Designing Photonic Materials for Effective Bandgap Modification and Optical Concentration in Photovoltaics

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***Abstract*—The limiting efficiency for photovoltaic energy conversion based on a semiconductor p-n junction is typically determined using the method of detailed balance put forth by Shockley and Queisser. Here, we describe how this theory is altered in the presence of a photonic structure that is capable of modifying the absorption and emission of photons and optimize a device with optical loss. By incorporating specifically designed photonic structures, higher maximum efficiencies can be achieved for low bandgap materials by restricting the absorption and emission of above bandgap photons. Similarly, restriction of the emission angle leads to increased optical concentration. We consider how both of these effects are modified in the presence of a nonideal photonic structure. Further, we find that the energy of the photonic bandgap that is needed for maximum efficiency depends critically on the reflectivity of the photonic crystal.**

***Index Terms*—Bandgap engineering, detailed balance, photonic crystal (PC), Shockley–Queisser limit.**

I. Introduction

In order to calculate the limiting efficiency of a solar cell, Shockley and Queisser developed a formalism that is based on the detailed balance of absorption and emission of photons that occurs at open circuit [1]. In the absence of nonradiative (NR) recombination and with infinite carrier mobility, the maximum efficiency is determined, which depends solely on the material's bandgap. Their method has been further generalized over the years [2]–[6] and is often the starting point for considering more advanced solar energy conversion processes [7].

Because the maximum conversion efficiency depends solely on the bandgap, it is worthwhile to explore further the connection between the bandgap energy and the efficiency. The semiconductor bandgap is important because it determines both which photons can be absorbed, and at open circuit, which photons must be emitted. Absorption of above bandgap photons gives rise to a current density J_L, which can be withdrawn from the device. Under open-circuit conditions, the cell still absorbs light; however, no current is removed by the external circuit. In order to maintain a detailed balance, radiative recombination leads to a flux of photons out of the cell equal in number to those entering the cell. The emitted flux comes from recombination across the bandgap. Thus, in the ideal case considered by Shockley and Queisser, the bandgap alone is all that is need to describe the absorption and emission processes, which are necessary to determine the conversion efficiency. The modification of the absorption and emission of a cell can lead to spectral shifts and effective bandgap modifications of the device [14]–[16]. We previously found that the introduction of even small amounts of loss in a photonic crystal (PC) that is placed atop a solar cell can result in significant efficiency degradations [14]. In the following analysis, we optimize the photonic bandgap energy depending on PC loss and find that with appropriate bandgap selection, the cell efficiency still improves. For a 90% reflective PC atop a 0.67-eV semiconductor, the unoptimized device yields an efficiency of 15.0%, while the optimized device yields 23.8%.

We also note that this effect is physically distinct from thermophotovoltaic devices where an intermediate structure is thermally isolated from the cell and is used as a modified emitter to effectively change the incident spectrum on the device [8], [9].

II. Photonic Aspects of Detailed Balance

In order to modify the semiconductor absorption and emission, we place a PC on top of the structure (see Fig. 1), where the PC has a photonic bandgap that extends from the semiconductor bandgap energy E_g^{SC} to the photonic bandgap energy E_g^{PC} (where $E_g^{\mathrm{SC}} < E_g^{\mathrm{PC}}$). This modification has two effects on the cell. First, J_L is decreased because incident photons with energies between E_g^{SC} and E_g^{PC} will be reflected off the top surface and will not reach the cell. Second, emission from the cell will be similarly limited. Photons that are created by radiative recombination will have energies greater than E_g^{SC}; however, only photons with energies greater than E_g^{PC} can escape the cell. Thus, photons with energies between E_g^{SC} and E_g^{PC} will be trapped within the cell, unable to escape. These photons can be reabsorbed by the cell in a process called photon recycling. The continuous absorption and reemission leads to a high concentration of carriers and, hence, an increased open-circuit voltage. Thus, the addition of a PC to the top of the cell leads to a decrease in the current density and an increase in the open-circuit voltage.

In order to determine the maximum efficiency, the equations of Shockley and Queisser can be used if the semiconductor

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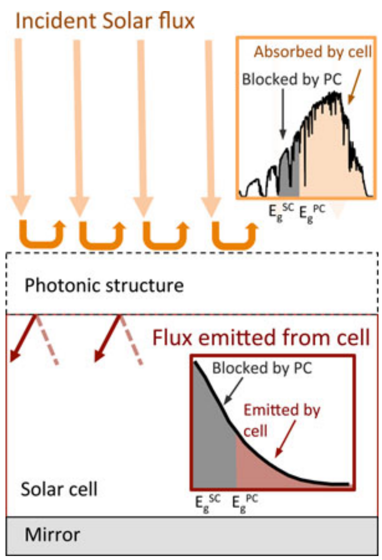

Fig. 1. PC structure reflects incident light from the sun and traps internally emitted light from the cell. This effect has two consequences. First, there is a decrease in the current due to fewer photons making it into the cell (top). Second, there is an increase in the voltage due to a buildup of the internal luminescence and, hence, carrier concentration because photons emitted near the semiconductor bandgap do not have enough energy to escape and are reflected by the PC (bottom).

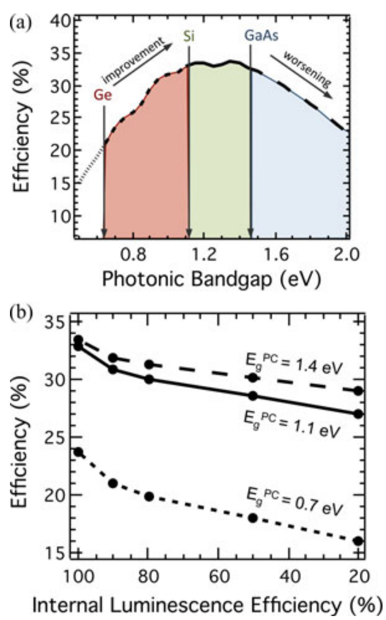

Fig. 2. Addition of an ideal PC causes the solar cell to behave as although it has a modified semiconductor bandgap energy. (a) PC improves the efficiency of low-bandgap semiconductors but has a detrimental effect on high-bandgap semiconductors. (b) Reduction in the internal luminescence decreases the overall cell efficiency; however, improvements persist for low-bandgap materials.

bandgap energy is replaced with the photonic bandgap energy (see [14] for details). Fig. 2(a) shows this calculation under AM 1.5G illumination, again in the absence of NR recombination. For low bandgap materials (<1.1 eV), the addition of a PC improves the efficiency. While for higher bandgap materials (>1.4 eV), the PC decreases the efficiency. For materials with bandgaps between 1.1 and 1.4 eV, the effects are relatively small. A few typical solar cell materials are shown in Fig. 2(a). For a low bandgap material like Ge, the current is high, but the voltage is low. Thus, restricting the absorption and emission allows the device to work at a higher voltage, which leads to an efficiency improvement. For a material like GaAs, there is already a nearly perfect balance between the voltage and current. Improving the voltage, while decreasing the current has a detrimental effect on the device performance [see Fig. 2(a)]. We should also note that under ideal conditions, it would appear that $V_{\rm oc} > E_g^{\rm SC}/q$ when $E_g^{\rm PC} \gg E_g^{\rm SC}$. This would suggest that lasing may be possible within the solar cell; however, as we shall see below, the introduction of optical loss reduces the carrier concentrations to levels such that $V_{\rm oc} < E_g^{\rm SC}/q$.

III. Effect of Loss Mechanisms

The total current density in the cell without NR recombination can be written as $J_{\rm tot} = J_L - J_{\rm dark}$, where $J_{\rm dark} = J_0 [\exp(qV/k_B T) - 1]$, J_0 is the reverse-bias saturation current density, q is the electron charge, V is the bias voltage, k_B is Boltzmann's constant, and T is the temperature of the cell. At open circuit, the absorbed solar photons create electron–hole pairs that subsequently recombine and reemit photons (photon recycling). Because only photons within the critical angle of the escape cone will exit the material, there is an intensity buildup within the semiconductor. The internal fluorescence within the cell is $4n^2/\sin^2\theta_e$ larger than the luminescence that escapes [10], where n is the index of refraction of the semiconductor, and θ_e is the emission half angle from the cell, which is usually $\pi/2$. If we allow an additional NR recombination pathway defined by a NR recombination current density $J_{\rm NR}$, then the internal luminescence efficiency can be written as

$$\eta_{\rm int} = \frac{J_{\rm dark}\left(4n^2/\sin^2\theta_e\right)}{J_{\rm dark}\left(4n^2/\sin^2\theta_e\right) + J_{\rm NR}} \tag{1}$$

where the total current is now $J_{\rm tot} = J_L – J_{\rm dark} – J_{\rm NR}$. Nonideal internal fluorescence reduces the overall efficiency of the photovoltaic device [see Fig. 2(b)]; however, the PC is still able to improve the efficiency of a low-bandgap semiconductor. As depicted in Fig. 2(b), even for low internal fluorescence, an ideal PC can improve the efficiency of a 0.7-eV bandgap material by ∼13% in absolute efficiency.

A very high quality photonic material is important to realize the aforementioned efficiency improvements. As an example, we consider a material with $E_g^{\rm SC} = 0.67$ eV covered by a PC with reflectivity R and a photonic bandgap from $E_g^{\rm SC}$ to $E_g^{\rm PC}$. $R = 90\%$ means that 90% of the incident photons over the energy range from $E_g^{\rm SC}$ to $E_g^{\rm PC}$ will be reflected from the cell, and 90% of the internal luminescence that would typically escape will be trapped within the cell. Fig. 3 shows that the largest efficiency gains are achieved with $R \geq 90\%$. Similarly, for $R < 100\%$, the $E_g^{\rm PC}$ required for maximum efficiency reduces rapidly with decreasing R (see Table I).

The current–voltage characteristic of a cell clearly demonstrates the decrease in current and the increase in voltage upon the addition of a PC. The PC reduces the maximum current by limiting absorption, but the overall cell performance improves because of an increase in the open-circuit voltage. Fig. 4 shows

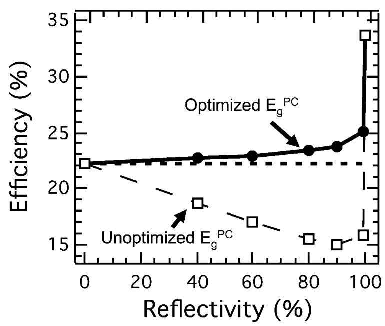

Fig. 3. Highly reflective PC is needed for significant improvement of the cell efficiency.

TABLE I
OPTIMIZED E_g^{PC} FOR MAXIMUM EFFICIENCY GIVEN R AND $E_g^{SC} = 0.67$ eV

E_g^{SC}(eV)	R(%)	E_g^{PC}(eV) (OPTIMIZED)	η (%)
0.67	--	--	22.3
0.67	100	1.37	33.6
0.67	99	0.79	25.1
0.67	90	0.73	23.8
0.67	80	0.72	23.4
0.67	40	0.71	22.7

Effect of nonideal PCs. The photonic bandgap energy necessary for highest photovoltaic efficiency depends on the reflectivity of the PC. R = 100% corresponds to an ideal PC that reflects all incident light that exists within the photonic bandgap. The top row corresponds to the reference cell with no PC.

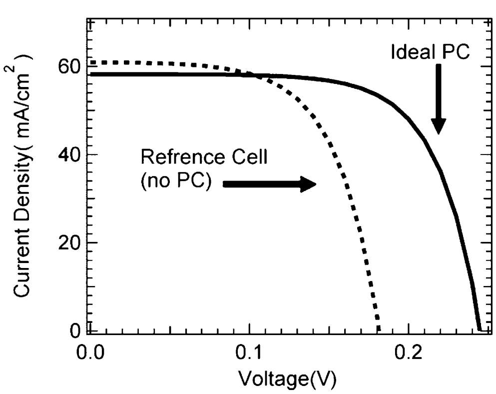

Fig. 4. Current–voltage characteristic of a $E_g^{SC} = 0.67$ eV solar cell with (solid line) and without (dotted line) a PC. The addition of a PC increases the open-circuit voltage but decreases the short-circuit current density.

this effect for a solar cell made from a material with a bandgap energy of 0.67 eV (e.g., Ge) and $\eta_{\rm int} = 0.1\%$. The addition of an ideal PC with energy bandgap from 0.67 to 0.74 eV results in a 2.9% absolute efficiency gain. Even with realistic material parameters, efficiency gains of several percent are possible. As an example, a solar cell's efficiency improves by 2.0% absolute for a PC with $R = 90\%$ compared with no PC. Table II shows the relevant cell parameters.

TABLE II
DEVICE PARAMETERS FOR A $E_g^{SC} = 0.67$ eV SOLAR CELL

	R(%)	J_{SC}(mA/cm^2)	V_{OC}(V)	η(%)
Reference Cell	--	61.0	0.182	6.84
Ideal PC	100	58.2	0.245	9.75
PC	90	58.5	0.226	8.80

The photonic crystal reduces the short circuit current, increase the open circuit voltage, and increases the energy conversion efficiency.

IV. EMISSION ANGLE RESTRICTION WITH OPTICAL LOSSES

It is well known that the emission solid angle plays an important role in determining the cell's $V_{\rm OC}$ [2], [11], [17]–[21]. In fact, the improvement in the $V_{\rm OC}$ due to restricting the emission angle is comparable with the improvement in the $V_{\rm OC}$ due to light concentration. In both cases, the voltage improvement is caused by an increase of the carrier densities. When the emission half angle θ_e is limited to that of the sun's half-angle $\theta_s = 0.267°$, the efficiency reaches that of 46 000 suns concentration.

The main limitation on emission angle restriction is generally thought to be due to NR recombination [2]. However, high-quality GaAs is thought to have an internal florescence yield of 99.7% [12], making it an excellent material choice. A GaAs solar cell that has a fully restricted emission angle may be able to achieve efficiencies >40% under 1 sun illumination if a photonic structure can be designed that is capable of fully restricting the emission of all photons. It is also known that PC structures can be used to modify the outcoupling of light in LEDs through a modification of the spontaneous emission radiation pattern [13], which could be useful for experimental realization.

Two important parameters that must be considered for emission angle restriction using realistic photonic structures are the bandwidth of the photonic structure $\Delta_{\rm PC}$ and the photonic efficiency, $\eta_{\rm ph}$, i.e., the fraction of photons that are restricted in their emission angle compared with the total number of photons that are emitted. If angle restriction is only possible over a range of wavelengths or $\eta_{\rm ph} \neq 100\%$, then the overall cell efficiency enhancement will be decreased (see Fig. 5).

Only a relatively small bandwidth is needed for significant efficiency improvement. A photonic structure with a bandwidth of only $\Delta_{\rm PC} = 170$ meV yields a ~3% absolute efficiency improvement for $\eta_{\rm ph} = 100\%$, and a structure with $\Delta_{\rm PC} = 570$ meV yields an efficiency >40%. However, when $\eta_{\rm ph} \neq 100\%$, the maximum achievable efficiency is significantly lower. While a perfect photonic structure could allow for a solar conversion efficiency of near 42%, a photonic structure with $\eta_{\rm ph} = 99\%$ results in a solar conversion efficiency below 37%. Thus, the development of extremely high-quality photonic structures is necessary.

Finally, we note the importance of high internal fluorescence yield. Fig. 6 shows the current–voltage characteristic for a semiconductor with $E_g^{\rm SC} = 1.43$ eV and $\eta_{\rm int} = 99.7\%$ (e.g., high-quality GaAs) that is fully angle restricted ($\theta_e = \theta_s$ and $\eta_{\rm ph} = 100\%$). For this case, an absolute efficiency enhancement of 1.7% is found.

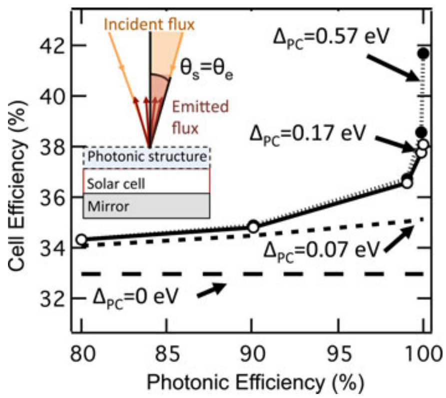

Fig. 5. Large efficiency enhancements are achieved for relative small bandwidth $\Delta_{\rm PC}$ photonic structures. However, these structures need a high photonic efficiency. Inset: A photonic structure is used to reduce the emission half-angle from the cell, which is typically 90°, to that of the sun, $\theta_s = 0.267°$.

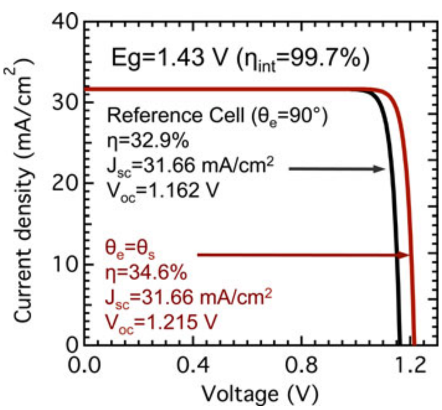

Fig. 6. Current–voltage characteristic of a solar cell with $E_g^{\rm SC} = 1.43$ eV and $\eta_{\rm int} = 99.7\%$. The addition of a photonic structure to reduce the emission angle has no effect on the short-circuit current but improves the open-circuit voltage.

V. Conclusion

We have shown a degree of freedom in a solar cell design by incorporating photonic structures that are constructed to restrict photon absorption and emission. Nonideal reflectivity and NR recombination are considered and found to play an important role in determining the maximum achievable efficiency. Such structures are capable of improving efficiencies by several percent when realistic material parameters are used. In addition to high-quality photovoltaic materials, the quality of the photonic structures is equally important. This leads us to emphasize the importance of developing new photonic structures for photovoltaics.

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