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OPTIMUM BANDGAP CALCULATIONS FOR A 4-TERMINAL DOUBLE TANDEM III-V CONCENTRATOR SOLAR CELL STRUCTURE

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ABSTRACT: A 4-terminal double tandem III-V concentrator solar cell, consisting of two mechanically stacked monolithic tandem cells, can achieve efficiencies of more than 40 %. Calculations were performed to determine the optimum bandgap combination for the InGaAsP subcells of this design, for an irradiance range of 1 to 1000 suns. Furthermore, the addition of Al to the compound that composes subcell 1 and allowing a certain degree of lattice mismatch were considered as methods to extend the bandgap ranges, in order to increase the efficiency. However, in a first order approximation the implementations of these methods seem to be difficult or to induce little effect.

Keywords: Multi-junction Solar Cell, Concentrator Cells, Modelling

1 INTRODUCTION

Anthropogenic CO₂ emissions are largely responsible for global warming and its associated damaging effects [1]. A sufficient reduction of this emission requires a dramatic decrease in the use of fossil fuels. One of the most promising long term solutions is to use solar cells to utilize solar energy. The reason that solar cells have not yet been implemented on a large scale is the fact that the cost of the electricity they generate is several factors higher than the prevailing electricity cost.

One way to significantly reduce the price of electricity generated by solar cells is to incorporate high efficiency cells into concentrator systems. For this reason, the department of Applied Materials Science (AMS) of the Radboud University Nijmegen has the long-term research strategy to develop concentrator solar cells with efficiencies of more than 40 %. Based on its theoretical maximum efficiency, on possibilities to actually grow the crystalline structures and on the specific capabilities available at the AMS department, a 4-terminal double tandem solar cell structure is considered to be a promising configuration to achieve this goal.

In the present study, the optimum bandgap combination for the subcells of the above mentioned structure was calculated for a series of irradiances ranging from 1 to 1000 suns, under the AM1.5D spectrum. Furthermore, two methods of extending the bandgap ranges of its subcells are discussed, since this can increase the efficiency of the configuration somewhat. These are the allowance of a certain degree of lattice mismatch, and the integration of Al to the compound that composes the top subcell.

2 THEORY

Many configurations are conceivable to design a high efficiency multi-junction III-V solar cell. One can choose to incorporate any number of junctions in the stack, the bandgap of each subcell can be varied, and there is the choice between monolithic and mechanical stacking. In theory, the efficiency of a solar cell stack increases with each junction added, but the efficiency gained gets smaller with each additional junction. Moreover, each junction that is added to a mechanical stack will require an additional growth run and associated processing, and

will add an extra set of terminals to the stack. In practice, each added subcell will also suffer from increasing shadowing losses and will make the structure more prone to mechanical impairment. These drawbacks do not accompany the addition of a junction to a monolithic stack. However, in this case the disadvantages are the fact that the potential improvement of the efficiency, by increasing the number of junctions, is limited due to current- and lattice matching restrictions. Also, the tunnel junctions required in this case have losses associated with them. In practise, therefore, the optimum number of stacked *pn*-junctions is limited for both mechanical and monolithic stacking methods. This explains the fact that the efficiency record for a multi-junction solar cell is currently held by a solar cell containing only three junctions [2].

An excellent way to achieve a high number of junctions, while largely circumventing the restrictions of both stacking methods, is by combining both forms of stacking in a 4-terminal quadruple-junction solar cell structure, referred to as a double tandem structure, as depicted in figure 1.

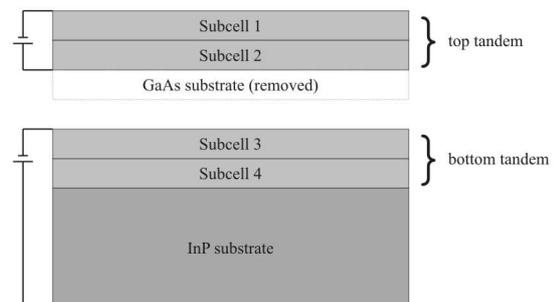


Figure 1: Schematic representation of the double tandem structure.

The envisioned double tandem structure consists of a thin-film semi-transparent monolithic tandem which is released from its GaAs substrate using the epitaxial lift-off (ELO) technique [3, 4], and mechanically stacked on top of a second monolithic tandem cell which is grown on an InP substrate. Recently Griggs *et al.* also performed calculations on such a structure [5]. Using lattice matched InGaAsP compounds as the materials for the junctions, the top and bottom monolithic tandems can cover the large bandgap ranges of 1.894 to 1.430 eV and

1.340 to 0.751 eV respectively[†], enabling a high total efficiency.

The optimum combination of subcell bandgaps in the above ranges, together with the associated theoretical maximum efficiency of the double tandem structure, was determined as a function of irradiance. This was done using the diode model, which describes the physics of a pn -junction solar cell. According to this model, of which a detailed derivation is given by Green [6], the relation between the voltage V and current density J of an ideal monolithic tandem cell consisting of subcells a and b , is given by:

$$V = \frac{kT}{q} \ln \left(\frac{(-J + J_{sca} + J_{0a})(-J + J_{scb} + J_{0b})}{J_{0a}J_{0b}} \right), \quad (1)$$

where k is Boltzmann's constant, T is the temperature of the monolithic tandem cell (taken as 25 °C) and q is the elemental charge. J_{sca} and J_{scb} represent the short circuit current densities for subcells a and b respectively, calculated for the case that all incident photons with an energy larger than the bandgap are absorbed, each exciting one electron in the process, while other photons are transmitted. Finally, J_{0a} and J_{0b} represent the diode saturation current densities (in units of Am^{-2}), for subcells a and b respectively, and were taken as:

$$J_{0i} = 1.5 \times 10^9 \exp \left(-\frac{E_{gi}}{kT} \right), \quad (2)$$

with E_{gi} the bandgap of subcell i ($i = a, b$). The numerical term is a reasonably estimated minimum value according to Green [6]. An expression for J_{mp} , the current density at maximum power output of the monolithic tandem cell, can be derived from equation (1) as:

$$J_{mp} = \frac{(-J_{mp} + J_{sca} + J_{0a})(-J_{mp} + J_{scb} + J_{0b})}{(-J_{mp} + J_{sca} + J_{0a}) + (-J_{mp} + J_{scb} + J_{0b})} \cdot \ln \left(\frac{(-J_{mp} + J_{sca} + J_{0a})(-J_{mp} + J_{scb} + J_{0b})}{J_{0a}J_{0b}} \right). \quad (3)$$

The efficiency η of the monolithic tandem cell can then be written as:

$$\eta = \frac{kTJ_{mp}^2}{qP_{in}} \left(\frac{1}{-J_{mp} + J_{sca} + J_{0a}} + \frac{1}{-J_{mp} + J_{scb} + J_{0b}} \right), \quad (4)$$

with P_{in} the total power per unit area in the light incident on it. The efficiency of the double tandem structure is simply the sum of the efficiencies of its constituting monolithic tandem cells. It was calculated for each logically possible bandgap combination that was allowed within the bandgap ranges of interest, in steps of 0.5 nm for the cut-off wavelength, which is defined as $\lambda_g = hc/E_g$. This was done for an irradiance E ranging from 1 to 1000 suns, with 1 sun defined as 1000 Wm^{-2} .

[†] All values for lattice constants and bandgaps used in this paper are taken from the computer program Abacuses version 3.6, © 1994-1999 by Olivier Duchemin.

The calculations were performed on the basis of the direct normal ASTM G-173-03 (AM1.5D) spectrum [7][‡], and equation (3) was solved numerically with an error $\leq 10^{-7} \text{ Am}^{-2}$.

3 RESULTS

The results of the computations for the double tandem structure are shown in figures 2 and 3. The first of these figures shows that the theoretical maximum efficiency is already 46.00 % at $E = 1$ sun, and increases approximately linearly with $\ln(E)$ to 55.91 % at $E = 1000$ suns. The kinks in the curves of the separate efficiency contribution of the top and bottom tandem indicate a change in bandgap of (some of the) subcells, as can also be seen in figure 3. However, this figure clearly shows that these changes are minimal and that the optimum bandgaps of the four subcells are virtually constant over the evaluated irradiance range. In addition, they lie close to the bandgaps that give optimum cell performance under the global tilt ASTM G-173-03 (AM1.5G) spectrum [7] at an irradiance of 1 sun, which are 1.894, 1.430, 1.111 and 0.772 eV, for subcells 1 to 4 respectively.

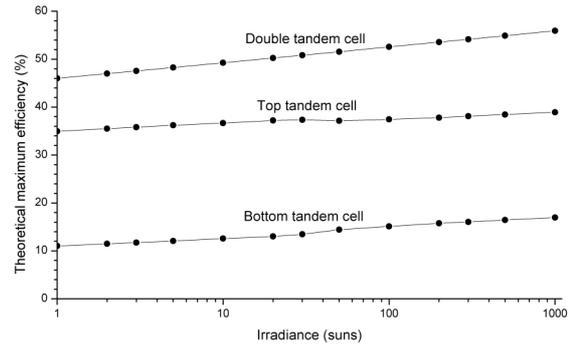


Figure 2: The theoretical maximum efficiency as a function of the irradiance, for double tandem configurations, under the AM1.5D spectrum. Bandgaps were restricted to the range of 1.894 to 1.430 eV for the top tandem and 1.340 to 0.751 eV for the bottom tandem. The separate contributions of the top and bottom tandem are also displayed.

It is hard to predict under which irradiance the highest efficiency will be achieved in practice, since this depends strongly on the resistance of the structure, which is unknown at present. Therefore, it will be a good approach to start experimental research towards the double tandem structure by focussing on the structure with the highest performance under standard 1 sun AM1.5G measuring conditions. With those bandgaps, the theoretical maximum efficiency of the double tandem

[‡] Note that additional data points were added to the AM1.5 spectra where necessary, to obtain a complete wavelength range of 0.5 to 4000 nm, in steps of 0.5 nm. This was done under the assumption that the spectral irradiance is zero for $0 < \lambda < 280$ nm and that it varies linearly in between the original data points. These values were then renormalized so that the total irradiance of the spectrum remained 1000 Wm^{-2} .

structure under the AM1.5D spectrum increases approximately linearly with $\ln(E)$ from 45.94 % at $E = 1$ sun to 55.74 % at $E = 1000$ suns, only marginally below the efficiencies using the optimum bandgaps. The compound compositions of subcells 1 to 4 in that case are $\text{In}_{0.4855}\text{Ga}_{0.5145}\text{P}$, GaAs , $\text{In}_{0.855}\text{Ga}_{0.145}\text{As}_{0.32}\text{P}_{0.68}$ and $\text{In}_{0.559}\text{Ga}_{0.441}\text{As}_{0.947}\text{P}_{0.053}$ respectively.

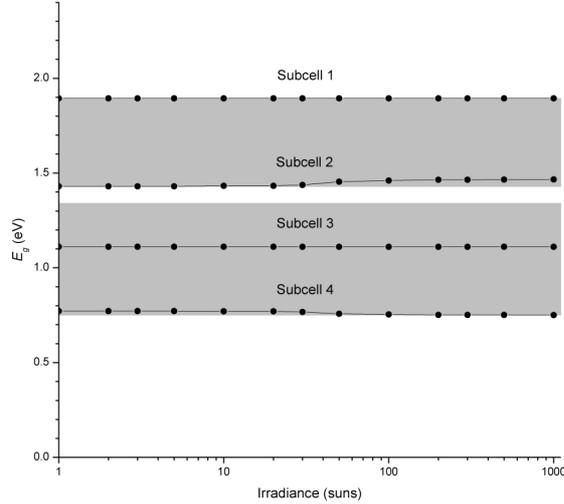


Figure 3: Variation in the optimum combination of bandgaps of the subcells in the double tandem structure, as a function of the irradiance, under the AM1.5D spectrum. The grey areas represent the ranges of available bandgaps of 1.894 to 1.430 eV for subcells 1 and 2, and 1.340 to 0.751 eV for subcells 3 and 4.

4 BANDGAP RANGE INCREASE

It should be noted that, apart from the bandgap of subcell 3, all the optimum bandgaps in figure 3 lie at one of the limits imposed by the restriction of lattice matching, for at least part of the intensity range. The bandgap of subcell 1 even lies at the highest available value of 1.894 eV for the entire irradiance range, which suggests that this is the main restriction on the maximum obtainable efficiency. This upper bandgap limit can be increased somewhat by integrating aluminium into the compound that composes subcell 1. However, III-V structures containing layers with a high Al fraction are very sensitive to the undesired incorporation of oxygen [8], which in practice decreases the performance of the solar cell. In addition, compounds containing a high Al fraction often have indirect bandgaps. Solar cells composed of such materials require thick layers to absorb the light, and therefore more material to achieve a high efficiency. For these reasons, the addition of Al is not considered to be a favourable option.

Another method by which the bandgap ranges can be extended is by allowing a small lattice mismatch in the subcells. This will, however, introduce a certain amount of stress in the subcells, and too much stress will cause so-called misfit dislocations between the substrate and the epitaxial layer, resulting in a rapid decrease of cell performance. In order to avoid this, the thickness of the epitaxial layer should not exceed the critical layer thickness h_c . According to the model of van de Leur *et al.* [9], which predicts values that closely match the

experimentally observed values, h_c can be found by numerically solving:

$$h_c = \frac{b}{4\pi|\varepsilon|} \frac{2-\nu}{1+\nu} \left[\ln \left(\frac{4\sqrt{6}\alpha h_c}{b} \right) - 2 \right]. \quad (5)$$

Here ν is Poisson's ratio of the film and α the dislocation core parameter. The variable b is the length of the Burgers vector, which equals $2^{-1/2}a_f$, where a_f is the lattice constant of the film. Lastly, ε is the strain of the film parallel to the substrate, and is equal to the lattice mismatch f between the film and substrate as long as no misfit dislocations have been generated, i.e. as long as the film thickness is below the critical thickness[§]. The lattice mismatch is defined as:

$$f \equiv \frac{a_s - a_f}{a_f}, \quad (6)$$

with a_s the lattice constant of the substrate.

In the present situation the required film thicknesses are known. Taking these as values for h_c , the limits of the lattice constants of the films can be calculated, and those in turn give the bandgap limits for the subcells in the monolithic tandems of the target structure. So inserting equation (6) and $b = 2^{-1/2}a_f$ into equation (5) and rewriting it for a_f , one gets:

$$a_f = \sqrt{\frac{4\sqrt{2}\pi h_c |a_s - a_f|}{\ln(8\sqrt{3}\alpha h_c) - \ln(a_f) - 2} \frac{1+\nu}{2-\nu}}. \quad (7)$$

Poisson's ratio can be expressed as:

$$\nu = \frac{c_{12}}{c_{11} + c_{12}}, \quad (8)$$

where c_{11} and c_{12} are the elastic constants related to the principle axes of the film. For a ternary compound $\text{A}_x\text{B}_{1-x}\text{C}$, such an elastic constant c_{ij} is the weighted average of those of the two associated binary compounds AC and BC, i.e.:

$$c_{ij,ABC} = c_{ij,BC} + x(c_{ij,AC} - c_{ij,BC}). \quad (9)$$

This means ν is a function of x , but x is not known until a_f is known. However, since it is assumed that the value of each lattice mismatch is small, the deviation in x will be small and it is reasonable to take the (known) x value of the compound that is lattice matched to the GaAs and InP substrates. The outcomes of the calculations later

[§] In the article of van de Leur *et al.* [9], this equation is actually stated with ε instead of $|\varepsilon|$. However, in practise this would result in a negative value for h_c in the case where the lattice constant of the film is larger than that of the substrate, i.e. when ε has a negative value. But when ε changes sign, the angle λ between the misfit stress and its Burgers vector, changes simultaneously to $\pi - \lambda$. And since $\cos(\lambda)$ appears in the Schmid factor, which is hidden in equation (5), and $\cos(\pi - \lambda) = -\cos(\lambda)$, this negative value of ε is compensated for.

confirm that this assumption is justified. For the compounds on the GaAs substrate this means $x = 0.4855$ for $\text{In}_x\text{Ga}_{1-x}\text{P}$, and $x = 0$ for $\text{In}_x\text{Ga}_{1-x}\text{As}$. On the InP substrate, these compounds will have x values of 1 and 0.5325 respectively.

It should be noted that equation (7) is given for a single epitaxial layer, while the present situation concerns a tandem cell structure on a substrate. In a first order approximation, equation (7) was therefore used to calculate the minimum or maximum lattice constant for a single film, with a thickness equal to that of the total tandem. For both substrates, this calculation was performed assuming the film consisted of $\text{In}_x\text{Ga}_{1-x}\text{P}$, and repeated assuming it consisted of $\text{In}_x\text{Ga}_{1-x}\text{As}$. Each resulting value was taken as the allowed lattice constant for its associated layer in the tandem cell structure. The predicted required film thicknesses are 0.7, 3.6, 2.0 to 3.6 and 3.6 μm for subcells 1 to 4 respectively. So the (maximum) required total thickness of the top and bottom tandems are 4.3 and 7.2 μm respectively. Using these values for h_c , together with the parameter values as stated in table I, the allowed lattice constant ranges for both tandem structures were determined.

Table I: Elastic strains, lattice constants and the dislocation core parameter, used to calculate the allowed lattice constants for $\text{In}_x\text{Ga}_{1-x}\text{P}$ and $\text{In}_x\text{Ga}_{1-x}\text{As}$ layers on GaAs and InP substrates, with the imposition that no misfit dislocations occur. The value of α cannot be determined exactly, but $\alpha \sim 4$ is a good approximation [9].

Variable	Value	Reference
$c_{11,\text{GaP}}$	14.05×10^{11} dynes cm^{-2}	[10]
$c_{11,\text{InP}}$	10.11×10^{11} dynes cm^{-2}	[11]
$c_{11,\text{GaAs}}$	11.90×10^{11} dynes cm^{-2}	[12]
$c_{11,\text{InAs}}$	8.34×10^{11} dynes cm^{-2}	[13]
$c_{12,\text{GaP}}$	6.20×10^{11} dynes cm^{-2}	[10]
$c_{12,\text{InP}}$	5.61×10^{11} dynes cm^{-2}	[11]
$c_{12,\text{GaAs}}$	5.34×10^{11} dynes cm^{-2}	[12]
$c_{12,\text{InAs}}$	4.54×10^{11} dynes cm^{-2}	[13]
a_s,GaAs	5.653 \AA	Abacuses
a_s,InP	5.869 \AA	Abacuses
α	4	[9]

For the top tandem this gives a lattice constant range of $5.6524 < a_f < 5.6536 \text{\AA}$, and for the bottom tandem $5.8686 < a_f < 5.8694 \text{\AA}$. So in both cases the allowed deviation from the substrate lattice constant a_s is less than 0.001 \AA , which is the accuracy of the lattice constants associated with the various bandgaps. Therefore, in a first order approximation the extension of the bandgap ranges by allowing strain in the layers, without the generation of dislocation centres, is calculated to be ineffective.

5 SUMMARY

For an irradiance range of 1 to 1000 suns, calculations were performed to determine the bandgap combination for the lattice matched InGaAsP subcells of a double tandem solar cell, for which the theoretical efficiency is maximum under the AM1.5D spectrum. The resulting optimum bandgap combinations turn out to be virtually constant over the entire irradiance range, and are

very similar to the optimum bandgap combination for the double tandem structure under standard 1 sun AM1.5G measuring conditions of 1.894, 1.430, 1.112 and 0.768 eV for subcells 1 to 4 respectively. The associated InGaAsP compounds for the subcells are $\text{In}_{0.4855}\text{Ga}_{0.5145}\text{P}$, GaAs, $\text{In}_{0.855}\text{Ga}_{0.145}\text{As}_{0.32}\text{P}_{0.68}$ and $\text{In}_{0.559}\text{Ga}_{0.441}\text{As}_{0.947}\text{P}_{0.053}$ respectively. The theoretical maximum efficiency for this configuration increases virtually linearly with $\ln(E)$ from 45.94 % at $E = 1$ sun to 55.74 % for $E = 1000$ suns under the AM1.5D spectrum.

Since an increase in the allowed bandgap ranges would result in somewhat higher efficiencies, the addition of Al to the compound that composes subcell 1 was considered, as well as allowing a certain degree of lattice mismatch. However, in a first order approximation the implementations of these methods seem to be difficult or to have little effect.

6 ACKNOWLEDGEMENTS

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