Perovskite solar cell stability enhancement using rGO interlayer: Opto–electro–thermal modeling

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***Abstract*—This study examines the effects of adding reduced graphene oxide (rGO) layer on the opto–electro–thermal properties of $MAPbI_3$-based perovskite solar cells (PSCs). The absorber and hole transport layers are separated by a rGO interlayer that is 5, 10, and 15 nm thick. Devices' peak temperatures are reduced when rGO is added as an interlayer to PSCs. The results show that rGO improves PSC thermal performance by lowering the maximum device temperature while slightly decreasing the power conversion efficiency (PCE). It should be mentioned that based on electro-thermal coupling results, the structure containing rGO with 10 nm thickness has the lowest PCE loss percentage (4%), that is even lower than the structure without rGO (4.48%). Therefore, the proposed structure with a 10 nm thick rGO interlayer is presented as the best option in order to achieve the lowest percentage loss in PCE. This study demonstrates how rGO can be used as a useful heat management solution to increase perovskite photovoltaics device stability.**

***Index Terms*—perovskite solar cell, opto–electro–thermal properties, reduced graphene oxide.**

I. Introduction

Single-junction perovskite solar cells (PSCs) have received attention due to their high power conversion efficiency (PCE), low fabrication cost, and simple fabrication processing [1]. However, concerns such as long-term stability still exist. Among them, thermal stability is particularly important, since these structures are more sensitive to heat. In this study, we investigate for the first time the impacts of reduced graphene oxide (rGO) as an interlayer between the absorber and hole transport layers on the opto-electro-thermal properties of a PSC as a beneficial thermal management strategy to boost device stability.

II. Theory and Modeling

In this study, a 3D numerical modeling of a PSC incorporating the rGO interlayer is performed using the finite element method (FEM). The schematic of the proposed PSC structure and the alignment of the energy level between layers are shown in Fig. 1.

The electromagnetic field (**E**) is obtained by solving the Helmholtz equation [2]:

$$\nabla \times (\nabla \times \mathbf{E}) - k_0^2 (n(\lambda) - ik(\lambda))^2 \mathbf{E} = 0 \tag{1}$$

The standard AM1.5G solar spectrum is considered the illumination input. After computing the distribution of **E**, the total photogeneration rate could be obtained as follows [2]:

$$G_{tot}(x,y,z) = \int_{300}^{1050} \pi \epsilon'' E^2(x,y,z,\lambda)/h \ \ d\lambda \tag{2}$$

In PSCs, the current density-voltage (J–V) characteristics are computed by solving the Poisson, continuity, and drift-diffusion equations using the $G_{tot}(x,y,z)$ [2]. The J-V curve gives the photovoltaic parameters, which include the open-circuit voltage (V_{oc}), the short-circuit current density (J_{sc}), the fill factor (FF), and PCE [2].

$$PCE = (FF\, J_{sc}\, V_{oc})/P_{in}; FF = (V_{mp}\, J_{mp})/(V_{oc}\, J_{sc}) \tag{3}$$

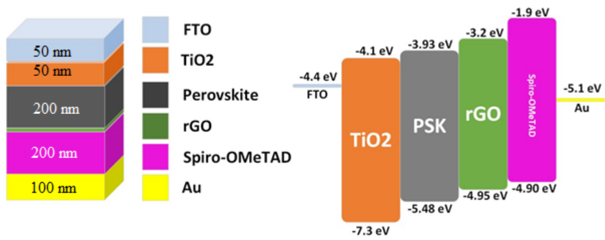

Fig. 1. A 3D schematic of proposed structure and energy level alignment.

In the final step, the carrier thermodynamic equations and simultaneous heat generation are solved. To calculate the heat distribution and thermal profile, the thermal conductivity (k), the heat capacity (C), and the heat transfer coefficient (h) of each layer are considered. The heat transfer equation is defined as follows [3]:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q \tag{4}$$

Here, T represents the material temperature, ρ is the density, C_p is the specific heat capacity, and Q includes heat sources such as joule heating and non-radiative recombination. The calculated temperature distribution is then applied to the semiconductor interfaces as the material temperature for further electrical property simulations [3].

III. RESULTS AND DISCUSSION

The thermal envelope results are shown in Figure 2 for the reference structure (without rGO) and the proposed structure (with rGO interlayers of various thicknesses). The reference structure's maximum temperature is 315.87 $^\circ K$, as shown in Fig. 2. The temperature drops to 313.32, 313.05, and 312.68 $^\circ K$ for the structure with rGO interlayer thicknesses of 5, 10, and 15 nm, respectively. Therefore, maximum temperature decreases by 2.55, 2.82, and 3.19 $^\circ K$, respectively. Also, thermal performance (relative temperature reduction percentage) increases by 0.81, 0.89, and 1.01 %, respectively.

Figure 3 shows how rGO affects electrical performance using J-V curve analysis. The parameters ($J_{sc}(mAcm^{-2})$, $V_{oc}(V)$, $FF(\%)$, $PCE(\%)$) for the reference structure are (22.76, 0.93, 82.23, 17.42) for the initial value with T=293 $^\circ K$ and (22.76, 0.90, 80.78, 16.64) for the coupled thermal effects. Therefore, photovoltaic parameters are decreased by (0, 3.23, 1.76, 4.48)% due to heat impacts. In proposed structure, when the thickness of the rGO interlayer are (5, 10, 15) nm, V_{oc} (FF) decreases due to heat impacts from its initial value of (0.936 (81.89), 0.925 (84.42), 0.933 (82.04)) V (%) to (0.908 (80.58), 0.899 (79.87), 0.907 (81.00)) V (%), and the PCE decreases by (4.75, 4.00, 4.02)%, from (17.27, 17.00, 16.65)% to (16.45, 16.32, 15.98)%. The structure containing 10 nm of rGO as the interlayer has a PCE loss percentage of 4% that is even lower than the reference structure's (4.48%). Therefore, the addition of a 10 nm interlayer is the best option to obtain a structure with the lowest percentage reduction in PCE. Also, the addition of rGO is beneficial for reducing thermal losses

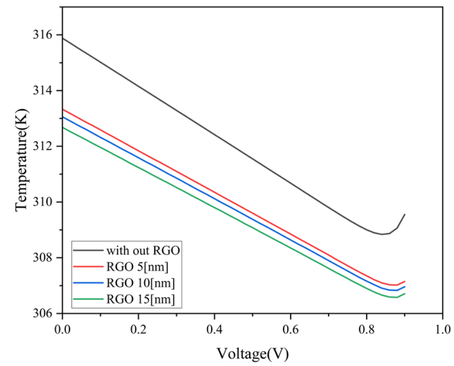

Fig. 2. Effect of rGO interlayer thickness on the T-V behavior of the PSC.

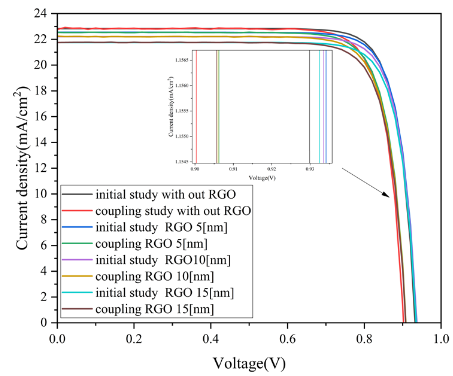

Fig. 3. J–V characteristics curve of PSCs without rGO and with different thicknesses of rGO interlayer under initial and thermally coupled conditions.

because high operating temperatures accelerate the perovskite absorber's degradation and negatively impact the long-term device stability.

IV. CONCLUSION

In this paper, the effects of the rGO interlayer on the opto-electro-thermal performance of $MAPbI_3$-based PSC were examined. According to the results of thermal simulations, the absorber layer's operating temperature was lowered when rGO was added as an interlayer to the PSCs. Furthermore, the electrical results demonstrated that rGO slightly reduced the electrical performance (PCE reduction) while increasing the thermal performance (temperature reduction). We demonstrated that adding a 10 nm rGO interlayer is the best option to create a structure with the lowest percentage loss in PCE (4%) with an improvement in thermal performance (0.89%).

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