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NUMERICAL MODELING OF NANOSTRUCTURE-ENHANCED SOLAR CELLS

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ABSTRACT
This paper presents a computational study of nanostructure-enhanced solar cells. The computer model is developed based on the FDTD solution of the Maxwell equations describing the light propagation in thin film solar cells. With the model, a combination of Ag nanoparticle arrays at the top, Ag nanoparticle embedded into absorption layer and nanograting structures at the bottom of a thin film solar cell is studied. Each nanostructure is known to be capable of enhancing the solar light absorption to a certain degree, with the effect of metal particles coming primarily from the light scattering, the embedded particles from the reflection and that of back reflector from light trapping and reflection. The preliminary data from model simulation illustrate that with an appropriate combination and arrangement of these nanostructures, an increase in both short and long wavelength range can be achieved, thereby overcoming the shorting comings of each of the nanostructures when applied alone.

INTRODUCTION
Solar cells are considered a promising candidate to meet the growing need of energy. Reducing the cost and improving the energy conversion efficiency of solar cells are two ways to enhance its competitiveness in the market. The most widely used type in the market now is the bulk silicon solar cell, which has a relatively high conversion efficiency but expensive for production. Compared to bulk silicon solar cells, thin-film solar cells and polymer solar cells reduce the cost but with a lower energy conversion efficiency. Thus, improving the conversion efficiency for these types of solar cells is intensively studied now. One promising way to enhance the energy conversion efficiency is to improve the absorption of light in these types of solar cells, which is usually done by the following methods. The first one is to add structures on the top of the cell, which scatters the light so that the reflection of the light is reduced. Nanostructure arrays (such as nanopillars [1], nanocones [2] [3], nanospheres and moth eyes [4]) are introduced to trap the light in the cell to increase the absorption of light. Another one is to add particles inside the absorption layer, which increases the absorption of the reflected light from the back reflector. The last one is to put the back reflector below the cell, such as grating [5], hollow cylinder [6] [7] and the recently reported upconverter layer [8]. All these methods show certain improvement in the light absorption, which leads to an enhancement in the energy conversion efficiency.

In this work, a combination of nanospheres on the top, inside the solar cells and the grating reflector below the cell is designed with a purpose to enhance the absorption of the light. The motivation for this work is derived from the need of enhancing light absorption over the entire range of sunlight frequency, which appears not able to be met with either of the nanostructures alone. The result shows that both short and long wavelength range are improved with the arrangement of combined nanostructure and light absorption enhancement appears to be better than each of the nanostructures applied alone. By this way, the conversion efficiency is improved, which makes the thin film and organic solar cells more competitive.

NUMERICAL MODEL
The simulation was done by Lumerical FDTD Solution software, which solves Maxwell's curl equations in non-magnetic materials:

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} \tag{1}$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E} \tag{2}$$

$$\mathbf{D}(\omega) = -\varepsilon_0 \varepsilon_r(\omega) \mathbf{E}(\omega) \tag{3}$$

where **H** is the magnetic field, **E** the electric field, **D** the displacement field, ω the frequency, and $\varepsilon_r(\omega)$ is the complex relative dielectric constant. The transmission is given by:

$$T(\lambda) = \frac{1}{2} \frac{\int real\left(\mathbf{P}(\lambda)^{Monitor}\right) \cdot d\mathbf{S}}{Source\,Power} \tag{4}$$

where T (f) is the normalized transmission, while **P** is the Poynting vector. The light absorption of a structure P_{abs} (λ) is then calculated by:

$$\text{Pabs}(\lambda) = T(z1, \lambda) - T(z2, \lambda) \qquad (5)$$

where z_1 and z_2 are the top and bottom surface of the structure. Under the assumption that all the electron-hole pairs contribute to the photocurrent, the short circuit current density J_{sc} is calculated by

$$J_{sc} = e\int \frac{\lambda}{hc} P_{abs}(\lambda) I_{AM1.5} d\lambda \qquad (6)$$

where e is the charge of a single electron, and $I_{AM1.5}$ is solar spectrum.

The above numerical implementation has been

RESULTS AND DISCUSSION

With the above model, effect of nanostructures on light absorption in solar cells can be studied. Numerical simulations for three types of nanostructures are presented below, along with the combination of these nanostructures. The simulations are done for both thin film Si solar cells and organic solar cells.

Thin film Si solar cells

Nanostructure on the top surface

The idea of adding nanostructure on the top surface of solar cells is discussed recently. Nanowire, nanocone and nanosphere are proved to have the ability to improve the absorption through scattering the light on the surface. Here, Ag nanosphere particles are used in simulation for the verification. The structure is shown in Figure 1.

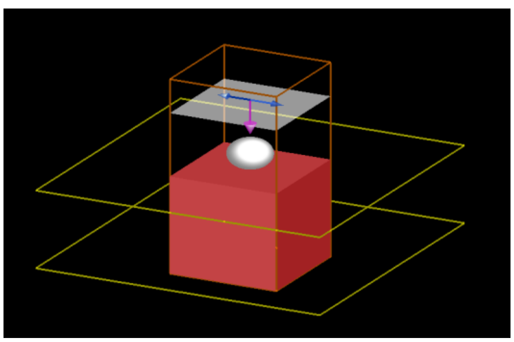

Figure 1. Ag nanosphere on the top of silicon

The thin-film silicon solar cells is simplified by the silicon layer since the dielectric function is not changed significantly when it is n doped silicon or p doped silicon. The source of the light is provided by a plane wave with a wavelength range between 350nm and 1100nm. The boundaries of x and y direction are set to periodic while z direction is PML (perfectly matched layer). The thickness of the Si layer is 500nm, the radius of each Ag sphere is 75nm while the distance between two Ag spheres is 375nm. Two transmission monitors are placed to calculate the absorption efficiency. One is on the top surface of the Si layer while the other is 0.4 μm below the surface.

The result is shown in Figure 2. From the result, we can see that the Ag sphere particles enhance the absorption in the short wavelength range especially from 380nm to 450nm. This is due to the strongly scattering effect on the surface.

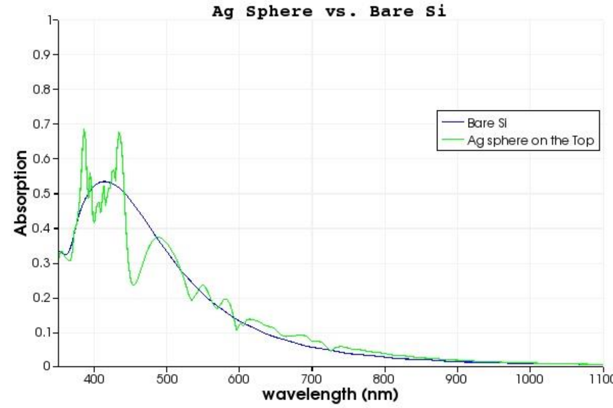

Figure 2. Absorption comparison between addition of Ag sphere structure with bare Si layer

Nanostructure at the back surface

While the 500nm thin-film Si layer is not thick enough for long wavelength range, the back reflector is designed to improve the absorption in this range since it enhances the path length. The grating structure of Ag at the back of the Si layer is verified in this work, which is shown in Figure 3. The interspace is filled with Si since the thin-film silicon solar cells can be deposited on the grating. The depth is set to 250nm while the length between each top end is 375nm.

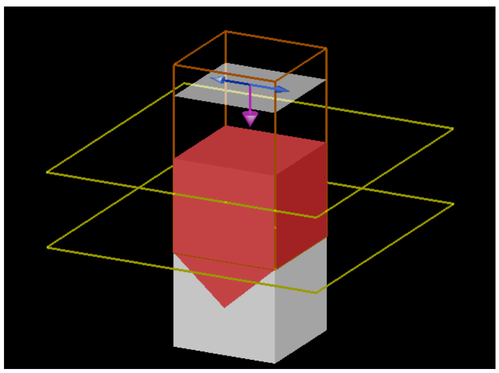

Figure 3. Ag grating at the back

The result is shown in Figure 4. The absorption of long wavelength range is improved especially between 530nm to 800nm. The reason is that when the grating structure is added, the path length is increased, which enhances the absorption according to Beer-Lambert law:

$$A = \varepsilon b c \qquad (7)$$

where A is the absorption of light, ε is the absorptivity, b is the path length and c is the concentration.

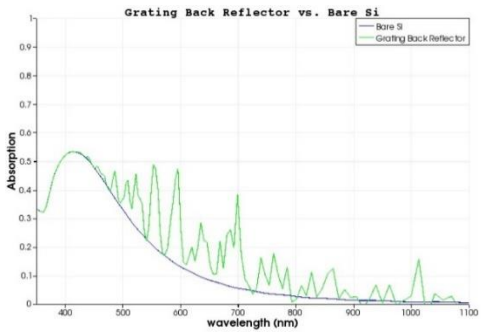

Figure 4. Absorption comparison between additions of grating back reflector structure with Si

Combination of above two nanostructures

The idea of combining above two nanostructures is to improve the light absorption in both short and long wavelength range, which can leads to more fully use of the solar spectrum. Here, the combination of Ag sphere on the top surface and Ag grating back reflector is simulated, which shows a reasonable improvement in both short and long wavelength range. The structure is shown in Figure 5 and the result compared with bare Si is shown in Figure 6.

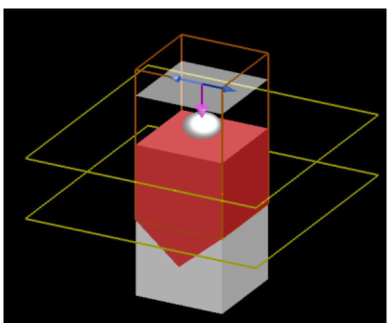

Figure 5. Combination of Ag sphere on the top and Ag grating at the back

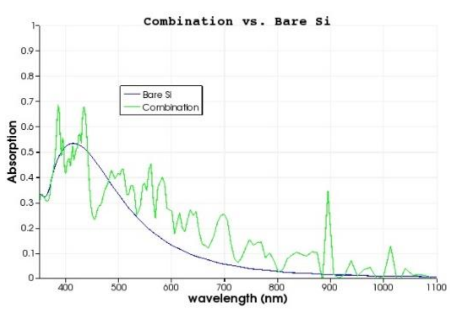

Figure 6. Combined structure vs. bare Si layer

From the result, we can see that the enhancement of the absorption is achieved in the entire wavelength range. There is no block of each other. This indicates that the idea of the combination is feasible.

The results of comparison of the combined structure with Ag sphere only is shown in Figure 7a, and the comparison of the combined structure with grating back reflector only is shown in Figure 7b.

a)

b)

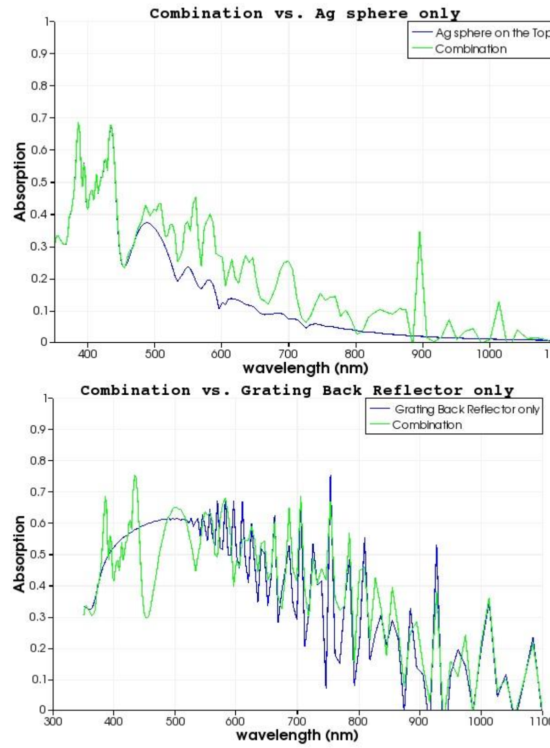

Figure 7. Absorption comparison of addition of combined structure with (a) Ag sphere particle only (b) grating back reflector only

Above two plots indicate interaction may exist between these two nanostructures. The future work will be done to better understand this interaction and to study different combined designs for optimized performance of solar light absorption.

Ag sphere embedded in the Si layer

The third nanostructure is to embed Ag sphere into the Si layer to absorb more light. The Ag sphere, which has a radius of 100nm, is embedded 300nm into the Si layer. The structure is shown in Figure 8 while the absorption result is plotted in Figure 9.

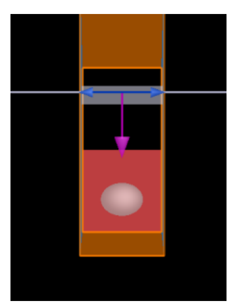

Figure 8. Ag sphere embedded into Si layer

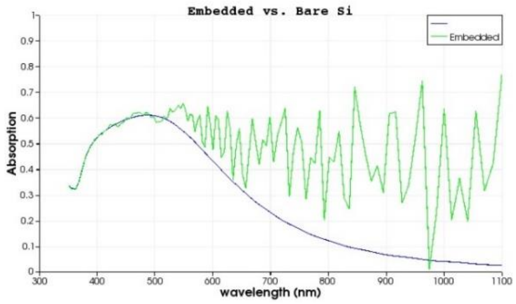

Figure 9. Embedded structure vs. bare Si layer

From the result, the absorption is increased at the long wavelength range, which is due to the absorption of the light reflected from the back reflector.

Combination of above three nanostructures

The idea of the combination of all above three nanostructures is aimed to enhance the absorption over the entire wavelength range. The structure and the absorption result of the combination of all above three nanostructure is shown in Figure 10 and Figure 11.

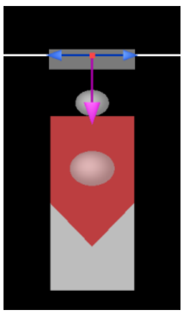
Figure 10. Combination of all these three nanostructures

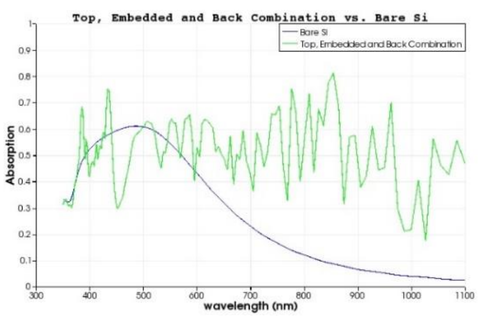

Figure 11. Combined structure vs. bare Si layer

The result shows that the absorption is improved at nearly all the spectrum. The best combination and dimensions will be optimized in the future work to enhance the absorption in the entire wavelength range.

Organic solar cells

The organic solar cells are intensively studied since the production cost is lower compared to thin film Si solar cells. However, the conversion efficiency of organic solar cells is lower than it of Si solar cells. Thus, the conversion efficiency of organic solar cells need to be increased. In this work, the above three types of nanostructures are added to organic solar cells and numerical simulation is done. The structure is shown in Figure 12.

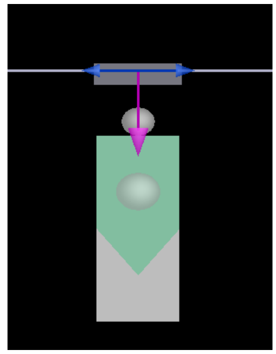
Figure 12. Nanostructures added to organic solar cells

Here, the material of the absorption layer is P3HT:PCBM3. The absorption at the wavelength below 600 nm is already relatively high, while the absorption at the long wavelength range is quite low. The idea is to improve the absorption at the long wavelength range. The absorption results of each nanostructure and the combination of all these three structures are shown from Figure 13 to Figure 16.

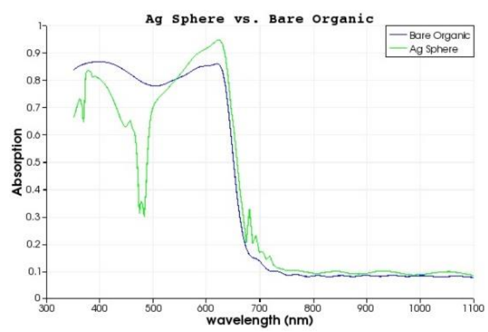

Figure 13. Ag sphere structure at the top vs. bare organic layer

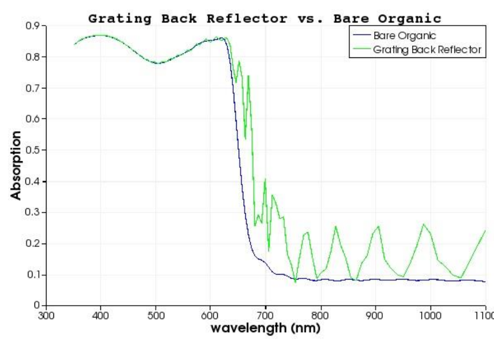

Figure 14. Grating back reflector vs. bare organic layer

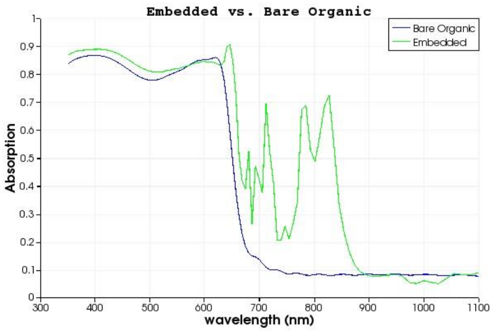

Figure 15. Ag sphere embedded vs. bare organic layer

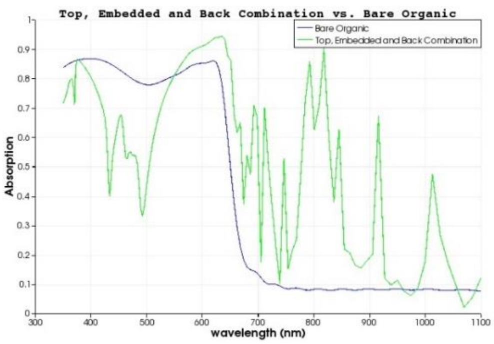

Figure 16. Combination of all three structures vs. bare organic

From above results, the absorption of the 600nm above wavelength range is improved, while it drops between 350nm to 550nm. At this point, the best combination is the embedded Ag sphere with the back reflector. The simulation result of this combination is shown in Figure 17.

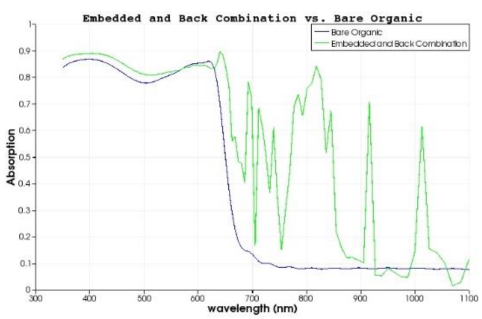

Figure 17. Combination of embedded Ag sphere and back reflector vs. bare organic layer

Electrical simulation of solar cells with nanostructures

The electrical simulation is carried out by Lumerical Device, which calculates the short circuit current and the efficiency by importing the generation rate from FDTD simulation result. The JV plot and power curve of flat silicon solar cells are shown in Figure 18 and Figure 19.

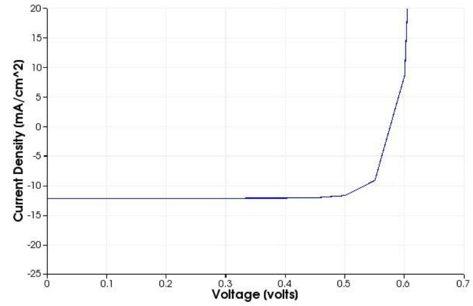

Figure 18. JV plot of flat silicon solar cells

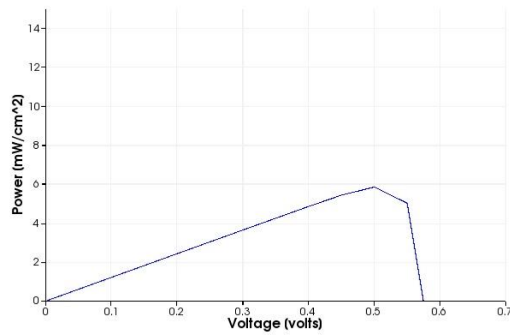

Figure 19. Power curve of flat silicon solar cells

From above results, the short circuit current Jsc=12.2(mA/cm^2). The efficiency equals the maximum power divided by the input power of 100 mW/cm^2, which is 5.9%.

The electrical simulation of Ag nanosphere on the top, Ag grating at the back and the combination of these two nanostructures are done. The results are shown in Figure 20 and Figure 21.

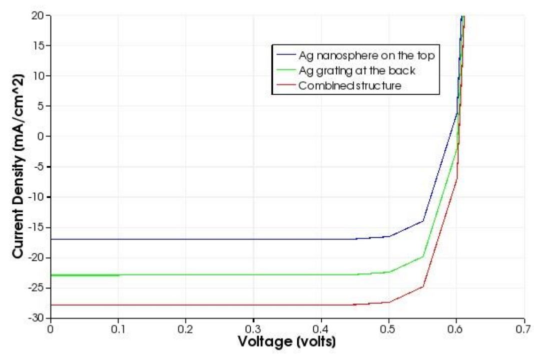

Figure 20. JV plot of all these three structures

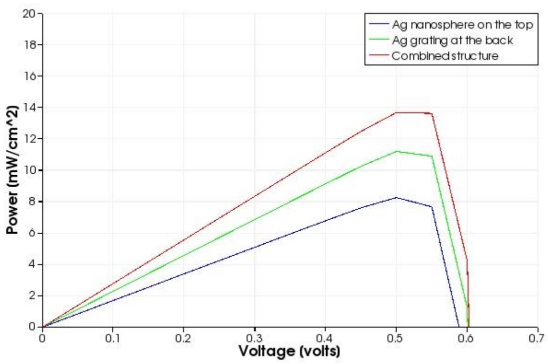

Figure 21. Power curve of all these three structures

From the results, the Jsc is improved from 12.2(mA/cm^2) to 17.0 (mA/cm^2), and the efficiency is increased from 5.9% to 8.26% by adding Ag nanosphere on the top of solar cells. By adding Ag grating at the back, the Jsc is improved from 12.2(mA/cm^2) to 22.9 (mA/cm^2), and the efficiency is increased from 5.9% to 11.2%. The combination of these two structures further improves both the Jsc and the efficiency, which yields the Jsc of 27.9 (mA/cm^2) and efficiency of 13.7%. The results confirm the idea that the combination of these nanostructures yields better improvement than each nanostructure applied alone.

CONCLUSION

In this paper, we have considered three kinds of nanostructures: Ag nanoparticles on the top, Ag nanoparticles inside of the solar cells and back grating reflector, which each has shown promise for improvement of the light absorption in thin-film solar cells. Preliminary data from numerical simulation shows that the idea of combining all these structures is feasible and may lead to the enhancement of light absorption in the entire wavelength range, which is better than each nanostructure applied alone.

Work is being continued with additional simulations for better understanding of the optical interaction between the nanostructures to optimize the design of the combined nanostructures for solar energy harvesting. The entire solar cells simulation will be done and experiments are being design to validate the above numerical data.

ACKNOLWEDGEMENT

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