



# Optical modeling of graphene contacted CdTe solar cells



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## ABSTRACT

For the first time, an optical model is applied on CdS/CdTe thin film solar cells with graphene front or back contact. Graphene is highly conductive and is as thin as a single atom which reduces the light reflection and absorption, and thus enhances the light transmission to CdTe layer for a wide range of wavelengths including IR. Graphene as front electrode of CdTe devices led to loss in short circuit current density of 10%  $\Delta J_{sc} \leq 15\%$  compared to the conventional electrodes of TCO and ITO at CdS thickness of  $d_{CdS} = 100$  nm. In addition, all the multilayer graphene electrodes with 2, 4, and 7 graphene layers led to  $J_{sc} \leq 20$  mA/cm<sup>2</sup>. Therefore, we conclude that a single monolayer graphene with hexagonal carbon network reduces optical losses and enhances the carrier collection measured as  $J_{sc}$ . In another structure design, we applied the optical model to graphene back contacted CdS/CdTe device. This scheme allows double side irradiation of the cell which is expected to enhance the  $J_{sc}$ . We obtained 16, 23, and 38 mA/cm<sup>2</sup> for back, front and bifacial illumination of graphene contacted CdTe cell with CdS = 100 nm. The bifacial irradiated cell, to be efficient, requires an ultrathin CdTe film with  $d_{CdTe} \leq 1$   $\mu$ m. In this case, the junction electric field extends to the back region and collects out the generated carriers efficiently. This was modelled by absorptivity rather than transmission rate and optical losses. Since the literature suggest that ZnO can increase the graphene conductivity and enhance the  $J_{sc}$ , we performed our simulations for a graphene/ZnO electrode (ZnO = 100 nm) instead of a single graphene layer.

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## 1. Introduction

Conductive electrodes used as the front and back contact in CdTe thin film solar cells are under extensive research [1]. Both electrodes require further optimization for enhancing the carrier collection and stability. The conventional Transparent conductive Oxide (TCO) materials suffer from low carrier mobility and the inefficient carrier collection as well as bandgap which is not sufficiently wide [2,3]. The conventional back contact materials, such as Cu/Au [4] cause performance degradation by migration to junction under stress conditions [5,6]. Graphene nanolayer can resolve all these issues by being highly conductive with an extremely high intrinsic carrier mobility (20000 cm<sup>2</sup>/V.s) and possessing a high/controllable work function ( $\geq 5$  eV). Graphene's continuous network of carbon honeycomb reduces the ion migration from the upper side of the CdTe layer to the CdS/CdTe junction through grain boundaries and therefore, the degradation sources are significantly

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surpassed [7,8]. The hybrid bonding of carbon atoms and CdTe surface is less damaged by thermal annealing, or metallic dopants as a favor to cell stability [9,10]. Nevertheless, such a hybrid interface between a nanolayer and a semiconductor plane material cannot be simulated by one dimensional modeling or simulators (i.e. AMPS-1D, SCAPS-1D) which solve the coupled current continuity equation and Poisson law. Alternatively, an optical approach allows modeling of short-circuit current density,  $J_{sc}$  and the optical loss effect (shown by  $\Delta J_{sc}$ ). The optical losses include light reflection at the interfaces, and absorption in the thickness of device components [11–13]. The optical approach was already introduced for regular CdTe thin film solar cell. Here we develop the same approach to the hybrid design of graphene front or back contacted CdTe devices (Fig. 1). The latter design (with graphene back contact) allows double side irradiation both from glass and transparent graphene layer. Graphene transparency is  $T_G \geq 90\%$  and is expected to improve  $J_{sc}$  significantly [3]. Note that the back side illumination seems to have a negligible effect in thin CdTe devices with a thickness of  $d_{CdTe} \geq 2 \mu\text{m}$  since the electric field at the back region is not strong to collect the carrier and the generated carriers face to surface recombination before being collected by the metallic contacts [14]. However, back side illumination might be considered about ultrathin films ( $d_{CdTe} \leq 1 \mu\text{m}$ ) where the depletion width extends from CdS/CdTe junction in the back region (CdTe/contact) and thus the extended electric field can collect the carriers from the whole CdTe layer [15]. The optical modeling is simple since it only requires optical constants of device components and graphene layer. We compare  $\Delta J_{sc}$  versus CdS thickness (which is the common layer in both designs) and then calculate how the back contact graphene improves the  $J_{sc}$  [16].

## 2. Modeling approach

The optical constants on the device components presented schematically in Fig. 1 were extracted from Refs. [11,13]. The value of refractive index,  $n$  and extinction coefficient,  $k$  within  $\lambda = 300\text{--}900 \text{ nm}$  for TCO, ITO were taken from Refs. [3,6] and from Refs. [17–19] for graphene monolayer/multilayer. Also the transmission rate of 1, 2, 4 and 7 layers of graphene were obtained from Ref. [3]. The refractive index is  $n^* = n - j\kappa$  and allows calculation of reflection coefficient,  $R$  of an interface of two different materials with refractive indices  $n_1$  and  $n_2$  [9],

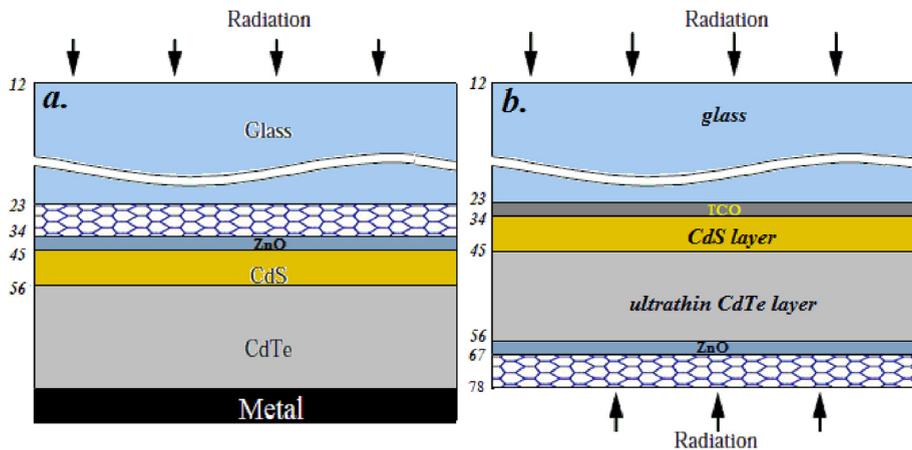
$$R^* = \left( \frac{n_1^* - n_2^*}{n_1^* + n_2^*} \right)^2 = \frac{(n_1 - n_2)^2 + (\kappa_1 - \kappa_2)^2}{(n_1 + n_2)^2 + (\kappa_1 + \kappa_2)^2} \tag{1}$$

The reflection at graphene interfaces,  $R_G$ , with other materials doesn't follow the above formula.  $R_G$  from interfaces of glass/graphene/ZnO and glass/graphene/CdS in Fig. 1a and from air/graphene/ZnO or air/graphene/CdS in Fig. 1b is given by Refs. [12,19],

$$R_G(\lambda) = \frac{r_1^2 + r_2^2 + 2r_1r_2\cos(2\beta(\lambda))}{1 + r_1^2 + r_2^2 + 2r_1r_2\cos(2\beta(\lambda))} \tag{2}$$

where  $r_{1,2}$  are reflection coefficients at both graphene interfaces and are similarly given by Eq. (1). For a graphene monolayer with  $d_G$  thickness,  $\beta$  is given by,

$$\beta(\lambda) = 2\pi n_G d_G / \lambda \tag{3}$$



**Fig. 1.** Schematic structures of thin film solar cells based on a. CdTe materials with graphene as transparent conductive electrode, and b. CIGS materials with graphene back contact. The graphene network was indicated in 2 dimensions just as to make it visible from the cross sectional view.

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