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Optimum band gap combinations to make best use of new photovoltaic materials

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ABSTRACT

The detailed balance approach has been used to analyze the optimum use of band gaps in a multi-junction device of up to 6 sub-cells. Results for the AM1.5G spectrum suggest that as the number of sub-cells increases the importance of the bottom sub-cell band gap becomes less critical, assuming the optimum band gap combination for that value can be obtained. Given this greater freedom in choice, the potential for the use of silicon as an active substrate is investigated along with a cell thinning 'current sharing' approach to improve current mismatch in the device. Results show a more robust design space of multi-junctions with active silicon substrates when the current sharing approach is used, with performances close to the optimum for a completely free choice of band gaps. The use of the AM1.5D spectrum for a concentration ratio of 100, shows similar results for the substrate and a slight increase in band gap sensitivity for the upper band gaps in the stack. Inclusion of optical coupling between the sub-cells lowers limiting efficiency, with luminescent coupling mitigating the band gap sensitivity. The results and approach outlined are useful for determining how best to deploy new photovoltaic materials in multi-junction solar cells.

1. Introduction

Multi-junction (MJ) solar cells stand alone as the only successful strategy for boosting solar cell power conversion efficiencies above the single band gap detailed balance limit found originally by Shockley and Queisser (1961), with MJ limits being determined in the ensuing years (Henry, 1980; Marti and Araujo, 1996, Brown and Green, 2002, Bremner et al., 2008). By stacking different materials (with different band gaps) the photon energy above the band gap energy, which is lost in a single band gap device, can be harnessed more efficiently, leading to a high voltage device with a current that is reduced, but gives an improved overall performance. This relies on the MJ solar cell having the band gaps chosen in such a way as to minimize the potential current mismatch between the sub-cells in the stack. For the most common case of a monolithic MJ solar cell, where layers of different materials are grown on top of each other with a common substrate, a further restriction is designing to minimize the lattice mismatch between materials, to ensure material of sufficient crystalline quality for high photovoltaic performance.

In recent years impressive results focused on the lattice matched GaInP-Ga(In)As-Ge triad have led a renewed interest in the development of high efficiency multi-junction solar cells (Jones et al., 2012). Further to these successes, has been the development of devices using metamorphic step-graded alloy buffer layers (King et al., 2007; Geisz, 2008), which have delivered performances at the same level as the lattice matched approaches, with the latest generation of 'inverted' metamorphic devices (Geisz, 2008) holding the current champion efficiency (Soitec, 2014). For these metamorphic approaches the need for very close lattice matching is relaxed, meaning an ever expanding palette of different materials can now be investigated for high performance Photovoltaic applications. Reports of highly efficient materials such as Perovskites (Green, 2014; Petrović et al., 2015), lower cost CZTS (Shin et al., 2013) and even breakthroughs for more conventional III-V material growth on silicon (Grassman et al., 2013), point to a much greater choice of materials to be deployed in MJ solar cells.

The detailed balance limiting efficiency for photovoltaic energy converter designs offers insights into the relative performance of real devices against the ultimate performance permitted by the laws of physics. It allows for the potential of different materials as PV solar cells to be assessed not just for homo-junction devices, but also for multi-junction devices, where a combination of band gaps will be used. This is a crucial question to researchers investigating new PV

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materials systems: how can this material be used to greatest effect in a general PV device? As an example, most materials will not have the band gap to be ideal for a single band gap device, indeed any material with a band gap in excess of around 1.5 eV will most likely be best used in a MJ device as an upper sub-cell. But is it best suited to a three or four sub-cell MJ or for a MJ with an even greater number of sub-cells?

In this paper we report on detailed balance modelling of multi-junction solar cells under 1 sun AM1.5G and 100 suns AM1.5D spectra, to help guide how best to use a material in a high efficiency photovoltaic device. Our results show that the choice of band gap for the active substrate in a multi-junction device becomes less critical as the number of band gaps is increased, providing the optimum band gaps for the upper layers can be implemented. A general approach to deciding the best use of a new PV material is outlined and as an example the use of silicon as an active substrate for a three band gap multi-junction solar cell is detailed for the 1 sun AM1.5G spectrum case. We show that despite the optimal use of its band gap being as the middle sub-cell, the use of thinner upper layers to create a 'current sharing' arrangement sees the use of silicon as an active substrate perform well, with a relatively large design space.

2. Model used

A detailed balance model (Shockley and Queisser, 1961; Henry, 1980; Marti and Araujo, 1996, Bremner et al., 2008), was used to calculate all limiting efficiencies in this work. This means that all transitions considered balance exactly with their inverse at thermal equilibrium. It is assumed that for each sub-cell absorption is 100% of photons with energy greater than the sub-cell band gap, but lower than the band gap for the sub-cell immediately above, for the top cell this means effectively an infinite band gap (we set this to 5 eV). Light generated current values were evaluated using data for the AM15G spectrum given by the ASTM G-173 Reference Solar Spectrum Irradiance (IEC, 2008). The digitized data was used to calculate incremental power and photon numbers between successive values of wavelength, with these values kept in a Look Up Table (LUT). The total input power P_{IN}, which corresponds to the sum of all of the incremental powers, was calculated as a cross-check that the data was being calculated correctly. For each sub-cell band gap the equivalent wavelength was found, allowing the LUT to be referenced and the short circuit current to be found without additional calculations. The AM1.5G spectrum was used for 1 sun concentration results in all of the calculations presented. Calculations for concentrated sunlight are performed using this method in a straightforward manner using the AM1.5D spectrum.

It is further assumed that each sub-cell has a single chemical potential difference across it (that corresponds to the sub-cells operating voltage) and that the dark current for the sub-cells is given by the radiative emission of each sub-cell behaving as a modified Blackbody (BB). The emission flux of a sub-cell at a temperature, T, and with chemical potential difference, μ, given by the Bose–Einstein (BE) integral:

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

for $0 < E_A < E_B$ and $\mu < E_A$. E_A and E_B are the energy limits of emission, and k is Boltzmann's constant. Ω is the étendue of the light emission, which is given by $\Omega = \pi n^2 \sin^2 \Theta_c$, where Θ_c is the half angle into which radiation can be emitted, and n is the refractive index of the medium light is being emitted into. As an example of finding the étendue, hemispherical emission into air ($n = 1$), such as a solar cell front surface emitting, means the étendue will be π. All of the light emission calculations done in this work assumed hemispherical emission. The BE integral was calculated using a rapid flux calculation technique based on Incomplete Riemann Zeta Integrals (IRZIs) previously shown to give greater speed and stability for these types of calculations (Bremner et al., 2008).

The efficiency was found for each combination of band gaps by first finding the open circuit voltage of each sub-cell and setting this as the upper limit for the chemical potential during subsequent calculations. Since the connection is series constrained, the light generated currents for each sub-cell was calculated, with the sub-cell with the lowest light generated current taken as a control sub-cell, since it is this sub-cell that will set the current through all of the sub-cells in the stack. The chemical potential across the control sub-cell, μ_{cont}, was ramped from zero to the open circuit voltage in steps of 1 mV, with the net current being calculated to give its operating point. The corresponding operating points for the other sub-cells in the stack was then calculated by finding the chemical potential across each sub-cell that gives the same net current as the control sub-cell. The sum of the chemical potentials across all of the sub-cells in the stack is thus found, and when multiplied by the net current in the stack, the output power found. The maximum power is updated for any increase with each increment of chemical potential allowing the maximum power output for a single band gap combination to be found. Finally, due to the non-continuous nature of the AM1.5 spectra, cycling through the band gap combinations was undertaken rather than using an optimizer.

3. Results and discussion

3.1. Free choice of band gaps

The palette of materials with potential use for photovoltaics is ever expanding, however, if one is restricting consideration to only a single band gap device, the suitability of a newly discovered material may be poor if its band gap is outside of the 1.0–1.5 eV range. Even if within this range there may be more value for using the new material as part of a multi-junction device, rather than as a single band gap solar cell. It therefore makes sense to have some idea of what band gaps are most useful for different numbers of band gaps in a multijunction stack.

To this end detailed balance calculations have been performed for different numbers of band gaps in a multijunction arrangement, with it assumed that each cell only emits through its front surface (and therefore the étendue is π). This corresponds to the rear of each cell having an idealized reflector that allows light below the band gap of the sub-cell in question to pass freely, but reflects 100% of the light that can be absorbed by the sub-cell in question. This situation represents the best efficiency that the multijunction stack can achieve (Rühle, 2016), since emission is minimized, while still allowing all sub-cells to access the solar spectrum efficiently.

A search of possible combinations of band gaps was undertaken for each number of band gaps in the multi-junction stack. For two, three, and four band gap stacks initial searches with resolutions of 0.01 eV were used, while for five and six band gap stacks a resolution of 0.02 eV was used. This was necessary due to the large number of band gap combinations to be searched in order to be certain the maxima were being captured correctly. Following the initial search a refined search limiting the search ranges was used with the digitised AM1.5G data resolution was used for the two, three and four sub-cell cases, a final resolution of 0.01 eV was used for the five and six sub-cell cases. The results of these searches are summarized graphically in Fig. 1 below. The color coding indicates the position in the stack for which the band gap is optimal. Note