Numerical simulation of eco-friendly 4-terminal all perovskite tandem solar cell using novel HTL structure in the bottom sub cell

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***Abstract*—In this paper, we proposed a free-pb 4-terminal (4T) all perovskite tandem solar cell (APTSC) as reference with the power conversion efficiency (PCE) of 26.42% . First, a 100 nm MgF_2 thin film is used as an antireflection layer (ARL) of the top sub cell to improve the total PCE of the reference structure. The total PCE has increased by 7.12%. Finally, a new structure hole transport layer made of CuSCN nanowire arrays in the bottom sub cell is applied. By comparing two different cross sections for CuSCN nanowire arrays, the total PCE of the circular-cross section CuSCN nanowire arrays is incresed 0.52% compared to square-cross section CuSCN nanowire arrays. Therefore, a free-pb 4T APTSC with circular-cross section CuSCN nanowire arrays as hole transport layer is the best based on the total PCE, which reached 29.21%. This is 10.56% higher than the reference structure's total PCE.**

I. Introduction

All perovskite tandem solar cells (APTSCs) have been attracted a lot of attention due to their ability to overcome the Shockley–Queisser theoretical power conversion efficiency (PCE) limit and low fabrication cost [1]. It has been reported that nanowire solar cells have a longer light path and a shorter carriers path [2]. As a result, they are effective to increase PCE. In this work, a lead-free APTSC with square- and circular-cross sections CuSCN nanowire arrays as the hole transport layer of the bottom sub cell is simulated to improve the PCE.

II. Theory and modeling

In this paper, a 3D numerical modeling of free-pb APTSC is performed. Four solar cell structures (Str.) are simulated using the finite element method (FEM), which are shown in Fig. 1. There are two sub cells in each case. In all structures, the semi-transparent top sub cell is made up of $Glass - ITO/TiO_2/MAGeI_3$ as free-pb wide band-gap (WBG) absorber layer/$Spiro{-}OMeTAD/ITO$, whereas the bottom sub cell is made up of $Glass - ITO/TiO_2/MASnI_3$ as free-pb narrow band-gap (NBG) absorber layer $/CuSCN/Ag$. Str.(I) is a APTSC as reference, while Str.(II) is a APTSC with a MgF_2 layer as antireflection layer (ARL) in the top sub cell. Str.(III) and (IV) are created by adding CuSCN nanowire arrays with a square- and circular-cross sections to the bottom sub cell of Str.(II), respectively. The FEM approach is used to solve the Helmholtz equation ($\nabla \times (\nabla \times \mathbf{E}) - k_0^2 \epsilon_r \mathbf{E} = 0$, k_0 is the wave vector of the incident light, and ϵ_r is the relative permittivity) and obtain the electromagnetic field ($\mathbf{E}$) from it. AM1.5 G solar spectrum is irradiated from the structure's top surface in the z direction, with Floquet periodicity boundary conditions in both the x- and y- directions. Scattering parameters are used to calculate light absorption and reflection as a function of lambda ($Absorption = 1 - (S_{11}^2 + S_{21}^2), Reflection = S_{11}^2$). Also, the absorption of non-absorber layers is referred to as parasitic absorption. The total photogeneration rate was determined using the following formula:

$$G_{tot}(x, y, z) = \int_{300}^{1050} \frac{\pi}{h} \epsilon'' E^2(x, y, z, \lambda) \ d\lambda. \qquad (1)$$

where ϵ'' is the imaginary part of the dielectric permittivity, h is the plank's constant.

Current density–voltage (J-V) characteristics are evaluated by solving the Poisson, continuity, and drift–diffusion equations. We used the G_{tot} function to solve these equations. Shockley–Read–Hall (SRH) recombination mechanism in each layer is considered by ignoring surface recombination. All optical and electrical properties of materials are taken into account as input from trustworthy source [3].

III. RESULTS AND DISCUSSION

The spectrum absorption of WBG and NBG absorber layers, parasitic absorption, and total reflection of Str.(I) are shown in Fig. 2. The 100 nm thickness of MgF_2 ARL coated on top of Glass-ITO substrate of top sub cell to get the best total PCE (the sum of the PCE of the top and bottom sub cells) is used in Str.(II). Fig. 3 shows the total reflection loss in Str.(I) and Str.(II). The total reflection loss is reduced by adding an ARL to the top sub cell, which closed the refractive indices of the top layer of the top sub cell with the PSC's external environment (air layer). Fig. 4 depicts the total absorption and absorption of the NBG absorber layer of Str.(II)-(IV). When comparing Figs. 2 and 4, the total absorption of Str.(II)

compared to Str.(*I*) has increased in several wavelength ranges due to the decreased reflection loss shown in Fig. 3. According to Fig. 4, absorption of the NBG absorber layer and, as a result, total absorption of Strs.(*III*) and (*IV*) are improved in several wavelength ranges compared to Str.(*II*) due to the increase in the length of the optical path in the collision with nanowire arrays. Also, the NBG absorber layer absorption and total absorption of Str.(*IV*) are greater than those of Str.(*III*). Nanowire dimensions should be (**a**,**h**,**W**) nm=(150,120,200) nm to achieve the best total PCE. Where, **a** is nanowire diameter with a circular-cross section and nanowire side with a square-cross section, **h** is nanowire height and, **W** is periodicity (the distance between the centers of two nanowires), respectively. Fig. 5 shows the J–V characteristic electrical simulation results for the top and bottom sub cells of Str. (*I*)-(*IV*). The J_{sc}, V_{oc}, FF and PCE values of top (bottom) sub cell have been obtained $8.08mA/cm^2$ $(19.76mA/cm^2)$, $1.70V$ $(0.93V)$, 0.92 (0.75), 12.64% (13.78%) for Str.(*I*), $8.77mA/cm^2$ $(20.91mA/cm^2)$, $1.70V$ $(0.93V)$, 0.92 (0.75), 13.72% (14.58%) for Str.(*II*), $8.78mA/cm^2$ $(21.74mA/cm^2)$, $1.70V$ $(0.94V)$, 0.92 (0.75), 13.73% (15.33%) for Str.(*III*) and $8.79mA/cm^2$ $(21.95mA/cm^2)$, $1.70V$ $(0.94V)$, 0.92 (0.75), 13.74% (15.47%) for Str.(*IV*), respectively. Str.(*II*) has a higher total PCE than Str.(*I*). Because the reflection loss of Str.(*II*) is lower than that of Str. (*I*), the J_{sc} of the top (bottom) sub cell is improved by 8.54% (5.82%), resulting in a 8.54% (5.81%) improvement in PCE. As a result, when compared to Str.(*I*), the total PCE of Str.(*II*) has increased by 7.12%. The J_{sc} (PCE) of the bottom sub cell in Str.(*III*) and Str.(*IV*) is improved 3.97% (5.14%) and 4.97% (6.10%) comparing to Str.(*II*), respectively. Therefore, the total PCE of Str.(*III*) and Str.(*IV*) is increased 2.69% and 3.22% because of the increase in the absorption of the NBG absorber layer and total absorption. By comparing Str.(*III*) with Str.(*IV*), the total PCE of Str.(*IV*) is increased by 0.52%.

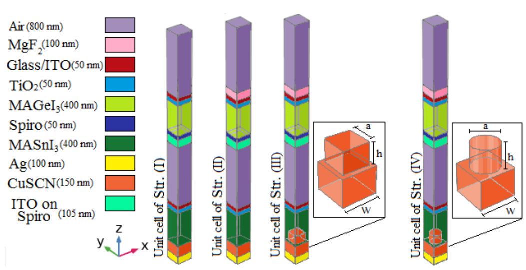

Fig. 1. A 3D schematic of the unit cell of all proposed structures.

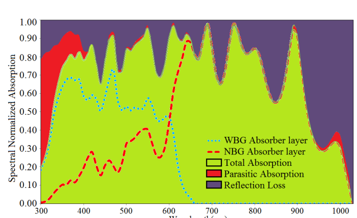

Fig. 2. Spectral normalized absorption of Str. (*I*).

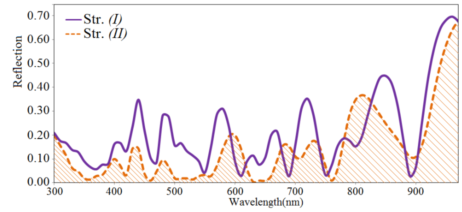

Fig. 3. Reflection loss of Str.(*I*) and (*II*).

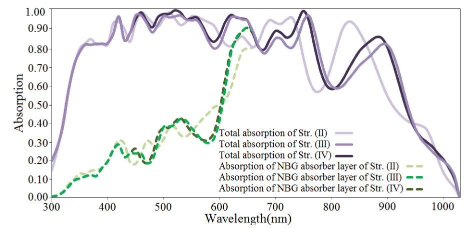

Fig. 4. Total absorption and absorption of the NBG absorber layer of Str.(*II*)-(*IV*).

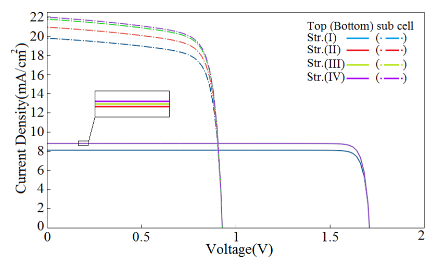

Fig. 5. The J-V characteristics of the proposed Str. (*I*)–(*IV*).

IV. Conclusion

In this study, the optical and electrical properties of free-Pb APTSC (Str.(*I*)), free-pb APTSC with MgF_2 ARL in top sub cell (Str.(*II*)), Str.(*II*) by adding square-cross section CuSCN nanowire arrays in bottom sub cell (Str.(*III*)), and Str.(*II*) by adding circular-cross section CuSCN nanowire arrays in bottom sub cell (Str.(*IV*)) were compared together. An ARL made of a 100 nm MgF_2 thin film was used to improve the PCE of Str.(*I*) (26.42%). The total PCE in Str.(*II*) was increased by 7.12% compared to Str.(*I*). Str.(*III*) and Str.(*IV*) were used to improve the total absorption with increasing the optical path length in the NBG absorber layer. In comparison to structure Str.(*II*), Str.(*III*) and Str.(*IV*) had a 2.69% and 3.22% increase in the total PCE, respectively. Finally, Str.(*IV*) was the best free-Pb APTSC, with a total PCE of 29.21%. Which is greater than the total PCE of the Str. (*I*) by 10.56%.

References

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[2] R. El-Bashar, et al., “Electrical performance of efficient quad-crescent-shaped Si nanowire solar cell,” *Sci. Rep.*, vol. 12, pp. 1–20, Jan 2022.

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