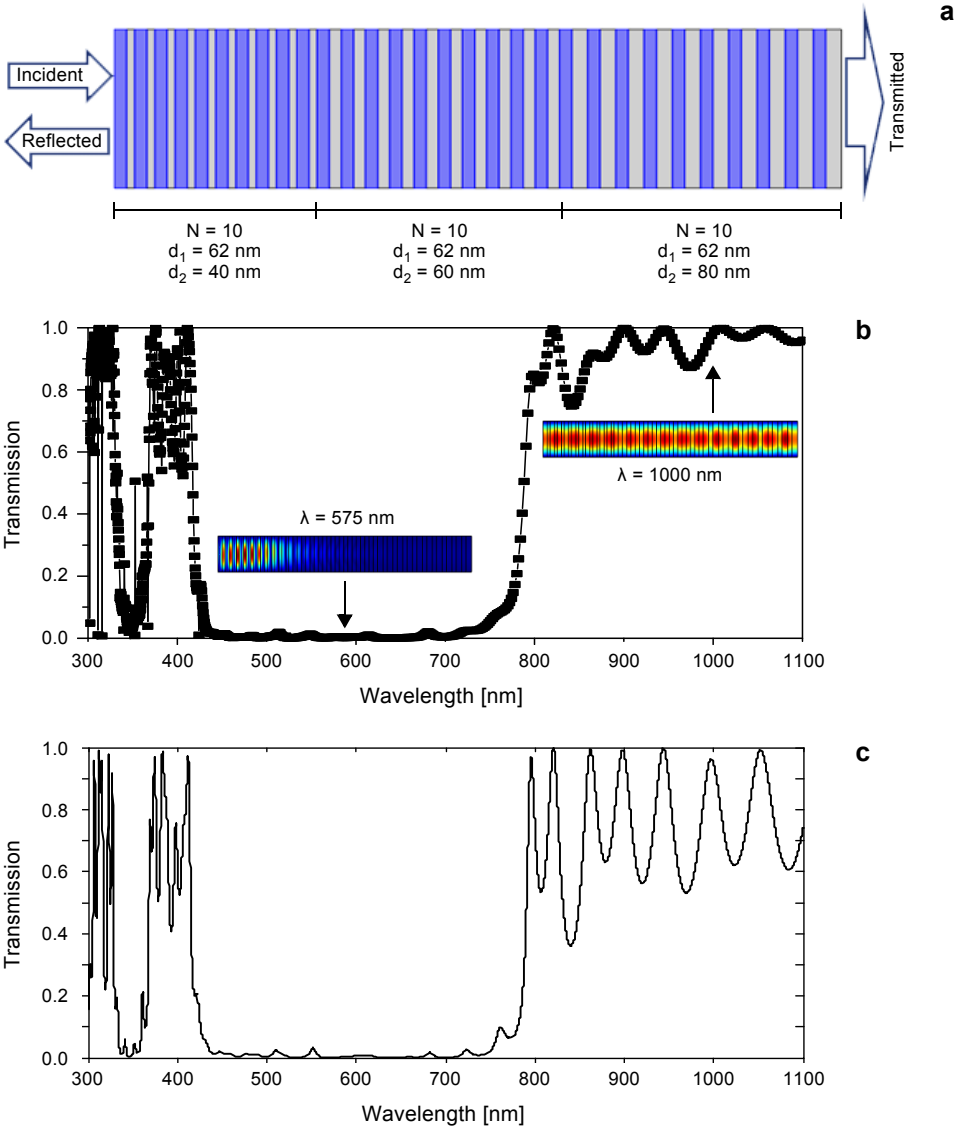

Fig. 8. One-dimensional binary photonic crystals of ZnO:Al with thickness 62 nm and μc-SiO_x:H with 40 nm for the first 10 periods, 60 nm for the second 10 periods and 80 nm for the third 10 periods. Schematic structure of the considered structure (**a**). Transmission behavior for the structure by COMOSL based on FEM (**b**). Transmission behavior for the structure by MATLAB based on TMM (**c**).

The results from 775 to 1100 nm behave as a window or ARC for the bottom cell because the transmission approaches unity. Finally, our results verify the optimum condition for ARC and IRL for an efficient tandem solar cell. We can say that, if we insert IRL and ARC in the tandem solar cell it will overcome a large portion of power dissipation and enhance the efficiency. In the next step, we plan to obtain the current density as well as the efficiency of the tandem solar cell.

4. Conclusion

Photonic crystals play an important role in reducing losses in solar cells. In this paper, we designed one-dimensional binary and ternary photonic crystals in ARC and IRL. Our simulation and calculation were carried out by using MATLAB program based on a transfer matrix method (TMM) and COMSOL Multiphysics based on a finite element method (FEM). In ARC, we embedded Si_3N_4 between two layers from SiO_2 to reduce the spectral reflectance and this seems to be suitable for low-temperature regions. In IRL we have used two layers of ZnO:Al and μc-SiO_x:H with different periods and thicknesses. In our structure, we have obtained the localization of photons energy on the appropriate cell and then reduced the energy losses by controlling the PBG.

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