Halide Perovskite Solar Cell Efficiency Improvements: New Device Type Simulation

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ABSTRACT

Trihalide perovskite photovoltaic (P-PV) solar cells have a promise to be connected into tandems with inorganic PV systems. In this paper, we present p-i-n GaAs & P-PV cells in either in a series way or parallel connection. Comparisons made for two types of tandems by a non-monolithic connection of two experimental sub-cells and results are being discussed based on simulation analysis. It is shown that the parallel connection is always preferable when the sub-cells photocurrent is not balanced while V_{oc} (open circuit voltage) is close to each other. Total efficiency over 20% is demonstrated for GaAs shading effect by MAPbI_{3} (methylammonium lead halide) film, with achieved J_{sc} - 41 mA/cm^{2} (short circuit current density) and high V_{oc}.

INTRODUCTION

Perovskite-based photovoltaics, that recently has created a fastest growing solar cell efficiency curve in the photovoltaics history, need improving [1]. Recently the new route has been suggested via the lead acetate precursor [2] which allows one to obtain the organic transport layer based planar PERO-PV with very high J_{sc} and the record efficiency ~18% for stable devices. Among the new perspective which developing of P-PV have opened, the most exact (including flexible, semitransparent design) is probably the promise to create high-efficiency tandems with the conventional inorganic solar cell are Si, CIGS, CdTe devices [3-5]. Although the sizable efficiencies achieved the photocurrent are quite modest (up to 26 mA/cm^{2}) [6] and the fundamental achievement for lower J_{sc} is the limiter thesis that in-series connection has - since it requires the balanced currents in two sub-cells. In-series tandem generates the minimal current of the sub-cell with lowest J_{sc} (short circuit current). In this paper, the motivation is to demonstrate that high-quality perovskite based-photovoltaics can be used to create high current tandems even with inorganic PV. For such
inorganic sub-cell, we have chosen p-i-n GaAs diodes, which are usually used as sensitive photodetectors due to their high charge carrier’s mobility and sample design. It is known that the high-efficiency PV device requires the GaAs/AlGaAs heterojunction that has large $\eta \sim 25\%$, due to the better charge separation at the heterojunction. But our goal is to demonstrate that even using simple p-i-n GaAs diodes the parallel tandem can be created with high photocurrents $\sim 40 \text{ mA/cm}^2$. It has been created for these two sub-cells: perovskite sub-cell that shows $J_{sc} \sim 22-23 \text{ mA/cm}^2$, $V_{oc} \sim 0.75 \text{ V}$, power conversion efficiency (PCE) 13.7 % and GaAs cell with $J_{sc} \sim 20 \text{ mA/cm}^2$, and $V_{oc} \sim 0.75 \text{ V}$. The two non-mono lithic connections are tested by traditional in-series connection, when GaAs is shadowed by the perovskite sub-cell film placed on it, and the parallel one.

**EXPERIMENTAL PART**

Figure 1 shows the tandem device front view, where perovskite sub-cell is installed directly on the top of GaAs sub-cell. The sub-cell positioning was made in shading configuration without taking into account the back perovskite electrode. The tandem connection was done with a combining of cathodes for negative charge accumulation in parallel mode as it presented in Figure 2 (in short circuit regime) in band diagram schematics. The in-series connection was done with combining of positive GaAs electrode and negative perovskite cathode (bias was applied to GaAs cathode and perovskite anode respectively).

The structure was grown by chloride vapor phase epitaxy (system Ga-AsCl$_3$-$\text{H}_2$) on the two-inch GaAs substrates with 400 micron-thickness and Si-doped to $2 \cdot 10^{18} \text{ cm}^{-3}$ level. Transitional buffer layer with 4 microns thickness was grown on the substrate and doped with sulfur to a concentration of $7 \cdot 10^{17} \text{ cm}^{-3}$ to reduce the influence of defects. Over the buffer, GaAs working layer was grown by chloride epitaxy high-purity film with resulting 5-micron thickness with background concentration on the level at $3 \cdot 10^{11} \text{ cm}^{-3}$. Perovskite sub-cell was created on ITO ($\text{In}_2\text{O}_3$: Sn) coated glass worked as a transparent electrode in the next order: hole transporting layer (30 nm thickness) PEDOT:PSS (poly(3,4-ethylenedioxythiophene) polystyrene sulfonate), absorbing film (450 nm) - MAPbI$_3$; electron transport layer (30 nm) - C$_{60}$ all films were deposited with spin coating method. Finally, a silver cathode with 100 nm thickness was deposited by thermal evaporation at $2 \times 10^{-6} \text{ Torr}$ pressure.

I-V performance measurements were done at standard 1.5 AM G spectrum of incident light ($100 \text{ mW/cm}^2$) with aperture mask usage (1 mm$^2$) to balance current densities of sub-cells. The tandem device in-parallel and in-series connection was investigated for I-V with Keithley 2400 SMU using Thermo Oriel ABA solar simulator and QE X6 system for external quantum efficiency measuring.

We used single diode model equations for tandem operation simulation. Output parameters, such as $R_{\text{Series}}$ (series resistance), $R_{\text{shunt}}$ (shunting resistance), $n$ (non-ideality factor), $J_0$ (dark saturation current density) were used for fitting of experimental and simulated curves and then a calculation and simulation for tandem I-V characteristics. For tandem operation regimes GaAs and perovskite sub-cells were connected in parallel and in-series, respectively (see Figures 3 a, b). GaAs sub-cell is showed as an equivalent circuit of diode (representing p-i-n structure); $I_{ph1}$ (representing GaAs sub-cell photocurrent); $R_{sh1}$
(representing shunt resistance of GaAs diode) and Rs1 (representing series resistance of GaAs sub-cell contacts with electrodes), while perovskite sub-cell is showed as equivalent circuit of diode (representing PEDOT:PSS–MAPbI$_3$–C$_{60}$ heterostructure); Iph2 (representing perovskite sub-cell photocurrent); Rsh2 (representing shunt resistance of perovskite cell heterostucture) and Rs1 (representing series resistance of perovskite sub-cell contacts with electrodes).

Figure 1. Tandem device schematics.
Figure 2. Tandem device sketch band diagram.
RESULTS

The cells connection can be either in-parallel or in-series. It is important to understand how the parameters and characteristics of individual structures influence the characteristics and efficiency of the tandem. Basic equation (1) for parameters calculation with later their comparing with experimental data was used:

\[
J = J_0 \left\{ \exp \left[ \frac{q(U - J \cdot R_{\text{in ser.}})}{n \cdot k \cdot T} \right] - 1 \right\} + \frac{U - J \cdot R_{\text{in ser.}}}{R_{\text{shunt}}} - J_{\text{ph}},
\]

where \( J \) - the current through the photostructure, A;
\( U \) - the voltage applied to the structure, V;
\( J_{\text{ph}} \) – the photocurrent, A;
\( n \) - the nonideality coefficient;
\( k \) - the Boltzmann constant, \( J / K \);
\( T \) – the temperature, K;
\( R_{\text{in ser.}} \) – the series resistance, Ohm;
\( R_{\text{shunt}} \) – the shunt resistance, Ohm.

Formula (1) describes the electrical model of the photodiode structure for a single diode. In the work, both structures for photovoltaic cells and structures with in-parallel and in-series connection were considered. The total current-voltage characteristic for a tandem structure can be described using the same expression. In this case, one of the aims in this work was to determine dependence between the characteristics (parameters) of the structure included in the tandem in-parallel or in-series, and of the individual structures included in the tandem.

In this work, the aim is to find trends for different tandem configurations using high – current sub-cells, based on GaAs p-i-n detector structure and CH\(_3\)NH\(_3\)PbI\(_3\) perovskite. So for
output parameters extraction, we simplified the calculation route to single diode model (see Figure 4).

In-parallel connection with unbalanced sub-cells, we have no such current loss because shunt and series resistances can be leveled in parallel circuit with the current sum, that’s why tandem operation tends to be closer for better sub-cell. Of course, this way has advantages only when $V_{oc}$ of sub-cells has similar value, in the opposite situation they can cut the power of tandem with the mismatch of current generation direction [6].

Analyzing the results of this work, it should be noted that GaAs and perovskite technologies are the most effective and promising at the moment for applications in their areas – substrate and solid-state technology, thin-film technology of organometallic semiconductors. The main advantage of this device is the high photocurrent production, which allows us to obtain high power. Therefore, in this paper, we have developed a tandem in a parallel, non-monolithic connection showing a high short-circuit current from a square centimeter 39 mA and obtained an efficiency of about 19%. The approach presented in this paper clearly shows the advantages of parallel tandems over in-serious ones with appropriate balancing the output characteristics: the filling factor and the idling voltage.

Band gaps for the sub-cells are 1.42 eV for GaAs and 1.58 eV for perovskite. Such difference - 0.16 eV gave a spectral window for GaAs sub-cell. It means that GaAs sub-cell will absorb light remained from perovskite in 420-760 nm region, mostly after 600 nm. Moreover, the near infra-red spectral window is fully absorbed by GaAs sub-cell, mostly contributing to sub-cells tandem operation.
CONCLUSIONS

In this work, we developed a tandem in-parallel, non-monolithic connection showing a high short-circuit current ~ 39 mA/cm² and obtained an efficiency ~19 %. Typical tandem devices today are mainly represented by various modifications of silicon-based solar cells with in-series connected elements for other types that need current balancing, which significantly reduces efficiency since each current of the sub-cells is usually much lower than in devices for this type in a single performance. The approach presented in this paper clearly shows the advantages of parallel tandems over successive ones with appropriate balancing of the output characteristics of the filling factor and the open circuit voltage. As shown by the experimental results, the parallel connection of GaAs and perovskite solar cells has an advantage over more than 5-7 % in-series connection even with a small perovskite spectral window for GaAs (about 100 nm in the long wavelength region). At the same time, the calculation using a simplified single diode model allows us to assume that it not only has an advantage in the sum of sub-cell currents but also eliminates shunt leaks and possible imbalance of the tandem in the filling factor. We see that the offered 4 electrode tandem concept development in the gradual integration of a monolithic connection and spectral separation opens wide possibilities for optoelectronic modifications of the perovskite bandgap to achieve record efficiency more than 25 %. Besides the quantitatively high output performance, the main result of this work is that the efficiency of more than 17-19 % in various configurations is a demonstration of the parallel architectures potential, which has obvious advantages in the operation of the device over in-serious tandems.

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