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A NEW DESIGN : THREE TERMINAL BAND OFFSET BARRIER ORGANIC/SI TANDEM SOLAR CELLS

J.P. Connolly^{1,2}, J. Alvarez^{1,2}, J.P. Kleider^{1,2}, P. Roca i Cabarrocas³, S. Chambon⁴, L. Hirsch⁴, L. Vignau⁴,
G. Wantz⁴, M.E. Gueunier-Farret⁴

¹ Université Paris-Saclay, CentraleSupélec, CNRS, Laboratoire de Génie Electrique et Electronique de Paris, 91192, Gif-sur-Yvette, France

² Sorbonne Université, CNRS, Laboratoire de Génie Electrique et Electronique de Paris, 75252, Paris, France

³ École Polytechnique, LPICM, CNRS UMR 7647, Institut Polytechnique de Paris, 91120 Palaiseau, France

⁴ Université de Bordeaux, IMS-CNRS, UMR 5218, Bordeaux INP, ENSCBP, F33405 Talence, France

ABSTRACT: Organic solar cells are particularly attractive for their very low fabrication cost, and lack of use of critical raw materials. While this has to date been hobbled by low efficiency, recent achievements demonstrate organic single junction technology at 20% efficiency approaching economically viable performance.

We survey the reasons for these recent high efficiency organic solar cell achievements. They include bulk heterojunction (BHJ) concepts, composed of electron donor materials, most often a semiconductor polymer and electron accepting materials, most often a small molecule, and the novel non-fullerene acceptor materials. The range of commercially available donor and acceptor materials available offers a large design flexibility for low or high band gap devices. A natural development for this emerging thin film technology reaching competitive efficiencies is its integration in tandem solar cells.

In the context of the breakthroughs in organic solar cell efficiency, this work presents first results of the ORGANIST project (2023 – 2027) supported by the French Research National Agency. The presentation of organic materials for top cells and their efficient integration on a high efficiency silicon IBC cell is discussed with a critical focus on the interface between top organic solar cell and bottom silicon IBC cell. We present preliminary theoretical results evaluating the performance of 3T devices being developed in ORGANIST and based on identified prototype materials for the organic cell, strategies for efficient optical and electrical connection between the two subcells, aiming for low cost three terminal organic / silicon tandems with high efficiencies above the Shockley-Queisser single bandgap limit for Silicon.

Keywords: Multijunction ; Organic ; Silicon; High efficiency

Author for correspondence : james.connolly@centralesupelec.fr

1 INTRODUCTION

Multijunction cells are the most efficient solar cell designs to date. These designs have historically been fabricated only with high cost III-V materials and have been restricted to space applications. Terrestrial applications under concentration which can significantly reduce cost. However they have not, to date, led to a breakthrough in applications due to underlying materials and fabrication costs, and to the additional complexity and associated cost of light concentration.

Concerning multijunction performances, a record certified terrestrial power conversion efficiency of 38.8% performance was achieved in 2014 [1] under standard AM1.5G test conditions but without notable subsequent progress [2]. The III-V approach, therefore, while promising, has not yet delivered for terrestrial applications though work is ongoing.

In that context, the obvious attraction of tandem solar cells with silicon lower bandgap subcells have emerged, based due to the observation that the silicon gap of 1.12 eV is nearly ideally suited to the bottom gap of a tandem solar cell [3]. This too has been the focus of much research for over a decade, and has now delivered high efficiency over 33% for both III-V/Si and perovskite/Si tandems [2].

And while other materials combinations on Si have been studied, we will not list them exhaustively, only remark that none has led to more promising performance so far. In this context, organic solar cell (OSC) performance has recently shown significant improvements, achieving 20% efficiency [4]. This makes this system a candidate for

tandem solar cells, in particular in developing high bandgap organic subcells associated with Si low bandgap subcells in silicon-organic tandem devices.

This paper presents early projections of expected device performance based on a brief survey of data from the literature, which lays the basis for device performance which may be achieved within the project.

2 DEVICE DESIGN

2.1 Ideal limits and materials compromise

We first look at achievable radiative efficiencies [3] for the materials under consideration. The donor and acceptor materials considered are PBDB and GS-ISO families respectively, which yield an organic subcell bandgap of the order of 2 eV.

The radiative efficiency limit of three terminal solar cells is shown in figure 1 in order to emphasise the tolerance of the three terminal (3T) design to subcell bandgaps. With the constraint of a Si bottom subcell bandgap of 1.12 eV, the ideal top subcell has a bandgap of 1.82 eV and the corresponding tandem efficiency is at 42.2% under standard AM1.5G test conditions. If we increase the top bandgap to 2 eV, the tandem efficiency is still at 41.7%, with a drop of just 0.5% compared to the optimum case. This 2 eV material is chosen on the basis of recent trends in the field which are non-fullerene wide bandgap acceptors coupled with PBDB-TF donor [4, 5].

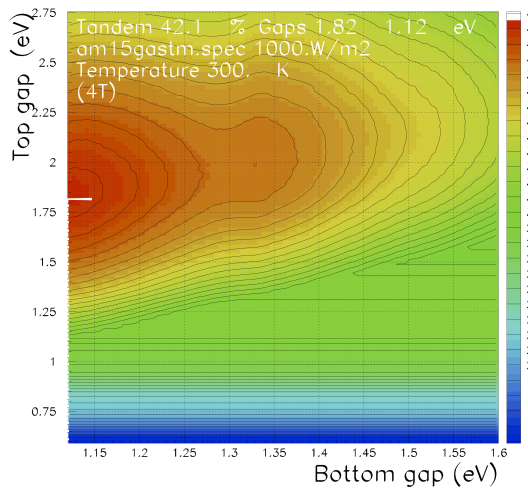


Figure 1 Three terminal tandem cell efficiency contour plot under standard AM1.5G test conditions, as a function of top and bottom subcell bandgaps in the radiative limit. Assuming a silicon bottom cell, the tandem cell maximum efficiency is 42.2% (bandgaps 1.12 and 1.82 eV).

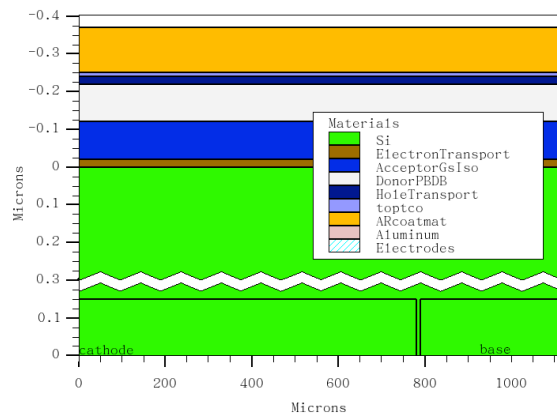


Figure 2 Sketch of the 3T OSC/Si-IBC tandem structure showing the OSC layer sequence for an n-type IBC.

2.2 Subcell design

We use a standard Si-IBC based on the ZEBRA design commercialised by ISC-Konstanz [6], partner of the ORGANIST project. We do not detail performance but note that the modelled cell efficiency is for an untextured IBC in order to facilitate OSC integration. The base Si-IBC has the following simulated performance: short circuit current density $J_{SC} = 32.3 \text{ mA/cm}^2$, open circuit voltage $V_{OC} = 0.73 \text{ V}$, $FF = 82\%$, and efficiency of 20%. When shaded by the OSC top cell, however, the efficiency of the Si-IBC is naturally reduced. We note that the J_{SC} is reduced to 13.4 mA/cm^2 , the V_{OC} to 0.71 V, and the fill factor slightly improved at $FF = 84\%$, leading to an efficiency in the 3T tandem of just 8%. The organic cell is modelled following the detailed modelling analysis of Koster et al. [7] and associated SILVACO example solarex07.in. This model includes organic semiconductor properties in particular exciton transport and dissociation at donor/acceptor interfaces.

The modelled structure in the first instance is a bilayer heterojunction with 100 nm donor and acceptor layer thicknesses, to be developed further to enable simulation of bulk heterojunction blended organic absorbers which offer advantages for carrier collection in these materials with very short exciton lifetimes and diffusion lengths. In the early stages of the ORGANIST project the modeling uses data obtained in the literature [8,9]. This approach yields the following simulated OSC performance : short circuit current density $J_{SC} = 10.6 \text{ mA/cm}^2$, open circuit voltage $V_{OC} = 1.48 \text{ V}$, $FF = 90\%$, and efficiency of 14.2%.

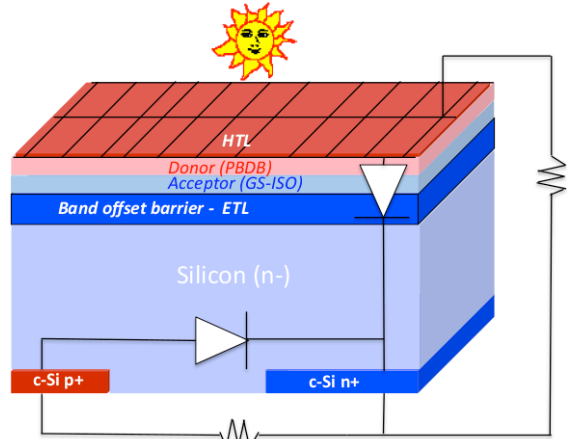


Figure 3 Sketch of the 3T OSC/Si-IBC tandem structure for an n-type IBC device.

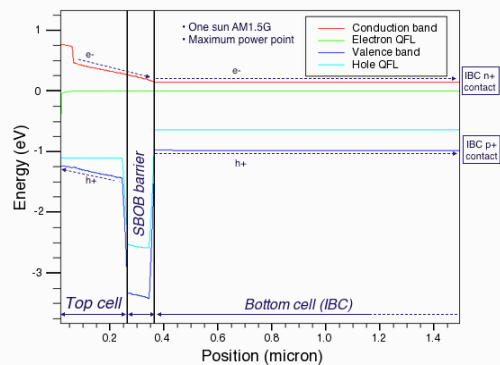


Figure 4 Schematic band diagram of the 3T-band offset barrier tandem, showing the band offset separating hole populations in top and bottom cells, and leading to different quasi-Fermi levels under one sun illumination, the simulation being at the maximum power point.

2.4 Three terminal OSC/IBC band offset barrier tandem

The 3T band offset barrier tandem device concept has been described previously [10] and is briefly summarised here. The device is sketched in figure 3 in the n-type IBC embodiment of the concept. The valence band offset barrier in this case prevents transport of holes between top and bottom subcells, such that hole populations in the two cells are decoupled, and each defined by an independent quasi-Fermi level.

Figure 4 shows the simulated band structure and quasi-Fermi levels at maximum power point voltage, under AM1.5G illumination. The different quasi-Fermi level separations in top and bottom cells allow independent

operation of the two cells meaning that this structure is not subject to the constant series current constraint which applies to two terminal tandems. The maximum efficiency of the 3T tandem is the straight sum of the efficiency of both subcells operating independently at their maximum power voltages.

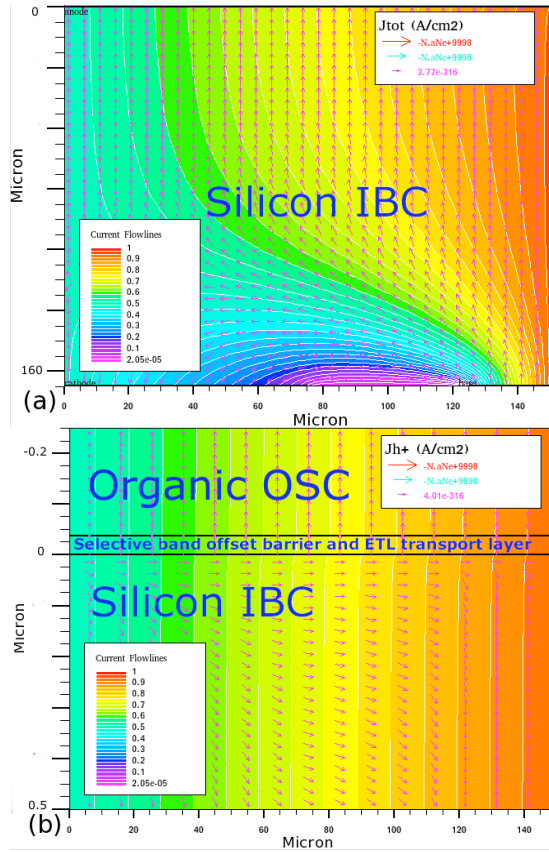


Figure 5 Numerical simulation of current flows at maximum power point showing (a) current flows in the Si-IBC between interdigitated contacts, and towards the organic cell and (b) showing hole currents only, such that the blocking behaviour of the band offset barrier can be seen.

3 CELL PERFORMANCE MODELLING

The three terminal organic / silicon tandem structure described in section 2 has been simulated with Silvaco ATLAS [11]. The current-voltage curves are simulated separately as validated by previous studies [12].

Figure 5 shows current flows in the structure at the maximum power point. Figure 5a shows current flow between the Si-IBC subcell interdigitated back contacts, and current flow into the top front surface anode. Figure 5b presents a close-up on hole transport at the front of the device, showing the organic subcell in its entirety and the top of the Si-IBC. One can see the blocking behaviour of the selective band offset barrier, such that holes in the Si-Si-IBC are blocked from flowing to the organic top cell, while organic subcell holes flow to the front surface p-type contact.

The resulting cell performance in figure 6 shows the independent power / efficiency curves of top and bottom OSC and Si-IBCs. The tandem efficiency is, in this case, 22%, which is the sum of OSC and Si-IBC subcell

efficiencies. We note that there is much potential for improvement, given that the radiative limit for these materials, as we have seen earlier, is close to 42%.

On a practical level, the route to increasing this 22% efficiency starts with the organic cell. The efficiency we have evaluated with a planar heterostructure and materials parameters taken from the literature is 14%. This is far from the best OSC results in the literature which as we have seen have achieved over 20% efficiency albeit for lower bandgap materials. The next steps are therefore optimisation of the OSC which will benefit from less stringent constraints on OSC bandgap.

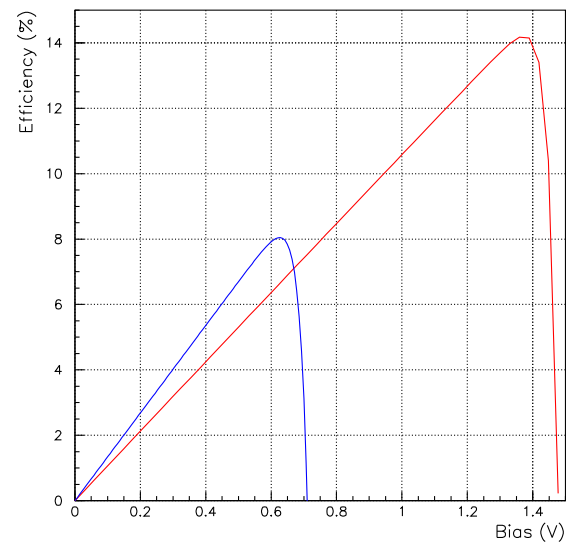


Figure 6 Performance of organic top (red) and bottom silicon (blue) cells, presented as power output relative to incident AM1.5G power, that is, subcell efficiency as a function of applied bias. The total power of the tandem is the sum of power output of each subcell.

4 CONCLUSIONS

We have presented the principles of operation of a novel tandem device, which is the three terminal selective band offset barrier tandem, based on organic and silicon materials. The performance of this device being significantly less sensitive to subcell bandgaps, the range of organic materials that can be adapted is broader. Preliminary evaluation of achievable efficiencies, using state of the art but untextured Si bottom cells, coupled with the highest efficiency organic cells but using high bandgap embodiments of donor and acceptor materials, yields a realistic efficiency potential in the short term of 22%. This being well below the radiative limit of 42.2% for these bandgaps, there remains much potential for subsequent increases in efficiency by optimising the high bandgap OSC.

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