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Modeling of optical losses in perovskite solar cells

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ABSTRACT

The optical losses within the structure of hybrid *perovskite* solar cells are investigated using only the optical properties of each layer e.g. refractive index and extinction coefficient. This model allows calculating the transmission/reflection rates at the interfaces and absorption loss within any layer. Then, the short circuit current density and loss percentage are calculated versus the perovskite and TiO_2 thicknesses from 50 nm to 150 nm. To make our calculations closer to reality, we extracted the optical properties of each device component from the literature reports on glass/TCO/TiO_2/perovskite/metal. The simulations were fitted with the experimental results of some relevant references. Our simulations show that ITO transmits the light better than SnO_2 as the TCO front electrode, and the light reflection at both sides of the perovskite layer, e.g. at TiO_2/perovskite and perovskite/Spiro-OMeTAD, is lower than 25%. The light interference and multiple reflections have been accounted in our calculations and finally we showed that a thicker TiO_2 and perovskite cause more optical loss in current density due to stronger absorption.

1. Introduction

The optical and electrical properties of hybrid organic/inorganic methylammonium lead iodide $CH_3NH_3PbI_3$ perovskite solar cells have been extensively studied in the last recent years [1,2]. Many research groups are now investigating these materials applications in solar cells. The main issues are with materials engineering to find a proper partner for perovskite layer [3], performance enhancement [4], and stability over time of such devices [5]. Perovskites have a proper energy bandgap, are simple to deposit, strong light absorption, low defect activity, and good carrier mobilities. However, they suffer from moisture sensitivity and instability decomposition under either high temperatures, high-intensity, and have finite mobility, and Pb toxicity. Modeling the device physics of such devices are extremely required for refining the device design and obtaining an insight into recombination/generation and carrier collection mechanism. However, this is not easy since the perovskites behave odd and unknown and it seems a specific device physics runs the photo-absorption and photo-generation. To avoid dealing with the complicated recombination mechanisms, an optical approach is used which considers only the absorption coefficient, α, refractive index, n and extinction coefficient, κ of any device component and their relation to device parameters e.g. the short circuit current density, J_{sc} [6,7]. This relation is via the Transmission/Reflection rates (T & R). We have recently developed such an approach for modeling the optical losses in CdTe and CIGS devices with a graphene electrode [8,9] and will apply this model to hybrid planar perovskite-based solar cells using the optical data given in literature especially in

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Ref. [10]. There are only a few publications in the literature on the optical modeling of perovskite solar cells [11–13]. They all developed a rigorous theoretical model based on the transfer matrix formalism which allows us to calculate the electric field intensity within each device component. However, we used a quite simpler model which does not require a rigorous modeling and computing calculation but can also calculate the reflection and transmission of the light from every interface in the device and the light absorption in any layer.

2. Modeling approach

The schematic structure of a perovskite solar cell and the optical constants of every layer have been presented in Fig. 1a and Fig. 1b and c, respectively. The heterostructure is made of glass/TCO/TiO_2/Perovskite/HTM/back-contact where HTM is Spiro-OMeTAD and the back contact can be Au, C or any metallic alloy [14,15]. The values of n and κ were taken within $\lambda = 150–1000$ nm from the relevant references e.g. for TCO/ITO from Refs. [9], for TiO_2 from Refs. [7], for perovskite from Ref. [10] and for HTM layer from Refs. [16,17], respectively. n varies slowly for a wide range of wavelengths and κ changes significantly only within a small range and ends to zero for longer λ almost for all the layers. The perovskite layer shows extinction coefficient peaks at 350–730 nm with κ values of 0.5–1.7 respectively, and the refractive index is $\geq$2.5 in the visible to near-infrared wavelength range in agreement with data presented in Ref. [18]. The κ values of the perovskite are slightly higher than those of inorganic materials such as CIGS, GaAs and CdTe in the wavelength range of 450 nm–750 nm. The perovskite layer exhibits a lower refractive index than that of CIGS, GaAs and CdTe, which will result in lower reflection at the perovskite interfaces and thus a higher absorption in the respective layer and higher J_{sc} values. Ziang et al., demonstrated that $n(\lambda)$ for CH3NH3PbI3 materials is a little smaller than, but very close to that of GaAs and much larger than that of c-Si in all wavelengths [19]. The thickness of the TiO2, perovskite, and HTM layers are quite thinner than the one of Si and chalcogenide materials too (nm versus μm). Therefore, optimized optical losses will assist in increasing the J_{sc} and reducing the recombination, reflection and absorption rates within the device components and at the interfaces. The device parameters of a few perovskite-based devices reported in literature such as the ones given in Ref. [15] are used in our simulations and are compared with our modeling results. The input data of our modeling are the thickness and the experimentally derived complex refractive index spectra for each layer. For the present report, we have analyzed the simple pin planar heterojunction stack although in principle the method and data could be used as a building block for the analysis of the many structures variation currently being explored in perovskite solar cells including mesoporous architectures, by employing an effective medium approximation.

To calculate J_{sc}, and ΔJ_{sc}, (due to light reflection and absorption in every layer before the light being absorbed in perovskite layer), the reader is referenced to our recently published papers [7–9]. The modeling approach is identical to previous ones. However, we briefly describe it here. First we obtain the Reflection, R_{12} from the interface of two different materials n_1 and n_2 [9]. This coefficient calculation maybe different if one of the two layers cause interference in light reflection [9,20]. In our case, the reflection coefficient at TiO_2/perovskite and perovskite/HTM was calculated using,

$$R_{45,56}(\lambda) = \frac{r_1^2 + r_2^2 + 2r_1 r_2 \cos(2\beta(\lambda))}{1 + r_1^2 + r_2^2 + 2r_1 r_2 \cos(2\beta(\lambda))} \tag{1}$$

where $r_{1,2}$ are reflection coefficients at both perovskite sides by β is given by $\beta(\lambda) = 2\pi\, n d_G/\lambda$ where n and d are the perovskite layer's refractive index and thickness, respectively. The reflection coefficient at the other interfaces are obtained normally. In addition of the reflection, the photoabsorption cause a loss in TiO_2 and HTM layers. The total transmission rate, T, is obtained using: $T(\lambda) = \sum_{i=1:5}^{j=2:6}(1 - R_{ij}) \times \exp(-\alpha_i \cdot d_i)$. This means that the transmission rate, T(λ), includes both reflection (at 12, 23, 34, 45, 56) and absorption in previous layers with the absorption coefficient given by $\alpha(\lambda) = \frac{4\pi}{\lambda}\kappa(\lambda)$. This allows calculation of J_{sc}

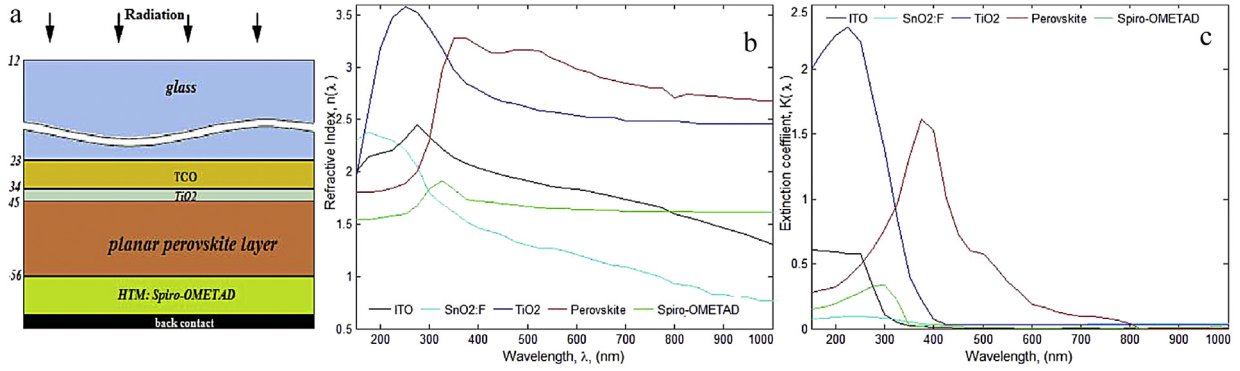

Fig. 1. a. schematic structure of a perovskite solar cell, b. refractive index and, c. extinction coefficient of every layer.