Configuration Optimization of a Nanosphere Array on Top of a Thin Film Solar Cell

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***Abstract* — Resonant dielectric structures placed on top of a solar cell can enhance light absorption and therefore increase its efficiency. Freely propagating sunlight diffractively couples into the resonant modes of a low loss sphere array. We numerically demonstrate this enhancement using 3D full field finite difference time domain simulations. The coupled energy is then transferred into the active layer underneath and significantly contributes to increase the calculated photocurrent of the solar cell. On a typical thin film amorphous silicon solar cell, a parametric analysis is done. For a hexagonally close packed sphere configuration, we vary the size of the spheres as well as the type of material used. Finally, we study a configuration where high index spheres are embedded in a lower index polymer. This last configuration has the advantage that it can easily be integrated upon solar cell fabrication.**

***Index Terms* — Nanospheres, Whispering gallery modes, Photovoltaic systems, amorphous silicon.**

I. Introduction

Guided whispering gallery modes in rersonant dielectric spheres can be coupled into particular modes of a solar cell and significantly increase the fraction of incident light absorbed [1]. As a reference, we use a typical flat ultra-thin amorphous silicon (a-Si) solar cell and we study the influence of a hexagonally close packed (HCP) array of nanospheres on top of it. The spheres can be of different materials. Here we look at silicon dioxide (SiO_2), polystyrene, and titanium dioxide (TiO_2) spheres. Due to their high refractive index, we also study the case of TiO_2 spheres embedded in ethylene vinyl acetate (EVA). EVA is a polymer that is commonly used as an encapsulant in the photovoltaics industry [2].

II. DESCRIPTION OF THE MODEL

Our approach here is to consider an array of hexagonally close packed resonant spheres on top of a solar cell. We demonstrated previously the interest of SiO_2 spheres directly placed on top of a-Si [1] and gallium arsenide (GaAs) [3] solar cells. We extend this concept and compare the influence of different types of spheres. We vary the size of the spheres and look at the effect on the absorption for an array of SiO_2, polystyrene, and TiO_2 spheres. The refractive index of SiO_2 is n1=1.46 and the refractive index of polystyrene is n2=1.59. The refractive index of TiO_2 is about n3=2.5. It is therefore possible to embed TiO_2 spheres in a lower refractive index polymer in order to achieve resonant sphere light-trapping. We choose EVA which is a commonly used encapsulant in the photovoltaics industry [2]. The refractive index of EVA is n4=1.48. This configuration has a great advantage over the others because the whole structure can be robust and protected.

Figure 1 describes one of the models used for the simulations. TiO_2 spheres are embedded in EVA and deposited on top of the a-Si solar cell. Here, the spheres are hexagonally close packed and the lattice constant a is equal to the diameter of the spheres D. Because the system is periodic, we only simulate one period of the structure corresponding to the rectangle of dimension a,b. We use periodic boundary conditions in our 3D FDTD simulations to account for the infinite periodicity of the structure, and a broadband normal incident plane wave source. In this HCP configuration, the dimensions of the unit cell are a and $b=a\sqrt{3}$. The symmetry of the unit cell and the orientation of the electromagnetic field allow us to simulate one quadrant of the unit cell, thus significantly reducing the time and memory requirements for the simulation [4].

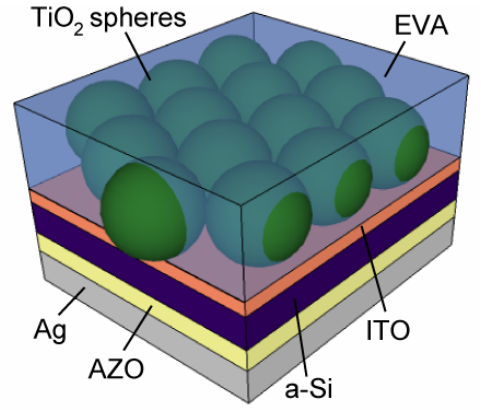

Fig. 1. Schematic of the solar cell with TiO_2 spheres embedded in EVA.

II. INFLUENCE OF THE SPHERE SIZE

To find the optimal configuration to maximize the absorbed light in the active layer of the solar cell, we vary the diameter of the spheres on top of the solar cell. The spheres remain in a HCP configuration, therefore, by varying their size, we also

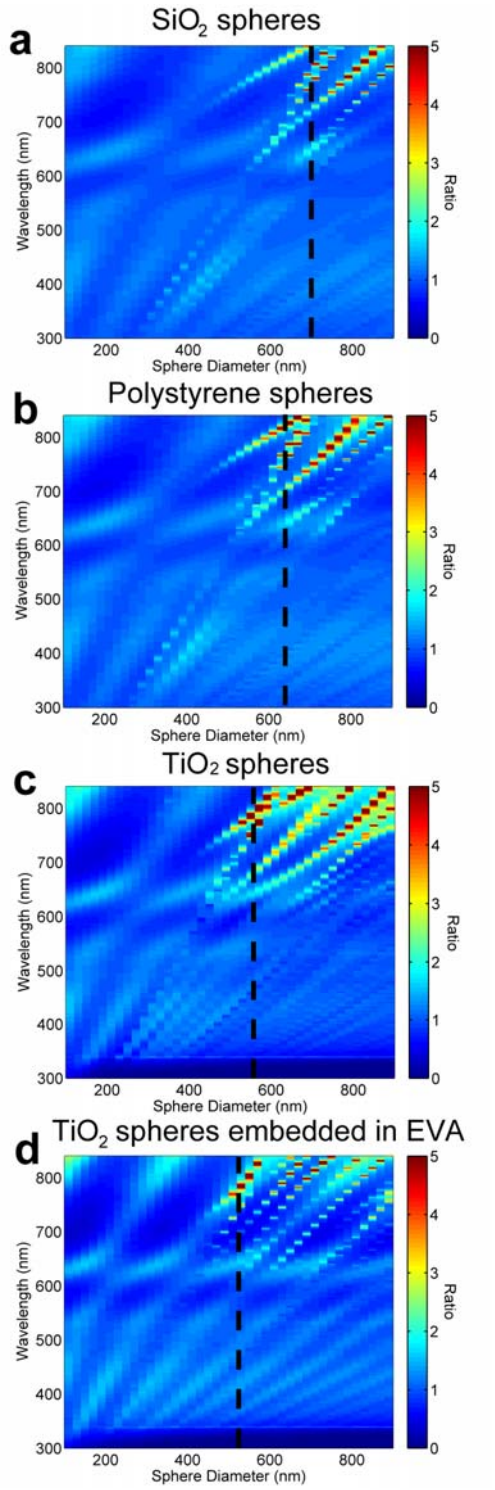

Fig. 2. Ratio between the spectral current density of an a-Si silicon solar cell with HCP spheres over the spectral current density of a solar cell without spheres for (a) SiO_2, (b) polystyrene, (c) TiO_2, and (d) TiO_2 embedded in EVA. The dashed black line shows for each case the sphere diameter which gives the highest current density when illuminated with the solar spectrum.

vary the lattice constant *a*. In order to excite the modes within the order of the wavelength scale by diffractive coupling [1], the lattice constant must remain on the order of the wavelength scale. Here, we compute for each type of sphere, a total of 41 simulations between a sphere diameter of 100 nm and 900 nm by steps of 20 nm. In order to clearly identify the influence of the sphere array on our solar cell, we illustrate in Fig. 2 the ratio between the spectral current density of a solar cell with HCP spheres over the spectral current density of a solar cell without spheres. In all cases, strong enhancement occurs corresponding to optical dispersion of the sphere array. Since the refractive index of the SiO_2 spheres is close to the refractive index of the polystyrene spheres, we can easily compare them. We observe that for the polystyrene spheres that have a slightly higher refractive index than the SiO_2 spheres, most of the optical dispersion lines are blue shifted. For TiO_2 spheres and TiO_2 spheres embedded in EVA, a larger number of optical dispersion lines corresponding to a larger number of modes appear. This is due to the higher refractive index of TiO_2 compared to SiO_2 or polystyrene. For each case, the dashed black line shows the optimal size of sphere. We note that the optimal sphere size for each material is one in which the array can support a large number of resonances on a region of the solar spectrum where a-Si is weakly absorbing.

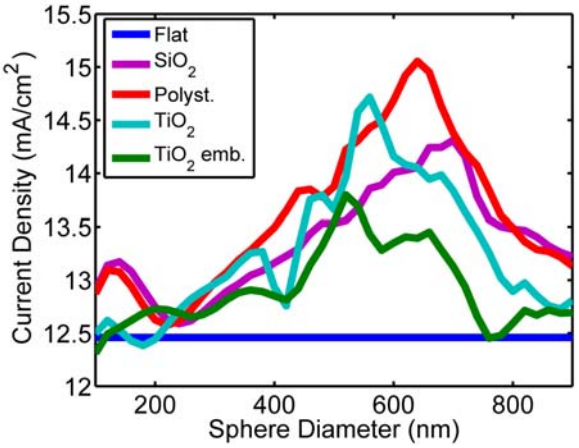

Fig. 3. Current density as a function of the sphere diameter for each considered case.

We compare, in Fig. 3, the calculated current density that can be obtained for each configuration as a function of the sphere size, assuming unity IQE. We find that the 640 nm diameter polystyrene spheres give the highest current density of J_{ph}=15.05 mA/cm^2 (Fig. 5b). This corresponds to an enhancement of more than 20% compared to the case without the sphere array. At λ=789 nm wavelength, the strong coupling of free space light into the whispering gallery modes of the spheres results into the enhancement of the electric field in the active layer bellow it. For SiO_2 spheres, the highest

value for the current density is obtained for the 700 nm diameter spheres and equals J_{ph}=14.31 mA/cm^2 which corresponds to an enhancement of about 15%. For TiO_2 spheres, the optimal case is J_{ph}=14.72 mA/cm^2 corresponding to an enhancement of almost 18% and is obtained for 560 nm diameter spheres. Surprisingly, even though the TiO_2 sphere arrays supports a larger number of optical dispersion lines, which correspond to optical modes, the highest absorption is obtained for polystyrene spheres. Since TiO_2 has a higher index than polystyrene, more light coming from the free space is reflected and therefore less light goes through the spheres or couples into the sphere array modes. Also, polystyrene spheres represent a smooth transition between the index of air and ITO that can facilitate the light absorption in the a-Si. As we can see in Fig. 3, polystyrene spheres are the right compromise to get the maximum light absorption in the active layer. Its index is high enough to support strong modes and low enough to reduce reflection. Finally, TiO_2 spheres embedded in EVA lead to an enhancement of more than 10%. This last configuration is the least efficient. However, from a practical point of view, it may be the most reasonable to implement.

VI. ANGULAR RESPONSE OF THE SPHERE ARRAY

Another important factor for any light trapping scheme is its angular response. Thus, we investigated the angular response of a SiO_2 sphere array in free space using rigorous coupled wave analysis (RCWA) using DiffractMOD software from RSoft. In Fig. 4 we show the transmission of a 500nm close packed SiO_2 sphere array. It can be seen that the resonant peaks in transmission change strongly as a function of angle. Effectively, this calculation maps out the 2-dimensional bandstructure of the sphere array. As the incident angle is changed, the in-plane momentum of the incoming planewave changes, allowing it to couple to different guided modes with appropriate in-plane wavevectors. This suggests that the angular response of the structure could be engineered as is desired by tailoring the in-plane bandstructure.

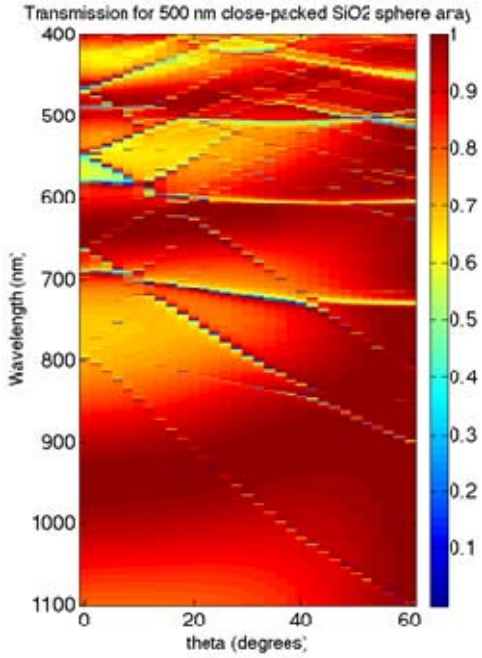

Fig. 4. Current density as a function of the sphere diameter for each considered case.

VI. CONCLUSION

The optimal configuration for the resonant dielectric nanosphere array was found for 600 nm diameter polystyrene spheres and numerically showed a photocurrent enhancement of more than 20% compared to a thin a-Si solar cell with anti-reflection coating. TiO_2 spheres embedded in EVA are a promising configuration for solar cell integration and lead to a photocurrent enhancement of more than 10%. Additionally, we show that the periodic nature of the sphere array can be used to tune the device's angular response by engineering the in-plane photonic bandstructure.

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