Analysis and optimization of perovskite-silicon tandem solar cells by full opto-electronic simulation

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***Abstract*—We present a comprehensive opto-electronic simulation framework for the computational analysis and optimization of perovskite-silicon tandem solar cells, consisting of a combination of a multiscale optical model for the simultaneous consideration of interference in thin coatings and scattering at textured interfaces with a mixed electronic-ionic drift-diffusion transport model that captures the peculiarities of the geometries and materials used in the tandem architecture.**

I. Introduction

Recently, the record photovoltaic performance of perovskite-silicon tandem solar cells of 29.15% [1] has surpassed the record efficiency of single junction devices made of silicon and equaled the global record efficiency for any single junction device established by Alta Device's thin film GaAs technology. However, there is still a substantial gap between the detailed balance efficiency limit based on optical simulations (>35%) and this realized record performance. While potentially avoidable optical losses are responsible for part of the difference, a significant source of performance overestimation is the use of idealized assumptions regarding the electrical properties, i.e., transport and recombination, in the detailed balance assessment of limiting efficiency. The aim of this contribution therefore is to present a tool for a more realistic performance assessment in the form of full opto-electronic device simulation of the entire tandem stack, including the interlayers connecting top and bottom sub-cells (recombination junction).

II. Approach

The optical component of the full model (Fig. 1) has been used successfully to identify high-efficiency designs for tandems with fully textured silicon heterojunction bottom cells [2], as realized in Ref. [3]. It consists of a transfer-matrix approach to compute the reflection and transmission of thin film components, a ray-tracer to evaluate the (angular) scattering properties of the textured interfaces, and a net-radiation algorithm that uses this information to quantity the light propagation in the entire layer stack. For the electrical model (Fig. 2), the standard drift-diffusion-Poisson simulation framework as implemented in Fluxim's device simulation software SETFOS is extended by drift-diffusion equations for mobile ions in the perovskite absorber, and by an integrated hopping model for charge transfer at hetero-interfaces [4]. Optical and electrical models are coupled in the standard way via the charge generation rate terms, and they are used together with an extended set of local and global optimization algorithms for the determination of the device configuration yielding the best performance.

While optical performance assessment and detailed balance approaches have been used since the early days of the research on perovskite-silicon tandem solar cells, the examples of full opto-electronic simulations are extremely scarce. To some extent, this is due to the required large number of material parameters that are not well known, especially in the case of the perovskite absorbers. However, we recently demonstrated that a consistent set of material parameters with a low degree of correlation can be obtained for perovskite materials by using the fitting of device characteristics from multiple experiments (steady-state, transient and frequency-domain) [5]. Nonetheless, the full opto-electronic optimization of perovskite-silicon tandem solar cells remains (numerically) challenging, due to the large disparity in layer thicknesses (from a few nm to hundreds of um), the large variation in charge carrier mobilities in the relevant case of silicon heterojunction bottom cells (from <1 $cm^2/(Vs)$ in a-Si:H to >1000 $cm^2/(Vs)$ in c-Si), the presence of mobile ions in the perovskite, the many hetero-interfaces with pronounced band offsets representing transport barriers, and the need to

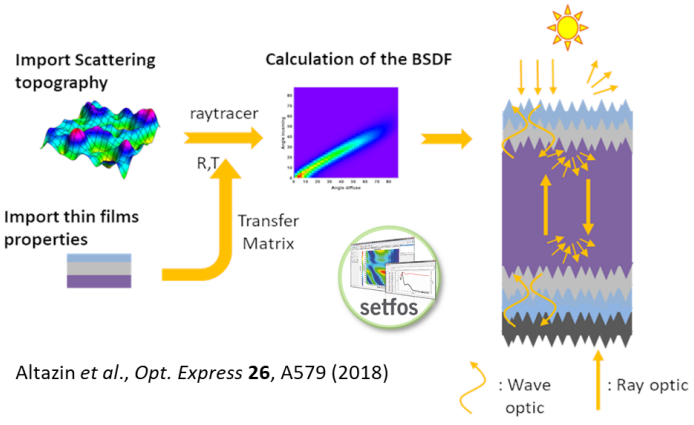

Fig. 1. Multiscale optical simulation approach based on the combination of transfer matrix simulations for coherent thin film components with ray-tracing treatment of light scattering at large-scale textures, as implemented in the device simulation software SETFOS.

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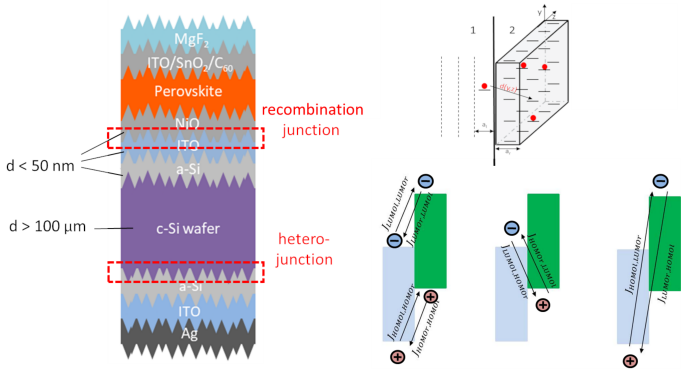

Fig. 2. Regarding the challenges for electrical simulation, the perovskite-silicon tandem device exhibits large disparity in the thickness of the component layers, and several hetero-interfaces, with either intra- or interband charge transfer. The latter is simulated here by an interface hopping model similar to the Miller-Abrahams theory for thermally activated transport.

describe charge transport across the recombination junction. The relevance of electrical optimization is demonstrated most impressively by the latest performance improvements in an architecture with rear-textured-only silicon wafer [1] as compared to the optically superior fully textured design of Ref. [3]. Indeed, while optical simulations supports the optimization of J_{SC}, electrical simulation allows for the optimization of device performance at maximum power point, i.e., under consideration of the recombination losses under operation, using directly the extracted electrical power density as the optimization target.

III. Results

Figure 3 shows the layer stack, energy levels and short-circuit current profile of the combined tandem device; note that for the SHJ bottom cell, the TCO-p contact is not simulated explicitly via a hopping interface, but the bottom ITO layer is directly used as the electrode in the electrical simulation. The additional interfaces at both sides of the silicon wafer are for the definition of light scattering due to the surface texture. Due to the current conservation inherent to the solution of the charge continuity equations, current matching is automatically enforced. Unbalanced optical generation therefore leads to increased recombination at steady-state operation. The current voltage characteristics for the planar single junction sub-cells and for an optically optimized (planar) tandem device are shown in Fig. 4(a). Interestingly, the current of the filtered SHJ device is lower than that of the perovskite subcell in tandem configuration (dashed lines), indicating additional recombination losses as compared to the single junction configuration. On the other hand, the voltage of the subcells adds nicely, demonstrating the efficient operation of the recombination junction modelled via the hopping interface. This is also apparent from the alignment of the quasi-Fermi levels at the recombination junction [Fig. 4(b)], i.e., the absence of a voltage drop. The efficiency for the opto-electronically optimized tandem structure is found to be slightly larger than that for the optically optimized device, and peaks at a lower perovskite thickness, which reduces recombination losses of photocurrent.

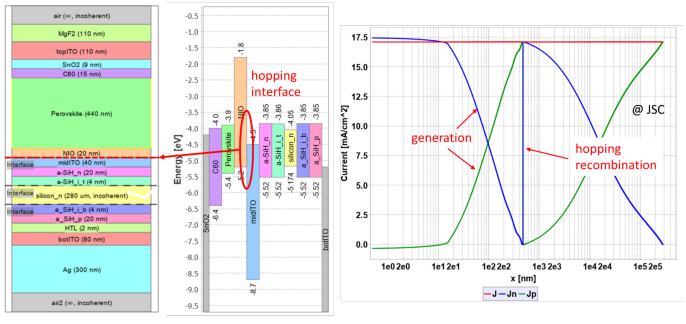

Fig. 3. Layer stack, energy levels and short circuit current profile of the perovskite-silicon tandem solar cell. The current profile (log x-axis) reflects photocurrent generation and inter-band transfer at the recombination junction.

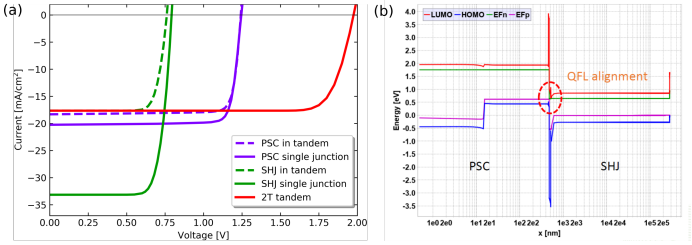

Fig. 4. (a) Current-voltage characteristics from full opto-electronic simulations of perovskite (PSC) top- and silicon heterojunction (SHJ) bottom cells in single junction configuration, as well as of the corresponding tandem device. (b) Band profile (log scale position axis) at MPP exhibiting the absence of a voltage drop at the recombination junction, which is reflected in the perfect alignment of electron and hole quasi-Fermi levels (QFL).

IV. Conclusions

We demonstrate the feasibility of and insight obtained from fully coupled opto-electronic device simulations of perovskite-silicon tandem solar cells, which enable device optimization at maximum power point directly.

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