Modeling polycrystalline effects on the device characteristics of CdTe based solar cells

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INTRODUCTION

Polycrystalline CdTe based solar cells represents one of the most attractive options for low cost photovoltaic module production [1]. However various efforts to grow polycrystalline CdTe based solar cells resulted in lower efficiencies. This is due to the fact that the grain size associated with polycrystalline thin films affects not only carrier lifetime and grain boundary limited recombination velocity but also enhance interface recombination that deteriorates the device performance significantly [2]. Researchers have focused primarily on modeling single crystalline CdTe cells but no complete model is presented until now taking into consideration the polycrystalline effects on the device J-V characteristics and the external quantum efficiency (EQE) of CdTe based cells [3]. We have developed a comprehensive model to analyze the J-V characteristics and the external quantum efficiency of CdTe cells based on minority carrier drift and diffusion processes that takes into account the grain size distribution due to the effects of $CdCl_2$ annealing treatment at elevated temperatures thereby affecting the carrier lifetime, grain boundary limited recombination velocity and interface properties. The model has been thoroughly investigated and matched well with the published experimental data.

THEORY AND MODELING

The total photocurrent density over all the incident photon wavelengths λ of the solar spectra is first calculated using [4]

$$J_L(V) = \int_0^{\infty} [J_e(\lambda,V) + J_h(\lambda,V)]d\lambda \qquad (1)$$

where

$$J_e(\lambda,V) = \frac{qG(\lambda)W}{(\tau_e^{-1} + \alpha(\lambda)W)}\left[\frac{(1-e^{(-\alpha(\lambda)W)})}{\alpha(\lambda)W} - \tau_e\left(e^{(-\alpha(\lambda)W)} - e^{(-\alpha(\lambda)W)-\frac{1}{\tau_e}}\right)\right]$$

$$J_h(\lambda,V) = \frac{qG(\lambda)W}{(\tau_h^{-1} - \alpha(\lambda)W)}\left[\frac{(1-e^{(-\alpha(\lambda)W)})}{\alpha(\lambda)W} - \tau_h\left(1 - e^{-\frac{1}{\tau_h}}\right)\right]$$

W is the width of CdTe layer, $\alpha(\lambda)$ and $G(\lambda)$ represents the wavelength dependent CdTe absorption coefficient and the carrier generation rate. We have also taken into account the effective mobility due to grain boundary of the polycrystalline CdTe films that directly effects the voltage dependent normalized carrier lifetime τ and can be written as

$$1/\mu_{eff} = 1/\mu_{mono} + \mu_{gbl} \qquad (2)$$

where μ_{eff} is the effective carrier mobility dependent on single crystal mobility μ_{mono} and grain boundary limited mobility μ_{gbl} can be expressed as

$$\mu_{gbl} = \frac{q\tau_g}{m^*} \qquad (3)$$

where m^* is the effective carrier mass and τ_g is expressed in terms of intra grain diffusion length L and average thermal velocity of carriers v_t. The effective diffusion length is related to the grain size g by

$$L_{poly} = \frac{L}{\sqrt{1 + \frac{2S_{gbl}L^2}{Dg}}} \qquad (4)$$

where S_{gbl} is the grain boundary limited recombination velocity in the CdTe active layer, and D is the diffusion coefficient.

Further a detailed study to calculate the effects on varying interface recombination velocities and CdTe doping on the external quantum efficiency *(EQE)* of the solar cell has been done. The internal quantum efficiency *IQE(λ)* is expressed as

$$\mathrm{IQE}(\lambda) = \mathrm{IQE}_{\mathrm{SCR}}(\lambda) + \mathrm{IQE}_{\mathrm{QNR}}(\lambda) \qquad (5)$$

where the *IQE* within the space charge region (SCR) region can be calculated as

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$$IQE_{\text{SCR}}(\lambda) = \int_0^{x_1} \alpha e^{-\alpha x} e^{\left(\frac{W'}{\mu_{eff}\tau' E_0}\ln(1-\frac{x}{W'})\right)} dx \qquad (6)$$

where $x1$ (< W'), W' is the width of the SCR region and E_0 is the electric field at the junction *(x=0)*. The internal quantum efficiency in the quasi neutral region *(QNR)* is calculated as

$$IQE_{QNR}(\lambda) = \int_0^{\infty} \alpha e^{-\alpha(x_1+x)} e^{-x/L_{poly}} e^{\left(\frac{W'}{\mu_{eff}\tau' E_0}\ln(1-\frac{x_1}{W'})\right)} dx \qquad (7)$$

The external quantum efficiency of the device can be written as

$$EQE(\lambda) = e^{-\alpha_{CdS}(\lambda)d_{CdS}}[1-R(\lambda)](1+\frac{S_f}{\mu_{eff}E_0})^{-1} IQE(\lambda) \qquad (8)$$

where S_f is the front interface carrier recombination velocity.

RESULTS AND DISCUSSION

The J-V characteristics of the CdS/CdTe structure as shown in Fig. 1 has been solved by the iterative improvement method and is plotted in Fig 2. It is observed that with increase in grain size from ~2 µm to ~5 µm, the short circuit current density increases by ~2.5 mA/cm^2 and the overall cell efficiency increases by ~3.2% which demonstrates the significance of the annealing treatment. From the EQE plot in Fig 3, it is observed that varying the treatment process, the interface recombination velocity changes as well as the effective CdTe doping from ~10^{16} cm^{-3} to low ~10^{15} cm^{-3} due to interdiffusion of CdS/CdTe layers.

The results from this study allow us to accurately formulate polycrystalline behavior of CdTe solar cells and provide recommendations to optimally choose parameters for increasing the photovoltaic conversion efficiency.

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REFERENCES

[1] Farid, S., Mukherjee, S., Jung, H., Stroscio, M. A., & Dutta, M. (2015). Analysis on the structural, vibrational and defect states of chlorine treated polycrystalline cadmium telluride structures grown by e-beam evaporation. Materials Research Express, 2(2), 025007.

[2] Beach, J. D., & McCandless, B. E. (2007). Materials challenges for CdTe and CuInSe2 photovoltaics. MRS bulletin, 32(03), 225-229.

[3] Sen, S., Konkel, W. H., Tighe, S. J., Bland, L. G., Sharma, S. R., & Taylor, R. E. (1988). Crystal growth of large-area single-crystal CdTe and CdZnTe by the computer-controlled vertical modified-Bridgman process. Journal of Crystal Growth, 86(1), 111-117.

[4] Anjan, M. S., & Kabir, M. Z. (2011). Modeling of current–voltage characteristics of CdS/CdTe solar cells. physica status solidi (a), 208(8), 1813-1816.

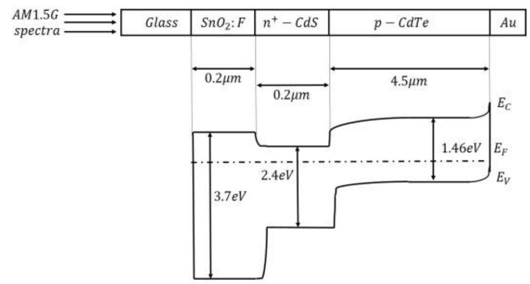

Fig. 1. Energy band diagram of CdS/CdTe solar cell.

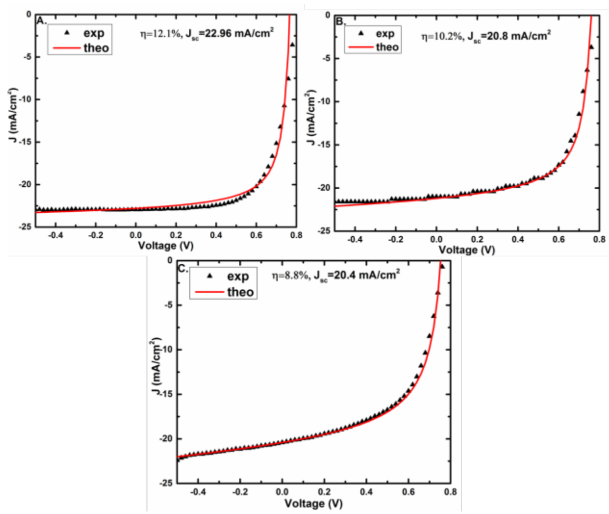

Fig. 2. Modeled J-V characteristics of CdTe/CdS cell with A) 12.2% efficiency, grain size ~ 5 µm, B) 10.2% efficiency, grain size ~ 2-3 µm, C) 8.8% efficiency, grain size g ~ 2-3 µm; dotted line shows experimental J-V data with varied annealing $CdCl_2$ treatments

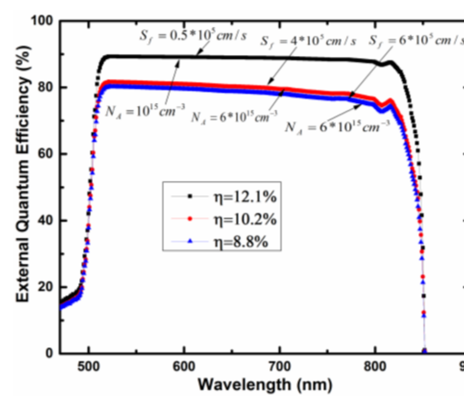

Fig. 3. External Quantum Efficiency for varied front interface recombination velocity (S_f) and effective CdTe doping (N_A).