Multiscale design of perovskite on silicon band offset barrier tandem solar cells

J. P. Connolly[1,2a], José Alvarez[1,2], Koffi Ahanogbe[1,2], Jean-Paul Kleider[1,2], Hiroyuki Kanda[3], Mohammad Khaja Nazeeruddin[3], Valentin Mihailetchi[4], Philippe Baranek[5,6], Philip Schulz[6,7], Malte Vogt[8], Rudi Santbergen[8], O. Isabella[8]

[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] *Group for Molecular Engineering of Functional Materials, Department of Chemistry and Chemical Engineering, Swiss Federal Institute of Technology, CH-1951 Sion, Switzerland*
[4] *ISC Konstanz e.V., Rudolf-Diesel-Straße 15, Konstanz 78467, Germany*
[5] *EDF R&D, Dept. EFESE, EDF Lab Paris-Saclay, 7 boulevard Gaspard Monge, 91120 Palaiseau, France*
[6] *IPVF, Institut Photovoltaïque d'Île-de-France, 30 route Départementale 128, 91120 Palaiseau, France*
[7] *CNRS, IPVF, UMR 9006, 30 route Départementale 128, 91120 Palaiseau, France*
[8] *Delft University of Technology, PVMD Group, Mekelweg 4, 2628 CD Delft, The Netherlands*

[(a)]*Correspondence: james.connolly@geeps.centralesupelec.fr tel. +33 783 03 92 70*

Abstract

A rare occurrence in the field of photovoltaics is the emergence of a new concept, an example of which is the three terminal (3T) Selective Band Offset Barrier solar cell (3T-SBOB [1] figure 1). The novelty of the device is delivering tandem efficiencies by preventing the transport of one carrier (holes or electrons) from one tandem sub-cell to the other (figure 2). This yields independent quasi-Fermi level separations, and therefore tandem solar cell efficiencies (figures 3 and 4).
The main advantages of this novel concept are, first, the lack of an intermediate conduction layer between sub-cells as required in 3T and 4T cells, second, the lack of a tunnel junction as required for 2T cells, and finally, the elimination of the 2T cell constant series current constraint.
This paper presents materials design principles for 3T-SBOB operation. Following these physical requirements, multiscale progress in full 3T-SBOB structure design on materials, electronic, and optical fronts for prototype designs is presented. The tandem structures considered are a silicon interdigitated back contact (IBC) bottom solar cell [2], an SBOB layer, and finally a perovskite (PSC) top cell.
The multiscale elements of this design work range from modelling at three scales. The first is two-dimensional device scale modelling using Silvaco software. The second scale consists of integrated materials properties modelling, which are developed and where possible validated by experimental data. A third scale is optical modelling complementing the electrical and materials modelling.
The structures considered are non optimum, consisting of the first materials envisaged at the design demonstration stage. As such, the IBC structure is a non-optimum untextured planar n-type design. The PSC structure is a simple three-layer design with PTAA [4] hole transport, a methylammonium lead triiodide (MAPI) perovskite absorber, and a SnO_2 [5] electron transport layer contacting the IBC.
The work presented consists of IBCs with planar front surfaces in order to focus on materials and optical properties, and validation of materials properties obtained from DFT modelling, yields the optimisation of the multilayer stack optical properties. This lays the foundations of multiscale optimisation of the 3T-SBOB device from electronic, optical, and materials perspectives.
Following this methodology, shortcomings of the prototype structure are identified, and routes towards optimised materials and structures proposed as evaluted within the H2020 Solar-ERANET project BOBTANDEM [6].

References

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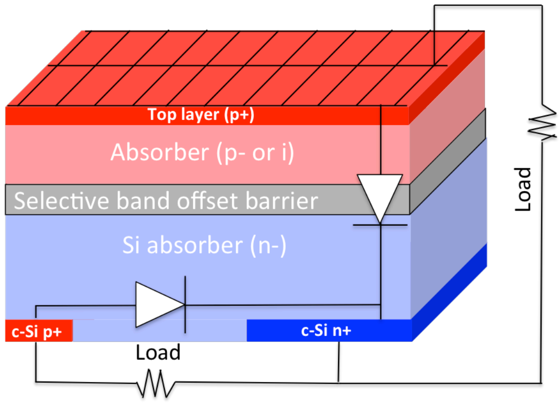

Figure 1 Three terminal band offset barrier tandem solar layer (3T-SBOB). The absorber in this work is perovskite.

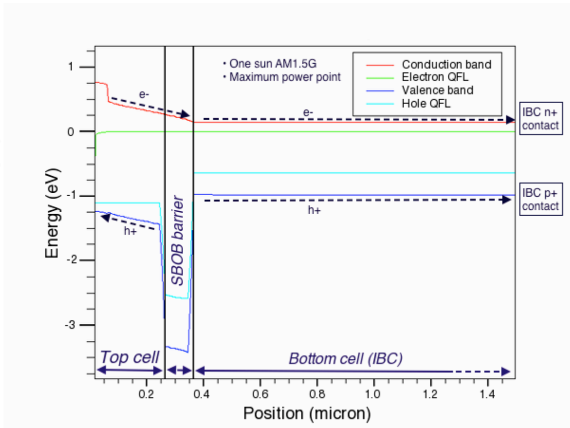

Figure 2 Numerical simulation of the band structure of the spectrum 3T-SBOB device under one sun illumination. The band offset in the valence band prevents hole transport. Independent quasi-Fermi level separations form in the top and bottom cells.

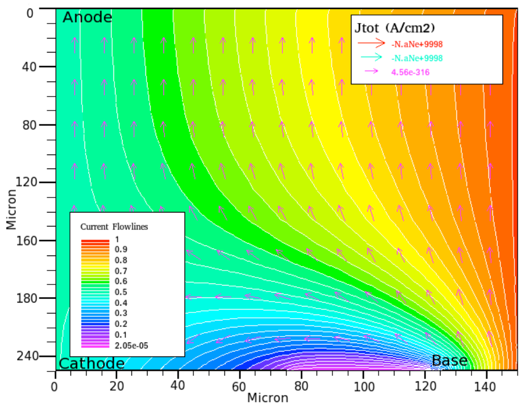

Figure 3 Current flow lines over the device for a thick IBC. The PSC is not resolved at this scale.

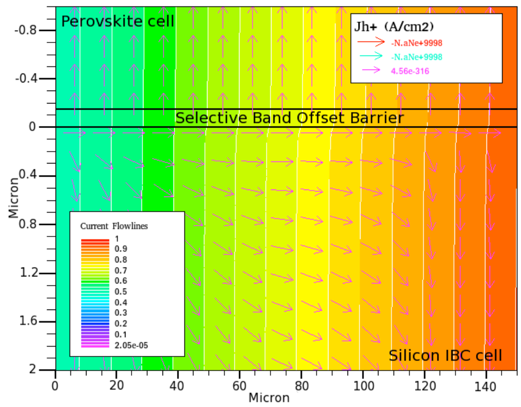

Figure 4 A zoom showing only the hole current flowlines over the top section of the 3T-SBOB. The IBC holes are seen to be repelled by the SBOB. Holes in the top cell are collected at the front contact.