J. Bangladesh Acad. Sci., Vol. 42, No. 1, 87-97, 2018

ABSORPTION ENHANCEMENT OF ORGANIC SOLAR CELL USING ALUMINUM OXIDE AS A PHOTONIC CRYSTAL

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ABSTRACT

Enhancement of light absorption in solar cell presents a strong challenge to its overall performance. We analyzed an Organic Solar Cell (OSC) with Photonic Crystal (PC) structure using Finite Difference Time Domain (FDTD) method. Aluminum oxide (Al_2O_3) has been used as photonic crystal structure and the lattice structure has been chosen to be hexagonal. Absorption enhancement has been observed by changing the height of the Hexagonal Lattice structure (HLS). When height is increased to 0.26 and radius to period ratio (r/a ratio) is set to 0.4, there is a significant increase of absorption in the middle wavelength region approximately from 463 nm to 575 nm and a significant decrease in lower wavelength. As the height is increased further, these changes in absorption begins to increase and at a certain value, these changes begin to reverse. Almost same phenomena occur when r/a ratio is 0.2 and 0.3 taken at approximately same height.

Key Words: Organic solar cell, Photonic crystal, Absorption enhancement, Energy pay back time, Guided modes, FDTD method

INTRODUCTION

The development and utilization of organic solar cells, nowadays, is proved to be a better way to produce clean and renewable energy because of its several advantages including the ease of fabricating them onto large areas of lightweight substrates. The first conceptual organic solar cell, which was developed by Kearns and Calvin in (1958), used magnesium phthalocyanine as organic material between two electrodes (Naichia *et al.* 2013; David *et al.* 1958). The Power Conversion Efficiency (PCE) was too low (in the order of 0.1% or lower) and it could not be increased for more than 20 years (Holger *et al.* 2004). In 1986, Tang developed bilayer hetero junction OSCs with a PCE of about 1% which is regarded as a major milestone for OSC (Tang C. *et al.* 1986; Prodhan *et al.* 2017; Cheyns *et al.* 2010; You J. *et al.* 2013).

The solution process ability of organic semiconductors provides a great potential for low cost (Deepti *et al.* 2016) fabrication of large area OSCs. Low temperature processing reduces energy consumption during manufacturing. OSCs have capability of decreasing the energy payback time and printing on top of plastic substrates results in

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applications. Not only having low efficiency compared to silicon solar cells but also the stability of OSCs is a limitation to worldwide commercialization (Vikram *et al.* 2012). Recently organic solar cell efficiency has been increased to more than 10% (K. Woods *et al.* 2013) using bulk hetero junction and tandem cell structure (Nusrat *et al.* 2017).

Using photonic crystal in OSC can improve efficiency nearly to 70% (Doo-Hyun *et al.* 2009). One-dimensional (1-D) photonic crystals can be made of layers deposited or stuck together. Combination of 1-D photonic crystal and dielectric material can increase the effectiveness of absorption (James G. *et al.* 2009). Two-dimensional 2-D photonic crystals are fabricated by photolithography, or by drilling holes in a suitable substrate. Both 1-D and 2-D photonic crystals (Fig. 1) are used in thin film (Angelo *et al.* 2012) and ultra-thin film (Emmanuel *et al.* 2010) solar cells to increase the effectiveness of light trapping and photon lifetime (Emmanuel *et al.* 2009). Three-dimensional (3-D) photonic crystals (Fig. 1) are made by drilling under different angles, stacking multiple 2-D layers on top of each other.

Indium tin oxide (ITO) is a ternary composition of tin, oxygen and indium. ITO is transparent and conductive and has a high value of conductivity as well as optical property. In solar cell, the main advantage of ITO is that it can be made as thin as possible. PC is usually inserted on the upper ITO electrode (Leo *et al.* 2014).

By inserting Phenyl-C61-butyricacidmethyl ester (PCBM) and Poly-3-hexylthiophene (P3HT) layer, maximum conversion energy for solar cell is reached to 10% (Alias *et al.* 2014). It is a combination of narrow-band donor and fullerene derivate which is a possible approach to efficient organic cells (Schmidt *et al.* 2015). Performance of P3HT: PCBM is linked with electron to hole mobility ratios (Omar *et al.* 2013) and it also works as buffer layer (Zurianti *et al.* 2012). Also, the performance and degradation of bulk heterojunction organic solar cell depends on P3HT: PCBM (Balderramaa *et al.* 2011)

Poly (3,4-ethylenedioxythiophene)-poly (styrenesulfonate), commonly known as PEDOT: PSS, is a widely used hole transport layer. It is also a spin cast film. It has an aqueous dispersion with a hygroscopic property. It increases the series resistance of the device but decreases fill factor and current.

In this research work, light absorption is

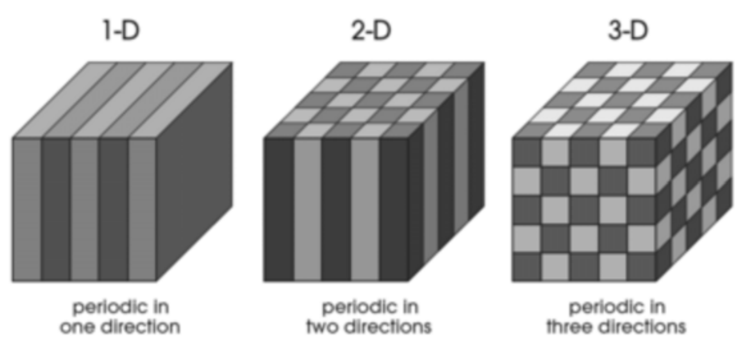


Fig. 1. 1D, 2D, 3D Photonic Crystal [Joannopoulos *et al.* 2008]

measured in P3HT: PCBM layer of the designed structure using FDTD simulations. Absorption profiles for OSC with different height and r/a ratio of the PC structure were compared and analyzed with that of flat solar cells.

METHODOLOGY

In order to analyze the light absorption, the structure shown in Fig. 2 is designed first using the FDTD solutions package of Lumerical Inc.

The structure has an aluminum layer at the bottom. Following up is a layer of Al_2O_3 adjacent with pillar type structure formed with Al_2O_3. A layer of P3HT: PCBM (poly-3-hexylthiophene [6,6]-phenyl-C61-butyric acid methyl ester) is employed then, which acts as a photoactive layer on PEDOT: PSS above of it. Sunlight is allowed to fall on a glass layer at the top of the structure beyond which an ITO layer is incorporated.

In setting up the structure, the geometry of each layer is fixed in terms of XY, YZ, and ZX dimensional positions. Three monitors are positioned to record the result. Those monitors are used to compare the results for OSC with photonic crystal layer and for flat surface with no extra layer. At first, period and diameter of the hexagonal PC structure are varied with fixed height to observe the absorption enhancement. Then height is varied with fixed period and diameter to observe the absorption enhancement (Fig. 3).

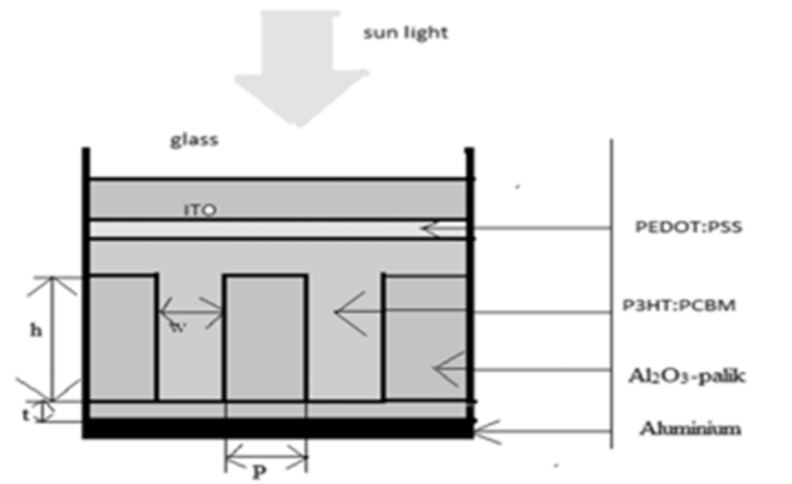


Fig. 2. Organic solar cell with aluminum oxide (Al_2O_3) as photonic crystal structure [Knowledge base, Lumerical Solution Inc.].

For every layer, rectangular structure and mesh order of 2 is used. Geometry is different for each layer. Sunlight is not directly used in this setup. Instead a normally plane wave source of wavelength ranging from 400 to 700 nm is used.

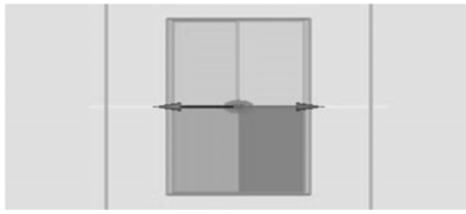


Fig. 3(a)

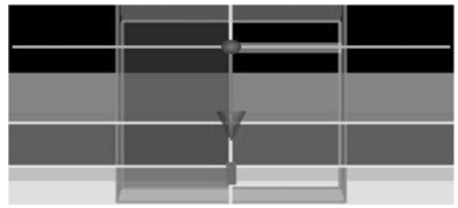


Fig. 3(b)

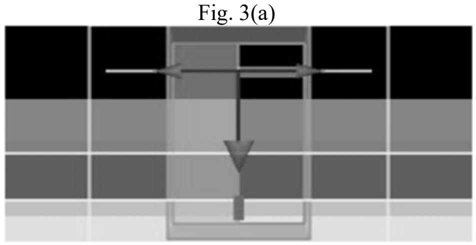


Fig. 3(c)

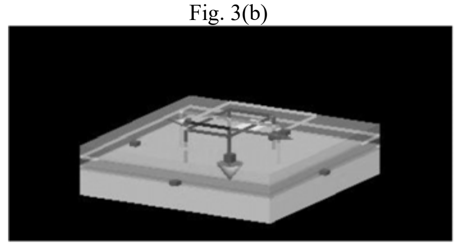


Fig. 3(d)

Fig. 3. Organic Solar cell 2D hexagonal lattice of photonic crystal are formed in the photoactive layer, (a) XY view, (b) YZ view, (c) ZX view and (d) perspective view.

Fig. 4 shows the normal coordinate view of a plane source.

For calculating the power absorption monitor_3 and monitor_4 is used. Monitor _3 is located boundary between P3HT: PCBM and PEDOT: PEDOT: PSS. Monitor_4 is located at the boundary between P3HT: PCBM and Al_2O_3.

The absorbed power P_{abs} is easily calculated by, Pabs(1) = –transmission ($monitor_3$)1 (–transmission ($monitor_4$)).

By using monitor 1, monitor 3, monitor 4 power absorption in ITO and PEDOT: PSS layer can be calculated. For absorption profile power monitor is required. In the

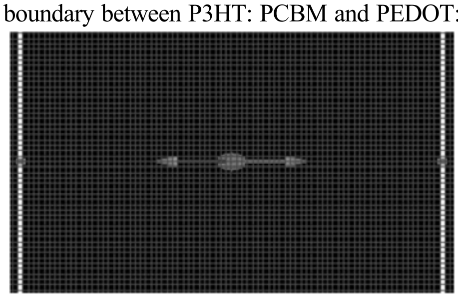


Fig. 4(a)

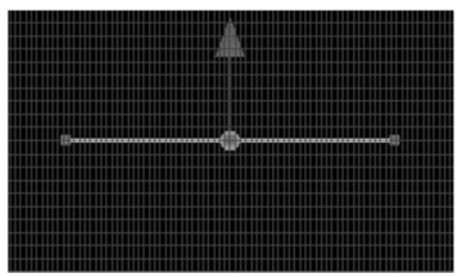


Fig. 4(b)

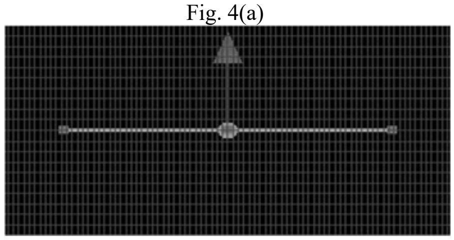


Fig. 4(c)

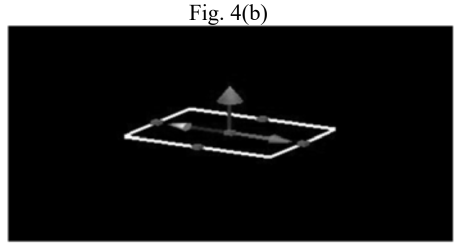


Fig. 4(d)

Fig. 4. (a) XY view (b) YZ view (c) ZX view (d) perspective view.

following table (Table-1) the general set up and geometry are shown.

Table 1. Simulation setup parameters and device geometry

	Monitor 1	Monitor 3	Monitor 4
Geometry	x = 0, y = 0, z = 0.2757 x span = 0.138, y span = 0, z span = 0.9018 (micron)	x = 0, y = 0, z = 0.198 x span = 0.2, y span = 2, z span = 0 (micron)	x = 0, y = 0, z = 0 x span = 2, y span = 2, z span = 0 (micron)
Time apodization	Apodization time (fs) = 500 Apodization time width (fs) = 100 Apodization freq width (fs) = 4.412	Apodization time (fs) = 0 Apodization time width (fs) = 250 Apodization freq. width (fs) = 1.76	Apodization time (fs) = 0 Apodization time width (fs) = 250 Apodization freq. width (fs) = 1.76

RESULTS AND DISCUSSION

Light absorption happened mainly in P3HT: PCBM layer. Absorption in P3HT: PCBM vs wavelength graph is calculated by changing period to diameter ratio and height. The thickness of the ITO and PEDOT: PSS are fixed to 178 nm and 50 nm, respectively, and that of P3HT: PCBM is fixed to 193 nm.

Fig. 5 shows the effect of height change on absorption enhancement of organic solar cell with photonic crystal when the period and diameter is fixed to 0.3 micron and 0.46 micron respectively where r/a ratio is 0.3 (Marko *et al.* 2001).

In Fig. 5(a), no significant change is observed between organic solar cell with photonic crystal structure and conventional flat solar cells. But in Fig. 5(b), there is a peak in higher wavelength region approximately at 674 nm where absorption ratio is 0.240 and also a slight decrease of absorption in lower wavelength region.

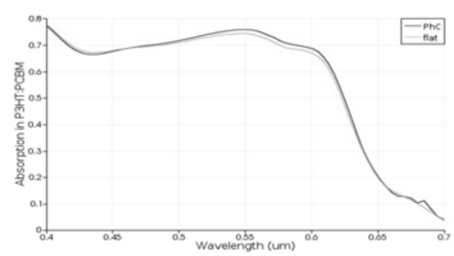


Fig. 5(a). Height of HLS is set to 0.03

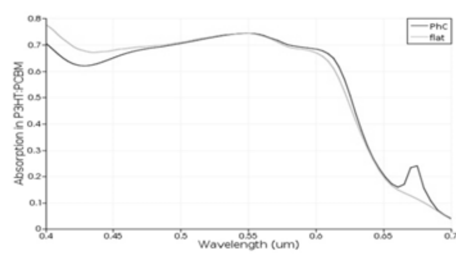


Fig. 5(b). Height of HLS is set to 0.11

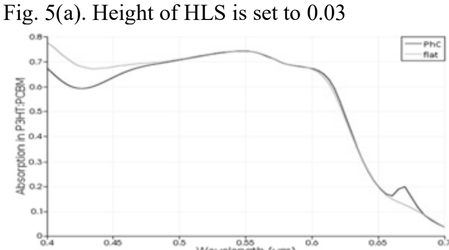


Fig. 5(c). Height of HLS is set to 0.13

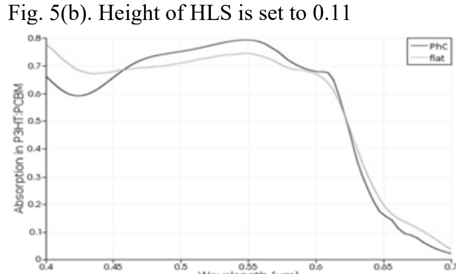


Fig. 5(d). Height of HLS is set to 0.21

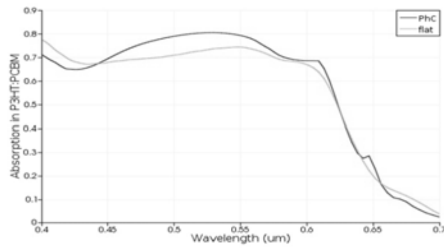


Fig. 5(e). Height of HLS is set to 0.29

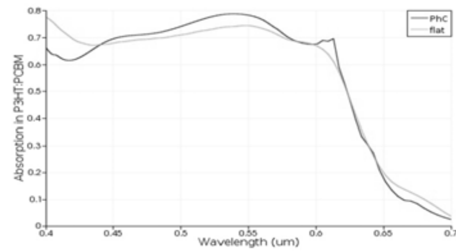


Fig. 5(f). Height of HLS is set to 0.37

A significant decrease of absorption in lower wavelength region which is 0.672 and the peak in the higher wavelength region at 669 nm begins to decrease and the absorption in the peak is 0.199 which is shown in Fig. 5(c). On the other hand, absorption in lower wavelength region (400 nm) decreases to 0.661 and there is increase of absorption in middle wavelength region between 457 nm to 617 nm in Fig. 5(d). The highest absorption in the middle wavelength region is 0.79 which is found at 548 nm.

Fig. 5(e) shows that absorption in lower wavelength region (400 nm) increases a bit. But the absorption in middle wavelength region widens more from 439 nm to 620 nm. The highest absorption in the middle wavelength region is 0.805 which is found at 529 nm. Besides, Fig. 5(f) shows that absorption in middle wavelength region begins to contract than before and absorption in lower wavelength start to increase. Absorption enhancement is seen between 437 to 582 nm and the highest absorption in the middle wavelength region is 0.788 which is found at 538 nm.

Fig. 6 shows the effect of height on absorption enhancement of organic solar cell with photonic crystal when r/a ratio is fixed to 0.368 micron and 0.46 micron respectively where r/a ratio is 0.4 (Emmanuel *et al.* 2009)

In Fig. 6(a), there is no significant change is observed between organic solar cell with photonic crystal structure and conventional flat solar cells. But in Fig. 6(b), a peak is shown in higher wavelength region approximately in 674 nm wavelength where absorption ratio is 0.235 and also a slight decrease of absorption in lower wavelength region.

A significant decrease of absorption in lower wavelength region which is 0.571 and peak in the higher wavelength region almost disappears in Fig. 6(c). On the other hand, absorption in lower wavelength region (400 nm) decreases to 0.547 and there is increase of absorption in middle wavelength region between 463 nm to 568 nm which is shown in Fig. 6(d). The highest absorption in the middle wavelength region is 0.79 which is found at 532 nm.

Fig. 6(e) shows that absorption in lower wavelength region (400 nm) increases a bit. But the absorption in middle wavelength region widens more from 463 nm to 575 nm. The highest absorption in the middle wavelength region is 0.81 which is found at 526 nm. Besides, Fig. 6(f) shows that absorption in middle wavelength region begins to contract than before and absorption in lower wavelength start to increase. Absorption enhancement is seen between

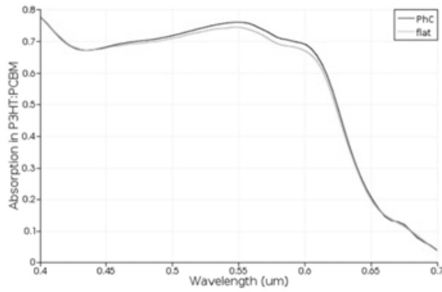


Fig. 6(a). Height of HLS is set to 0.01

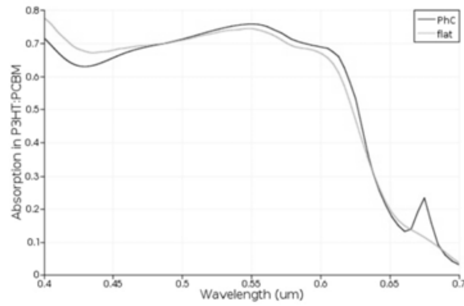


Fig. 6(b). Height of HLS is set to 0.09

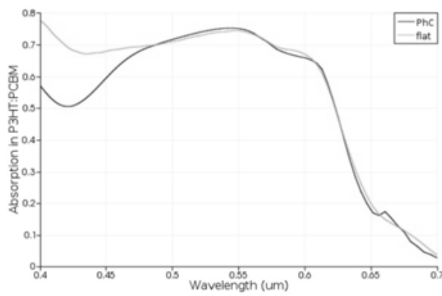
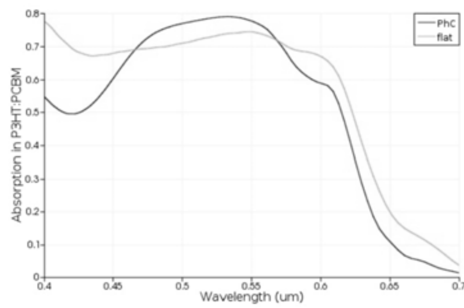


Fig. 6(c). Height of HLS is set to 0.14



F Fig. 6(d). Height of HLS is set to 0.20

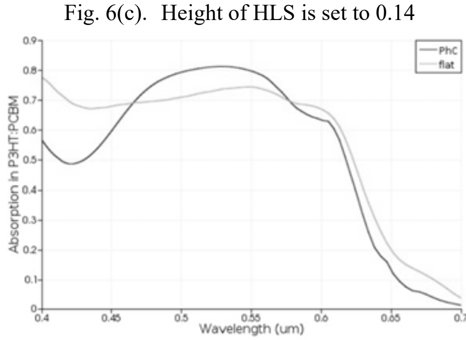


Fig. 6(e). Height of HLS is set to 0.26

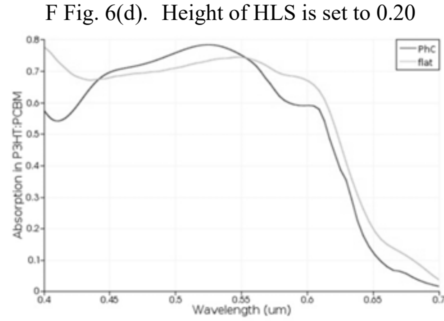


Fig. 6(f). Height of HLS is set to 0.36

439 to 551 nm and the highest absorption in the middle wavelength region is 0.78 which is found at 523 nm.

Fig. 7 shows the effect of height on absorption enhancement of organic solar cell with photonic crystal when the period and diameter is fixed to 0.184 micron and 0.46 micron respectively where r/a ratio is 0.2 (Masud *et al.* 2012).

In Fig. 7(a), there is no significant change is observed between organic solar cell with photonic crystal structure and conventional flat solar cells. But in Fig. 7(b), a peak in higher wavelength region approximately in 679 nm wavelength where absorption ratio is 0.179 and also a slight decrease of absorption in lower wavelength region.

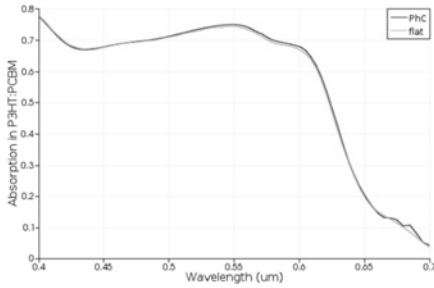


Fig. 7(a). Height of HLS is set to 0.04.

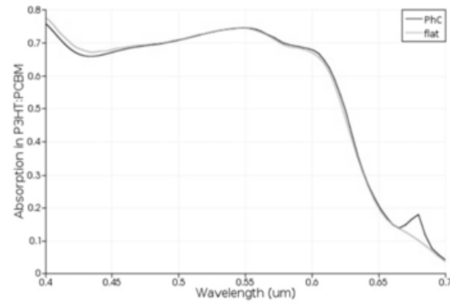


Fig. 7(b). Height of HLS is set to 0.10.

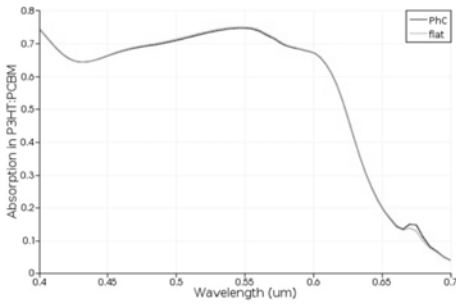


Fig. 7(c). Height of HLS is set to 0.15.

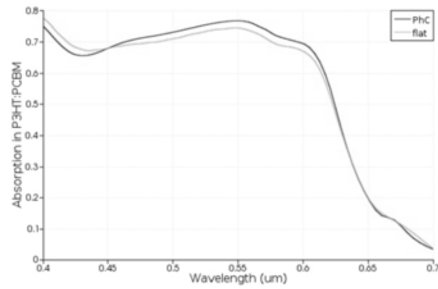


Fig 7(d). Height of HLS is set to 0.21.

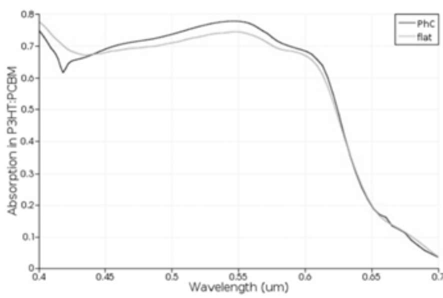


Fig. 7(e). Height of HLS is set to 0.34.

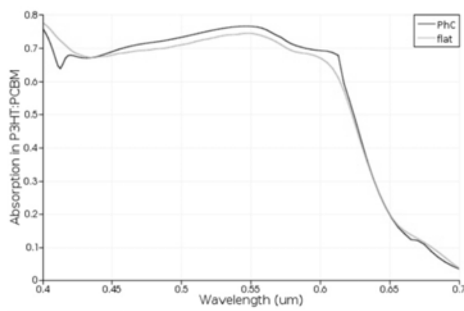


Fig. 7(f). Height of HLS is set to 0.40.

Fig. 7(c) shows that no change of absorption compared to flat solar cell in lower wavelength region. Peak in the higher wavelength region almost disappears. Besides, in Fig. 7(d), absorption in lower wavelength region (400 nm) decreases to 0.749 and there is increase of absorption in middle wavelength region between 450nm to 625 nm. The highest absorption in the middle wavelength region is 0.767 which is found at 551 nm.

Absorption in lower wavelength region at 417 nm decreases to 0.615. The absorption in middle wavelength region widens more from 439 nm to 625nm which is shown in Fig. 7(e). The highest absorption in the middle wavelength region is 0.778 which is found at 545nm. On the other hand, in Fig. 7(f), absorption in middle wavelength region begins to contract than before and sudden decrease of absorption in lower wavelength shifts at 410nm. Absorption enhancement is seen between 437 to 620 nm and the highest absorption in the middle wavelength region is 0.765 which is found at 548 nm.

These graphs compare absorption enhancements between organic solar cell with photonic crystal structure (aluminum oxide as photonic crystal) and conventional silicon flat solar cells. The three groups of graphs show the effect of height from these graphs, it can be seen that the absorption at the longer wavelength can be enhanced by photonic crystal. Here, the period, the diameter and the height of the PC are fixed to P = 460nm, D = 300nm. and h = 120nm, respectively and the thickness of the Al_2O_3 is set to t = 150nm. Users can optimize the design by the built-in optimization algorithm.

CONCLUSION

It is concluded that the photonic crystal structures of aluminum oxide can be modeled as a photoactive layer and analyzed using Finite Difference Time Domain to determine and observe the absorption enhancement and the effects of changes in height with different fixed periodicity and diameter. As height is increased with constant period and diameter, absorption at lower wavelength region decreased a lot and absorption in middle wavelength region approximately tends to reverse. The changes in absorption also happens because of guided modes created by aluminum oxide. Different material is taken as photonic crystal and aluminum oxide seems to achieve the most favourable results. Silicon dioxide (Khai Q. *et al.* 2015) shows almost similar absorption enhancement compared to aluminum oxide.

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(*Received revised manuscript on 27 March, 2018*