Utilizing Principles of Wave Photonics to Address Solar Cell Inefficiencies

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The Shockley-Queisser Limit informs us that the maximum efficiency of a conventional single p-n junction solar cell lies around 33.7%. With that in mind, we propose methods that may work around this inefficiency to achieve a higher overall energy output as compared to the conventional solar cell, given the same black body radiation. This method is two fold: (1) introducing a new material to work in tandem with our silicon cell and (2) adding thin layer anti-reflective coatings optimized for the PV system. We hope to demonstrate in this paper that a Perovskite-silicon Tandem cell can exceed the Shockley-Queisser Limit and that an anti-reflective coating can significantly decrease lost solar energy.

I. INTRODUCTION AND MOTIVATION

Electors are set to vote Joseph R. Biden into office on Dec. 14th. Biden, who campaigned on sweeping climate reform, set a goal for a switch to completely renewable energy by 2050 [1]. In order to achieve this goal, our energy grid will have to rely ever more heavily on energy sources like solar power. Fossil fuels generate 2.582 billion mega-Wh of energy annually for the United States, as of 2019 [2]. Solar cells generate around 15 watts per square foot, meaning that if we want to recoup even 1% of our fossil fuel output through solar, we would need upwards of 466 acres of land. Clearly, seeing as land is a valued commodity and that increased area leads to increased maintenance cost, there is a need to increase the efficiency of today's solar panels while still maintaining a competitive price.

II. BACKGROUND AND LIMITING FACTORS

A great deal of research has already been done in the field of multi-junction solar cells and anti-reflective coatings. For example, one of the main challenges with a tandem cell is determining the proper perovskite cation to achieve the right band gap in multi-perovskite systems. One of the biggest challenges surrounding viable perovskite PV cells was their instability, especially in materials with a smaller band gap. Some proposed methods to overcome these limits is to incorporate tin into the AB3 structure in place of lead is known to be fairly stable. Tin perovskite cells have a significant stability challenge, facing substantial oxidation around the cathode [3]. For this reason of insufficient stability from potential materials for the bottom layer of a tandem solar cell, we are interested in modeling a lead perovskite - silicon tandem PV cell over a monolithic perovskite cell. In addition to materials research, there has been research into geometric ways of retaining light within the cell [4]. We hope to expand upon these studies, simulate our model, and condense our findings into a proposed tandem solar cell.

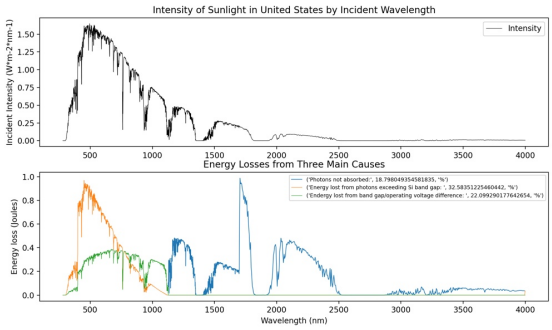

FIG. 1. **Incident light energy by frequency and constituent inefficiencies** Above figure depicts the incident energy of light across the United States [5]. Together inefficiencies describe energy loss for a 1.1 eV single junction Si cell per square meter.

A. Shockley-Queisser

The first of our two limiting factors for our solar cells can be described by the Shockley-Queisser limit. Shockley-Queisser describes the upper limit on the amount of energy a single P-N junction solar cell can produce. We begin with the energy that falls upon our solar cell, defined by the black body radiation from the sun averaged across the united states. Then we consider our chosen semi-conductor, with a given band gap. Our S-Q limit describes two inefficiencies: (1) photons whose energy is less than our band gap that are not absorbed and (2) lost energy from photon energy that exceeds the operating voltage of the cell – assuming that our cell operates at a voltage equal to that of our band gap.

As we can see in FIG. 1, most of our loss originates from photon energy that exceeds our material's specified band gap. Thus, this provides for the highest potential target when trying to optimise our cell, representing 32.58% of our loss. FIG. 1 also depicts lost energy due to differences between operating voltage and band gap voltage of our semiconductor material, with the assumption that our 1.1 eV Si cell operates at 600 mV. This inefficiency comes inherent with our materials and, for the sake of the rest of this paper, will not be considered.

B. Reflectivity

Next, we encounter our next inefficiency when investigating the amount of light entering our cell vs that that is reflected. This limitation defines the upper limit of energy that can reach our cell. We can use transform matrices to investigate the amount of light reflected from our single P-N junction Si solar cell.

$$T_{\mathrm{ij}} = \frac{1}{t_{\mathrm{ij}}} \begin{bmatrix} 1 & r_{\mathrm{ij}} \\ r_{\mathrm{ij}} & 1 \end{bmatrix} \tag{1}$$

$$r_{\mathrm{ij}} = \frac{E_{\mathrm{B}}(x_{\mathrm{i}\text{-}})}{E_{\mathrm{F}}(x_{\mathrm{i}\text{-}})} = \frac{n_{\mathrm{i}} - n_{\mathrm{j}}}{n_{\mathrm{i}} + n_{\mathrm{j}}} \tag{2}$$

$$t_{\mathrm{ij}} = \frac{E_{\mathrm{F}}(x_{\mathrm{i}+})}{E_{\mathrm{F}}(x_{\mathrm{i}\text{-}})} = 1 + r_{\mathrm{ij}} \tag{3}$$

$$R = r^2 = r_{\mathrm{ij}}^2 \tag{4}$$

The second of our paper's assumptions is the angle of incident for our light: a normal incident of light because that is the angle at which we would want to optimise a solar cell. With that in mind we can look to equations (1) to determine the reflectivity of our bare Si solar cell. With a refractive index n = 3.5, we find that our percent reflectivity, R = 30.86%. This informs us that upwards of 30% of the energy approaching our cell at the normal is not entering the cell, in of itself a greatly significant inefficiency. In this paper, we will take advantage of the properties of destructive interference and a material's reflectivity to minimize the amount of light 'lost' from our system.

C. Optimization Function

Below we will attempt to find the optimum refractive indices and thicknesses for our anti-reflective coating so as to minimize reflected light out of our solar cell system. Powell's conjugate direction method proved both most efficient and accurate. It can be described succinctly in [6].

III. OPTIMIZATION SIMULATION METHODS

Here we will be discussing the methods in which we modeled tandem solar cells to demonstrate transcending the Shockley-Queissar limit. Then, we will address our reflectivity inefficiency with a simulation of a simple two layer anti-reflective coating.

A. Optimizing a Tandem System

Our tandem solar cell will incorporate silicon as our base layer with a 1.1 eV band gap. We will then attempt to diminish our primary solar cell inefficiency: energy lost to photons whose energy exceeds our cell's band gap. Again, we will be ignoring inefficiencies associated with silicon as a semi-conductor and operate under the assumption that the cell's operating voltage is equal to its band gap.

$$I = 1.602 \times 10^{-19} \sum photons \tag{5}$$

$$P = I_{limiting} \times (V_{Si} + V_{Perovskite}) \tag{6}$$

From (5) we can determine the limiting current by summing photons that are a high enough frequency to excite electrons in one of our layer's junctions. We will consider photons of an energy that can be absorbed by the top layer will not be absorbed by our base Si layer. The layer that produces the lesser current will then dictate the power that the cell can produce.

Now, we will run through three viable perovskites structure for methylammonium lead trihalide (CH3NH3PbX3). Perovskites are attractive materials because of their relative low cost and ease to manufacture. However, perovskite cells prove less stable and long-lasting than their simpler Si counterparts. We will consider this material for mixed lead halides: these have experimentally varying band gaps that lie between 1.55 and 2.3 eV, and we will investigate this range at even intervals to determine the optimum material. Then we will compare our entire cell's efficiency as compared to our single junction Si cell.

$$P_{max} = 450.489 \quad W/m^2 \tag{7}$$

B. Creating Anti-reflective Coating

Figure 2 depicts our working model for an anti-reflective coating. We will operate with constant refractive indices of our ITO and Cell layer of n = 1.9 and n = 3.5 respectively. In addition, our ITO layer will have a thickness of 80 nm. We will then use a series of transform matrices to model the ultimate reflection of a given wavelength of light. What is left for us is to then determine the optimum combination of the two refractive indices n1 and n2 and thicknesses d1 and d2. To achieve that we will be utilizing our Powell conjugate direction model to estimate a minimum possible reflectivity and the four parameters associated with that.

$$T_{\mathrm{i}} = \begin{bmatrix} e^{j\Phi_i} & 0 \\ 0 & e^{j\Phi_i} \end{bmatrix} \tag{8}$$

$$\Phi_{\mathrm{i}} = k_{x,i} d_i = 2\pi n_i d_i \tag{9}$$

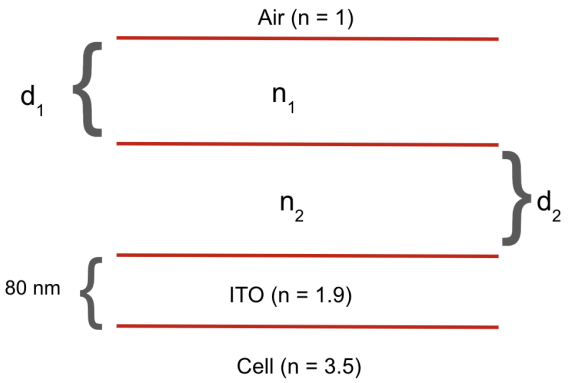

FIG. 2. **Model for a simple solar cell to determine optimal parameters for a two-layer Anti-reflective coating** Above figure is the system of layers used to simulate a solar cell, simplified to two anti-reflective layers, an ITO layer, and a solar cell base, which we estimate to be the refractive index of our Si layer.

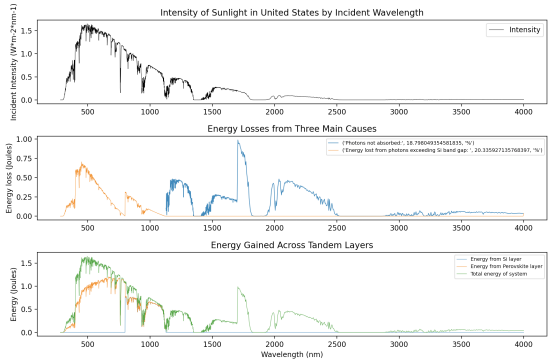

FIG. 3. **Efficiency and energy model of a tandem cell with band gap 1.55 eV** The top figure is once again our black body radiation, followed by the inefficiencies for our tandem cell from photons whose energy exceeds the band gap and from photons who are not high enough energy to excite an electron. The final graph demonstrates how the perovskite cell fills in the high energy photon inefficiency gap to make for an overall more efficient cell.

Using (7), (8), and (1) we can form a transform matrix:

$$T_{04} = T_{01}T_1T_{12}T_2T_{23}T_3T_{34} \tag{10}$$

We set our expected value for our Powell function to have our refractive indices n to be $1 < n < 1.9$ and thicknesses d to be $d > 80$ nm.

IV. RESULTS AND DISCUSSION

In our findings we modeled band gaps at even intervals. For readability, we included our efficiency findings

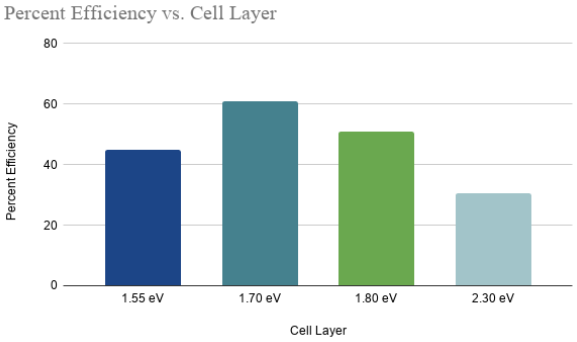

FIG. 4. **Efficiency of Tandem Cell with Different Perovskite Top Layer and 1.1 eV Si Bottom Layer** The figure depicts percentage efficiency for lead-halide perovskite cells with band gaps ranging between 1.55 eV and 2.3 eV.

for band gaps of 1.55, 1.70, 1.80, and 2.30 eV as shown in FIG. 4, again based on AM1 spectrum data. When varying the band gap for our top layer, we see that the Si layer represents the current limiting cell for lower band gap top layers and perovskite for the larger band gaps.

We find that for most band gaps for our perovskite top layer, we could have an efficiency ceiling of above 40%, an improvement from the 33% limit to our single junction Si cell as defined by the Shockley-Quisser limit. We can see that a 1.70 eV material may even give us an efficiency of above 60%. This is a difficult number to reconcile, but this determined efficiency leaves out material inefficiencies and compounded resistance and may represent an absolute upper limit for our cell system. If we use our 1.70 eV material as our optimum perovskite layer, this could possibly correlate with $MAPb(I_{0.74}Br_{0.26})_3$[7].

Next, we can discuss our findings for our two-layer anti-reflective coating optimization model. We found that we can reduce our reflectivity to 2.6% almost statistically insignificant given the 30% reflectivity of our simple Si cell.

$$n_2 = 1.0100 \tag{11}$$

$$n_2 = 1.1934 \tag{12}$$

$$d_1 = 171.8697 \quad nm \tag{13}$$

$$d_2 = 108.4766 \quad nm \tag{14}$$

$$E_{reflected} = 9.747 \quad J \tag{15}$$

From here we can see that our total reflected energy is 9.347 J with a given input of 450.49 J from (7). We can also plot our optimization function as a function of wavelength as seen in FIG. 5.

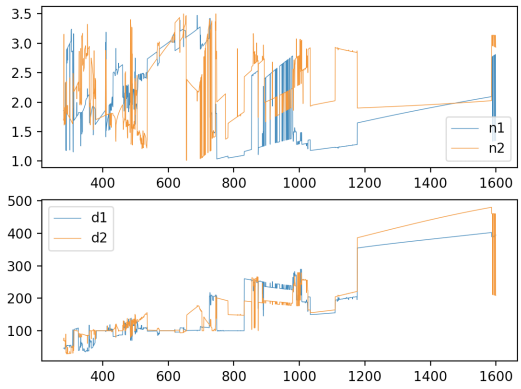

FIG. 5. **Optimum refractive indices n1, n2 and thicknesses d1, d2 for a given wavelength** The top figure shows the relation ship between n1 and n2 as we traverse our spectrum. The bottom figure does the same for d1 and d2.

V. OUTLOOK AND CONCLUSIONS

While our simulations successfully demonstrate the potential for a solar cell that exceeds the Shockley-Queisser limit and drastically diminishes lost light, a few issues and opportunities for further research presented themselves. First, we see can consider our Powell optimization function. Because it traverses our function as estimated only from a second degree, we may not be accurate enough to have a fool proof algorithm. As evident in FIG. 5, we would expect to see our n2 (orange) to always be at a higher index of refraction than n1 (blue) to form a gradient into our cell. However, we can see that this is indeed not the fact for a good portion of our spectrum. The same can be said of d2 an d1, where we would want our d1 (blue) to always be greater than d1 (orange).

Second, we can consider our outputted index of refraction. Given such a small range from air (n = 1) to our ITO layer (n = 1.9) we now must reconcile a top anti-reflective coat to want to have a reflective index of n = 1.01. Manufacturing glass with such a precise index of refraction and with high enough quality may not be feasible or cost effective. Additionally, our simplified model may have over estimated the index of refraction of our cell layer, which would surely have a more layers between the silicon (n = 3.5) layer and our ITO layer. Future research is needed to determine a more robust algorithm for our multi-layer anti-reflective coating and how that will play along with our proposed tandem cell.

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[3] K. A. Bush, A. F. Palmstrom, J. Y. Zhengshan, M. Boccard, R. Cheacharoen, J. P. Mailoa, D. P. McMeekin, R. L. Hoye, C. D. Bailie, T. Leijtens, *et al.*, 23.6%-efficient monolithic perovskite/silicon tandem solar cells with improved stability, Nature Energy **2**, 1 (2017).

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