

## RAPID DETAILED BALANCE CALCULATIONS FOR MULTIPLE ENERGY GAP SOLAR CELLS

S. P. Bremner, M. Y. Levy, C. B. Honsberg  
University of Delaware  
Newark, Delaware USA

**ABSTRACT:** A rapid flux calculation method has been used to determine the detailed balance limiting efficiency for tandem solar cell stacks. This method uses Incomplete Riemann Zeta Integrals as a replacement for the Bose-Einstein integral when calculating the photon fluxes from blackbodies. Results are presented for up to 8 stacked tandem solar cells under the terrestrial AM1.5G spectrum and also under maximum concentration for comparison. The results obtained using this method agree with previous calculations with one exception highlighting the need for caution when calculating limiting efficiencies under spectrums with a piece-wise continuous nature. Finally, the band gap sensitivity of tandem solar cell stacks is investigated for the case of current constrained five solar cells, an arrangement of current interest in research. It was found that the sensitivity of the stack is fairly robust with a limiting efficiency in excess of 56% over a 0.15eV variation in the top band gap. The method presented provides an extremely useful tool for researchers to assess not just the optimum band gap arrangements of solar cell stacks but also the impact of non-optimum band gap values.

### 1 INTRODUCTION

Since first being used by Shockley and Queisser [1] in 1961, application of the detailed balance principle has been the standard approach to calculating the limiting efficiency for a solar cell. These limiting efficiencies [2,3,4] provide researchers with an upper limit to the efficiency of a particular solar cell design providing a framework for assessing novel device designs [5,6] and a guide as to the losses encountered in real devices.

In recent years there has been intense research into the development of ultra-high efficiency tandem solar cells. Along with reports of efficiencies in excess of the single band gap limit [7] there is increasing interest in tandem solar cells with 5 band gaps [8]. As the number of band gaps present in tandem solar cell stacks increases the ability to rapidly and reliably calculate the limiting efficiency for a large number of band gaps has taken on greater importance.

The detailed balance approach makes a number of assumptions in relation to the types of transitions that are present. It is assumed that all transitions are radiative with no non-ideal non-radiative transitions – the so called radiative limit. It is also assumed that both the sun and solar cell emit light as blackbodies with the fluxes given by the so called Bose-Einstein integral. The calculation of these fluxes for a single band gap solar cell is relatively straightforward but for multiple band gaps this is not always the case. The common reason for difficulty is that the test bias may be close to the band gap of the solar cell meaning the calculation is being performed near a singularity.

We have used Incomplete Riemann Zeta Integrals (IRZIs) to overcome this difficulty in calculating the photon fluxes [9] necessary for finding the limiting efficiency of a tandem solar cell stack. Results found using this method are presented for tandem stacks of up to 8 solar cells under the AM1.5G spectrum for 1x and maximum concentrations. The increased rapidity and stability offered by this method has also allowed us to calculate over a large range of band gaps meaning the band gap sensitivity of tandem stacks can be assessed. Results found for a current constrained tandem solar cell stack of 5 band gaps are presented and discussed.

### 2 RAPID FLUX CALCULATIONS USING INCOMPLETE RIEMANN ZETA INTEGRALS

#### 2.1 Tandem Solar Cell Arrangement

The two tandem solar cell arrangements considered in this work are shown in Figure 1. Figure 1a shows the unconstrained case where each solar cell in the tandem stack has its own external circuit that can be tuned to achieve optimum efficiency. Figure 1b shows the constrained case where the solar cells are connected in series meaning mismatch in performance between the devices needs to be minimized for highest efficiency.

It is assumed that each solar cell absorbs all incident photons with energy greater than its band gap and is transparent to photons with energy lower than its band gap. The solar cell with the highest band gap below the energy of the photon is assumed to absorb the photon in all cases. Energy selective reflectors are positioned between the solar cells for optimum performance [4].

#### 2.2 Transforming the Bose-Einstein Integral

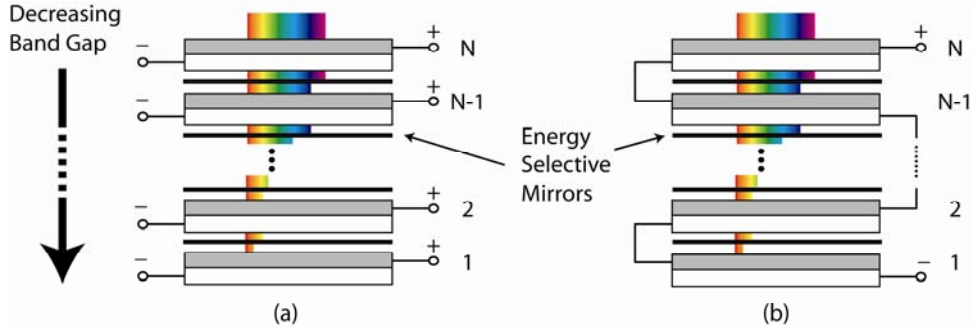
In general the Bose-Einstein integral, used for calculating the flux from a Blackbody has the form:

$$\Phi(E_A, E_B, T, \mu) = \frac{2\pi}{h^3 c^2} \int_{E_A}^{E_B} \frac{E^P dE}{\exp\left(\frac{E-\mu}{kT}\right) - 1} \quad (1)$$

for  $0 < E_A < E_B$  and  $\mu < E_A$ . It is zero for all other values.  $E_A$  and  $E_B$  are the lower and upper energy limits of emission,  $\mu$  is the chemical potential,  $T$  is the emitter temperature and  $k$  is Boltzmann's constant. The value for  $P$  is 2 for particle flux and 3 for energy flux. By substituting  $x = kT/(E-\mu)$  into Equation 1 the flux can be restated as follows (the dependence of  $\Phi$  on  $E_A$ ,  $E_B$ ,  $T$  and  $\mu$  remains but is omitted for brevity):

$$\Phi = \sum_{p=1}^{P+1} a_{p-1} \int_{x_B}^{x_A} \frac{dx}{x^{p+1} [\exp(1/x) - 1]} \quad (2)$$

Where  $x_A = kT/(E_A-\mu)$  and  $x_B = kT/(E_B-\mu)$ . In this form the evaluation of improper integrals is avoided and look up



**Figure 1: Tandem solar cell arrangements for the a) unconstrained and b) constrained cases with energy selective reflectors between solar cells**

tables (LUTs) can be constructed. A domain  $D_x$  exists for which Equation 2 is stable and computable, outside of  $D_x$  limiting expressions must

be found for the cases where  $x < \min(D_x)$  and  $x > \max(D_x)$ . Within the domain  $D_x$ , Equation 3, below gives the expression used for evaluation of the flux. The middle term is found by the consultation of LUTs for both  $x$  and the computed values of the IRZI between successive entries of  $x$ . The first and third terms are simply the remainders when  $x$  lies between values of  $x$  listed in the LUT. These remainders are computed each time a new range of  $x$  is used.

$$\Phi = \sum_{p=1}^{P+1} a_{p-1} \left( \int_{x_N^p}^{x_A} \frac{dx}{x^{p+1} [\exp(1/x) - 1]} + \sum_{k=n}^{N-1} \int_{x_k^{(p)}}^{x_{k+1}^{(p)}} \frac{dx}{x^{p+1} [\exp(1/x) - 1]} + \int_{x_B}^{x_n^{(p)}} \frac{dx}{x^{p+1} [\exp(1/x) - 1]} \right) \quad (3)$$

For the case of  $x < \min(D_x)$  and/or  $x > \max(D_x)$  the first and third terms in Equation 3 are approximated by the following expressions respectively:

$$\Phi^{high} = \sum_{p=1}^{P+1} a_{p-1} \int_{\max(D_x)}^{x_A} \frac{dx}{x^p} \quad (4)$$

$$\Phi^{low} = \sum_{p=1}^{P+1} a_{p-1} \int_{x_B}^{\min(D_x)} \frac{dx}{x^{p+1} \exp(1/x)} \quad (5)$$

Both Equation 4 and 5 are analytic and so speed and precision is maintained. The stability and rapidity offered by this method of consultation of LUTs and calculation of the small remainders [10] makes it an ideal method for calculating the efficiency of tandem solar cells stacks. As will be shown, not only does it allow the maximum limiting efficiency to be calculated but the sensitivity of the efficiency to deviations in band gap values away from the maximum can be assessed.

### 2.3 Calculation Method Used

The calculation method used consisted of taking an initial value for the lowest band gap in the tandem stack and then using a subroutine to determine the remaining band gaps that gave a short circuit current match. This

arrangement stood as the initial guess for the routines used. In the case of the constrained stack the initial guess provided by this approach was always close to the optimum band gap combination but this was not the case for the unconstrained case.

The photocurrent available was found by using the IRZI method for a blackbody at 6000K and zero chemical potential for maximum concentration calculations. For the case of a numerical spectrum the photocurrent was digitized into a LUT to minimize the re-calculation of the photocurrent for a particular band gap combination.

For the unconstrained case a LUT approach was employed where the efficiency of a solar cell absorbing between two band gap values was calculated and listed. The efficiency for a band gap combination was found by summing the contributions from each solar cell in the stack found by consulting the LUT for the relevant entry. In all of the calculations the band gap step size was set to 0.01eV.

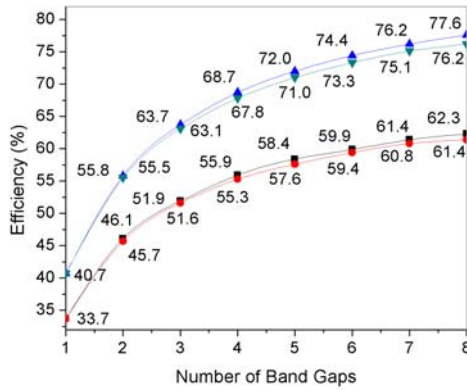
In calculations for the constrained case the following method was employed: for each band gap combination the band gap giving the lowest short circuit current was found and used as a control device for the stack. The bias was varied across this control cell and the biases required for the other solar cells to match the current output of the control cell were found. These biases were summed to give the total bias across the tandem stack and hence the efficiency was found. The band gap step size was set to 0.01eV.

## 3 RESULTS AND DISCUSSION

### 3.1 Maximum Limiting Efficiency of Tandem Stacks Under AM1.5G Spectrum

The maximum limiting efficiency was found by calculating over a large range of band gap combinations. The AM1.5G spectrum data was that of ASTM G173-03 with linear interpolation and trapezoidal integration used for photocurrent calculations. No optimizer routine was employed.

Summarised in Figure 2 are the results found for up to 8 solar cells for the unconstrained and constrained cases. The lower curves are for AM1.5G whilst the upper curves are for maximum concentration i.e. a blackbody at 6000K.



**Figure 2:** Limiting efficiency as a function of the number of band gaps in a tandem stack. The two cases of unconcentrated AM1.5G spectrum and maximum concentration (blackbody) are included for both constrained and unconstrained cases.

Included in Table I are the optimum band gap configurations for the AM1.5G spectrum results. All of the results returned for up to 6 solar cells were consistent with previous published figures [4][11] with the exception of the unconstrained 3 solar cell case (marked with asterisk).

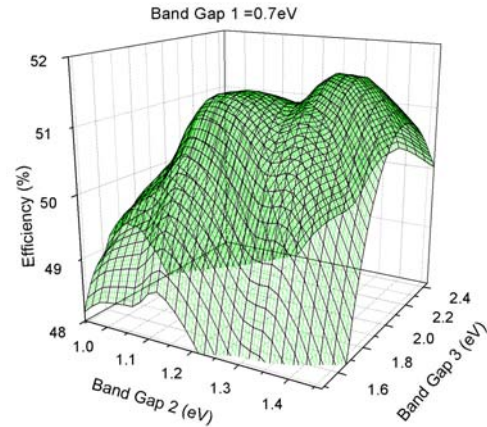
We have ascribed this discrepancy to the two humped nature of the efficiency surface as a function of band gaps

under AM1.5G. A secondary maximum with a peak efficiency very close to the absolute maximum (sometimes smaller than 0.1%) was found in all of the AM1.5G cases suggesting the calculation method may be influencing the maximum obtained.

This situation is illustrated in Figure 3 for the case of an unconstrained 3 solar cell tandem stack under AM1.5G. This is believed to be due to the piece-wise continuous nature of the AM1.5G spectrum.

**Table I:** Listing of optimum band gaps for tandem stacks of up to 8 solar cells. All values are in eV.

$E_1$	$E_2$	$E_3$	$E_4$	$E_5$	$E_6$	$E_7$	$E_8$
<i>Unconstrained AM1.5G Spectrum</i>							
1.34	-	-	-	-	-	-	-
0.94	1.73	-	-	-	-	-	-
0.93	1.40	2.05	*	-	-	-	-
0.70	1.13	1.64	2.23	-	-	-	-
0.69	0.98	1.38	1.81	2.40	-	-	-
0.69	0.94	1.19	1.53	1.92	2.45	-	-
0.69	0.94	1.15	1.41	1.72	2.11	2.57	-
0.51	0.70	0.94	1.15	1.41	1.73	2.11	2.57
<i>Constrained AM1.5G Spectrum</i>							
1.34	-	-	-	-	-	-	-
0.94	1.60	-	-	-	-	-	-
0.94	1.37	1.90	-	-	-	-	-
0.71	1.11	1.49	2.00	-	-	-	-
0.70	1.01	1.33	1.67	2.14	-	-	-
0.69	0.96	1.20	1.47	1.79	2.24	-	-
0.69	0.93	1.14	1.37	1.60	1.90	2.33	-
0.51	0.75	0.98	1.18	1.40	1.63	1.92	2.35



**Figure 3:** Limiting efficiency for an unconstrained 3 solar cell tandem stack under AM1.5G with the lowest band gap fixed at 0.7eV. Note the two maxima.

By foregoing an optimizer, the possibility that the optimizer returns a false result for the absolute maximum [11] is avoided. No such features were found for the blackbody calculations suggesting an optimizer can be used with confidence for the maximum concentration case but under any spectrum with a piece-wise continuous nature optimizers should be used cautiously.

### 3.2 Band Gap Sensitivity of a Five Solar Cell Tandem

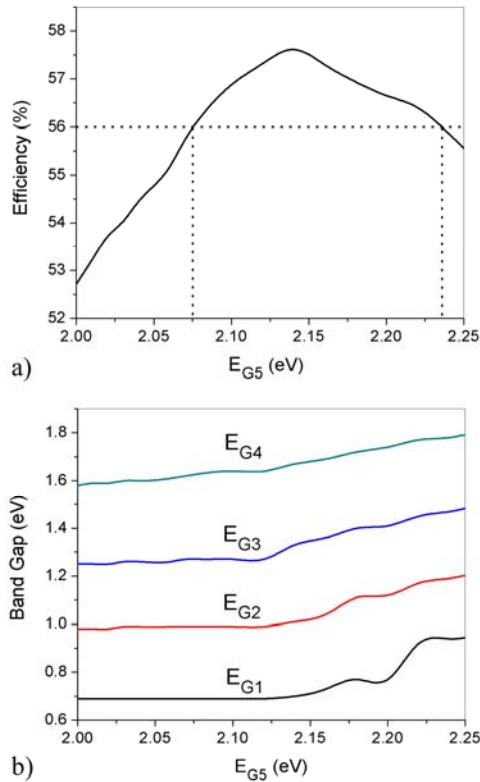
The rapidity and stability of the IRZI based method allows the investigation of a large design space of band gaps. This large design space means that the band gap sensitivity of a tandem solar cell stack can be assessed. Due to the interest in developing tandem stacks of 5 solar cell the case of a constrained 5 band gap tandem was investigated.

The optimum value for the top (highest value) band gap in a 5 solar cell stack was found in the previous section to be 2.14eV. This value of the top band gap (highest value) was varied around 2.14eV, between 2.0eV and 2.25eV. At each value of  $E_{G5}$  the tandem stack was optimized with the remaining four band gap values being varied.

The results obtained for the 5 solar cell stack are summarized in Figure 4 below. Figure 4a shows the optimized efficiency for the 5 solar cell stack as  $E_{G5}$  was varied. As can be seen, the drop-off in efficiency as  $E_{G5}$  is varied is relatively slight over a large range. The dashed lines highlight that the limiting efficiency remains above 56% from  $E_{G5} = 2.08\text{eV}$  through to  $E_{G5} = 2.23\text{eV}$ .

Figure 4b shows how the optimized values of the lower band gaps in the solar cell stack varies with the change in  $E_{G5}$ . Interestingly, the optimized values remain essentially the same for the case of  $E_{G5}$  being lower than its optimum value. Once  $E_{G5}$  exceeds its optimum, however, this is no longer the case meaning a significant re-design would be needed for an optimized device.

This result is of relevance to current attempts to fabricate 5 solar cell tandem stacks. The most pressing issue in the development of tandem devices with a large number of solar cells is obtaining a top band gap in excess of 2.0eV [8]. So far this has proven to be problematic [13][14].



**Figure 4: Results from the optimization of a 5 solar cell constrained tandem stack under 1x concentration AM1.5G spectrum. a) shows the optimum efficiency as the value of the highest band is varied. B) shows the corresponding optimum values of the remaining band gaps.**

The results presented here suggest that it may not be necessary to obtain a top band gap with the optimum value returned by detailed balance analysis. If a device can be fabricated that has a top band gap slightly lower than the optimum the limiting efficiency of the tandem stack drops by a small amount and the four lower solar cells may not require any re-design in order to achieve optimum operation.

#### 4 CONCLUSION

A rapid flux calculation method based on the use of Incomplete Riemann Zeta functions as an estimate of the Bose-Einstein Integral has been presented. This method offers improved stability and rapidity when calculating the photon fluxes necessary for detailed balance analysis of solar cells in the radiative limit.

The IRZI method has been used to calculate the maximum limiting efficiency of tandem stacks of up to 8 solar cell stacks in both the constrained and unconstrained arrangements. The results agree well with previously published data with one exception. A possible reason for the disagreement was identified as being due to the multiple maxima nature of the efficiency versus band gap surface. This multiple maxima feature was ascribed to the piece-wise continuous nature of the AM1.5G spectrum.

Finally the band gap sensitivity of a constrained 5 solar cell tandem stack was analysed as the top (highest) band gap was varied. It was found that the drop off in efficiency as the top band gap deviates from the optimum is as little as 1.5% absolute over a change in the top band gap of 0.15eV. Interestingly the optimum values for the remaining band gaps in the tandem stack show little variation when the top band gap is lower than its optimum value but are altered significantly when the top band gap is higher than its optimum. This suggests that tandem stacks with a top band gap that is lower than the optimum would not require a re-design for the lower band gaps.

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