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Current voltage characteristics modeling of polycrystalline CdTe-CdS solar cells for different grain-sizes of CdTe

Bahniman Ghosh, Bhuktare Swapnil, Priyesh Surana, M. W. Akram*

Department of Electrical Engineering, Indian Institute of Technology, Kanpur 208016, India

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Abstract

A model is developed to explain the current-voltage (J-V) characteristics of polycrystalline CdTe-CdS solar cells with different grain sizes of CdTe. Analytical expressions are derived for J-V characteristics by solving the continuity equation for electrons and holes using appropriate boundary conditions. The grain size (g) effect is taken into account via the parameters like mobility, diffusion length and life-time of carriers. The model developed is fitted with the experimental data and it shows a good agreement.

Keywords: modeling, drift-diffusion, thin film solar cells, polycrystalline, grain size.
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1. Introduction

Thin film solar cells, especially CdTe-CdS have been an active area of research because of their low cost and better efficiency. Various models have been proposed focusing on the different aspects of the cell like front region [1] , back contact[2] , carrier collection efficiency [3] etc. to explain the J-V characteristics. The present model focuses upon the grain size effect on the performance of the CdTe-CdS solar cells.

CdTe thin films are polycrystalline. The major drawback of polycrystalline material is the presence of grain boundaries and the intra grain defects which increase the recombination of carriers and thus degrade the performance of the device. Some researchers have investigated the effect of grain size on the performance of the solar cell[4-6] but it seems that they have focused upon certain important aspects like open circuit voltage (V_{oc}), short circuit current (J_{sc}), fill factor (FF) and efficiency (η) only. In the present paper however, we try to model the entire J-V characteristics of the solar cell for different grain sizes of CdTe. The grain size effect has been taken into account using suitable models which give the impact of grain size on parameters like mobility and diffusion length. Then with the assumption of constant electric field, we solve the continuity equations for electrons and holes in the p-type region only incorporating suitable generation-recombination rates to get the J-V characteristics. The model is verified with the experimental data and shows a good agreement.

*) For correspondence, E-mail: mwakram@iitk.ac.in

2. Model

2.1.Modeling of Grain Size Effect

Various models have been presented to study the effect of grain boundaries on the charge transport in semiconductor devices [7-11].One can assume a potential barrier of a finite width at the grain boundary and analyze the structure as has been done by Bourezig et al. [10] or Seto [11] or one can use the models like those proposed in [7-9] which gives the effect of grain size on the parameters like mobility or diffusion length and then use these parameters to study the effect of grain size on the performance of the device. We are adopting the later approach. We are using a very simple model. The effective mobility in poly-crystalline material can be given by:

$$\frac{1}{\mu}=\frac{1}{\mu_S}+\frac{1}{\mu_G} \tag{1}$$

Where μ_S is the mobility in a single crystal and μ_G is the grain boundary limited mobility. μ_G can be written as:

$$\mu_G=q\tau_G/m^* \tag{2}$$

Where q is the electronic charge, τ_G is the grain-boundary controlled relaxation time and m^* is the effective mass of the carrier. The average thermal velocity of the carriers, v is given by:

$$v=\sqrt{\frac{3kT}{m^*}} \tag{3}$$

Where k is the Boltzmann's constant and T is the absolute temperature. τ_G can be expressed in terms of L, the grain boundary limited mean free path and v as:

$$\tau_G=L/v \tag{4}$$

We used $m_e^*/m=0.14$ [12] and $m_h^*/m=0.35$ [12]. L was taken as a fitting parameter. The diffusion co-efficient can be obtained from mobility using Einstein relation:

$$\frac{D}{\mu}=\frac{kT}{q}=V_t \tag{5}$$

The effective diffusion length in poly-crystalline material can be expressed as [13]:

$$L_{eff,poly}=\frac{L_{eff,mono}}{\sqrt{1+\frac{2S_{GB}L^2_{eff,mono}}{D\times g}}} \tag{6}$$

Where $L_{eff,mono}$ is the diffusion length in a single crystal, S_{GB} is the grain boundary recombination velocity, D is the diffusion co-efficient and g is the grain size. S_{GB} and $L_{eff,mono}$ were again taken as fitting parameters. The effective lifetime of carriers (τ) was then obtained using

$$\tau = L^2_{eff,\ poly} / D \tag{7}$$

$L_{eff,mono}$ was taken as 20 μm and the single crystal mobility values for electrons and holes were taken to be 1050 cm^2/Vs [14] and 80 cm^2/Vs [14] respectively . The Table 1 lists all the simulations parameters used.

Table 1: Simulations Parameters Used

Different Parameters Used	Grain size (3 μm)	Grain size (4 μm)	Grain size (5 μm)
Mean free path for electrons Ln (in A^0)	53.4152	65.2548	75.0393
Mean free path for holes Lp (in A^0)	1.929	2.063	2.7963
$\mu_{Gn}(cm^2/Vs)$	214.334	257.829	301.103
$\mu_{Gp}(cm^2/Vs)$	4.8806	5.2197	7.0748
$\mu_n\ (cm^2/Vs)$	178	207	234
$\mu_p\ (cm^2/Vs)$	4.6	4.9	6.5
S_{GBn} (m/s)	13.2689	7.3091	1.198
S_{GBp} (m/s)	6.78847	3.9829	0.8099
$L_{eff,poly\ n}$ (μm)	6.803	1.0375	1.744
$L_{eff,poly\ p}$ (μm)	1.546	2.257	4.111
τ_n (μs)	0.1	0.2	0.5
τ_p (μs)	0.2	0.4	1

2.2. Modeling of J-V Characteristics

If J_n and J_p are the electron and hole current densities respectively, the continuity equation for electrons and holes in steady state become:

$$\frac{-1}{q}\frac{\delta J_p}{\delta x} + G(x) - R(x) = 0 \tag{8}$$

$$\frac{1}{q}\frac{\delta J_n}{\delta x} + G(x) - R(x) = 0 \tag{9}$$

Where G(x) and R(x) are the generation and recombination rates of carriers respectively. If n(x) and p(x) are the electron and hole concentrations respectively, then using drift-diffusion model, $J_n$and J_p is given by:

$$J_n(x) = q\mu_n n(x)E(x) + qD_n\frac{\delta n}{\delta x} \tag{10}$$

$$J_p(x) = q\mu_p p(x)E(x) - qD_p\frac{\delta p}{\delta x} \tag{11}$$

Where E(x) is the electric field and D_n and D_p are the electron and hole diffusion-coefficients respectively. The doping concentration Na in p-CdTe is 10^{16} cm^{-3} and Nd in n-CdS is 10^{18} cm^{-3}. As Nd is very high compared to Na, the depletion region will extend primarily in the p-type region. To simplify the analysis, we invoked the full depletion approximation. If V is the applied voltage, V_o is the junction voltage and d is the width of the p-type layer, then (neglecting series resistance for the time being) we could assume the voltage dependent electric field in the p-type region to be given by:

$$E(x)=\frac{V_0-V}{d}=E \qquad (12)$$

Kabir and Anjan [15] had also used similar expression in their analysis.V_o was taken as a fitting parameter to be equal to 0.8V as suggested by Kabir and Anjan [15]. The generation rate can be taken as:

$$G(x)=G_o e^{-\alpha x} \qquad (13)$$

Where G_o is the carrier generation rate at x=0 and α is the absorption coefficient of CdTe. G_o and α were taken as fitting parameters. G_o was taken to be equal to 4.64×10^{26} $m^{-3}s^{-1}$ and α to be $10^5 m^{-1}$ in all cases. The recombination rates for electrons and holes were taken as $n(x)/\tau_n$ and $p(x)/\tau_p$ respectively. If we substitute all these expressions in the continuity equation, we get the following second order differential equations in terms of n(x) and p(x). For convenience we drop the notation n(x) or p(x) and will write simply as n and p:

$$D_p\frac{\partial^2 p}{\partial x^2}-\mu_p E\frac{\delta p}{\delta x}-\frac{p}{\tau_p}+G_o e^{-\alpha x}=0 \qquad (14)$$

$$D_n\frac{\partial^2 n}{\partial x^2}+\mu_n E\frac{\delta n}{\delta x}-\frac{n}{\tau_n}+G_o e^{-\alpha x}=0 \qquad (15)$$

The equations can be solved analytically. The complete solution which will be the sum of a general solution and a particular solution is given below:

$$p(x)=C_1 e^{\lambda_1 x}+C_2 e^{\lambda_2 x}+K_1 e^{-\alpha x} \qquad (16)$$

$$n(x)=C_3 e^{\lambda_3 x}+C_4 e^{\lambda_4 x}+K_2 e^{-\alpha x} \qquad (17)$$

Where,

$$\lambda_{1,2}=\frac{1}{2}\frac{E}{V_t}\pm\frac{1}{2}\sqrt{\frac{E^2}{V_t^2}+\frac{4}{D_p\tau_p}} \qquad (18)$$

$$\lambda_{3,4}=\frac{-1}{2}\frac{E}{V_t}\pm\frac{1}{2}\sqrt{\frac{E^2}{V_t^2}+\frac{4}{D_n\tau_n}} \qquad (19)$$

$$K_1=\frac{-G_o}{D_p(\alpha^2+\frac{E}{V_t}\alpha-\frac{1}{D_p\tau_p})} \qquad (20)$$

$$K_2=\frac{-G_o}{D_n(\alpha^2-\frac{E}{V_t}\alpha-\frac{1}{D_n\tau_n})} \qquad (21)$$

And C_1, C_2, C_3, C_4 are constants to be determined by appropriate boundary conditions. We have used following conditions: At x=0, $n=n_1$ and $p=p_1$ and at x=d, $n=n_2$ and $p=p_2$

Finally C_1, C_2, C_3, C_4 can be written, as given below:

$$C_1=\frac{p_2-K_1(e^{-\alpha d}-e^{\lambda_2 d})-p_1e^{\lambda_2 d}}{e^{\lambda_1 d}-e^{\lambda_2 d}} \tag{22}$$

$$C_2=p_1-C_1-K_1 \tag{23}$$

$$C_3=\frac{n_2-K_2(e^{-\alpha d}-e^{\lambda_4 d})-n_1e^{\lambda_4 d}}{e^{\lambda_3 d}-e^{\lambda_4 d}} \tag{24}$$

$$C_4=n_1-C_3-K_2 \tag{25}$$

At x=0 i.e. at the junction, n and p will be zero because if any carrier is generated then it will be swept by the field instantly so we can take $n_1=0$ and $p_1=0$. The other boundary condition can be obtained at the contacts by equating the current with the surface recombination current. That will require the values of surface recombination velocity of carriers. Instead of taking surface recombination velocity as a fitting parameter, we have taken directly the electron and hole concentration there as fitting parameters. Using these boundary conditions, we can determine n(x) and p(x). Then from n(x) and p(x), we can get $J_n(x)$ and $J_p(x)$ directly. The total current density J will be sum of hole and electron current density, as given below:

$$J=J_n(x)+J_p(x) \tag{26}$$

Including series resistance R_s:

The series resistance R_s can be included in the analysis by modifying the expression of E given earlier i.e. Eq. (12) as:

$$E(x)=\frac{V_0-V-(J/A)R_s}{d}=E \tag{27}$$

Where A is the cross sectional area of the device. R_s were taken as a fitting parameter equal to $3.5\times10^{-4}\ \Omega\ cm^{-2}$ for all cases.

3. Results and Discussions

For the simulation, Matlab 7.10.0 (R 2010a) was used to solve the equations iteratively and get the results. The model was fitted with the experimental data (Detailed discussion is made in the Appendix). In the drawn plot + points are the experimental ones and the continuous line shows the simulated results. From the plot drawn (Fig. 1, Fig. 2, and Fig. 3), it is observed that the simulated results are in good agreement with the experimental ones. The discrepancy may be because of the assumption of constant electric field. We had taken G_o and α same for all cases. This may not be true in real situation. The optical losses may be slightly different for each case and the initial deviations for g=4µm case may be because of that.

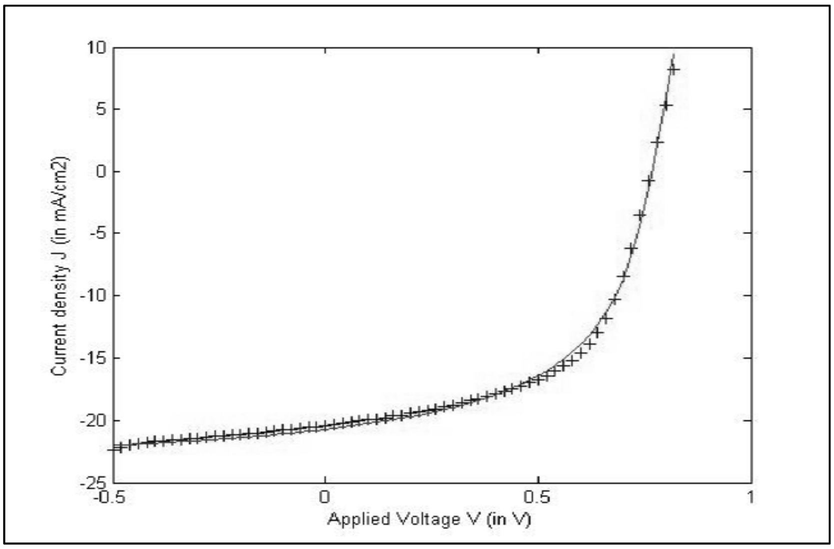

Figure 1: J-V Characteristics for g=3µm.

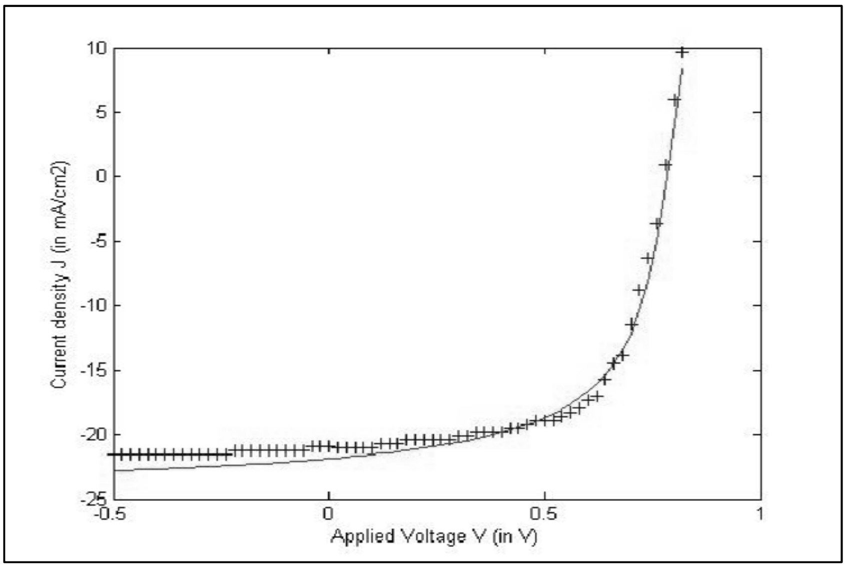

Figure 2: J-V Characteristics for g=4µm.

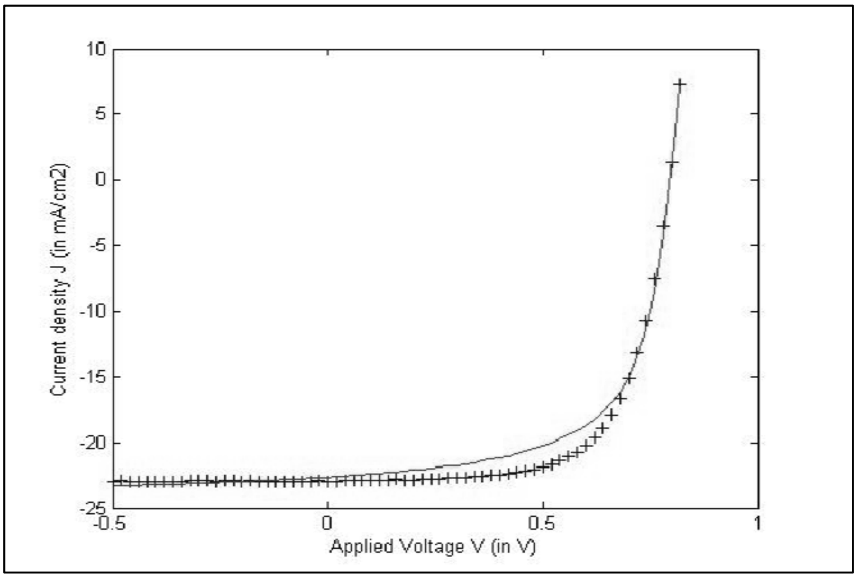

Figure 3: J-V Characteristics for g=5µm.

4. Conclusion

A theoretical model based upon simple drift-diffusion formulation is developed to study the J-V characteristics of a solar cell. The continuity equations are solved with suitable generation-recombination rates and appropriate boundary conditions. The grain size effect is incorporated using parameters like mobility and diffusion length of the carriers. The model is fitted with the experimental data and it shows a good agreement.

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References

[1] Alex Niemegeersa and Marc Burgelman, J. Appl. Phys. **81** (1997) 2881

[2] Amal K. Ghosh, Charles Fishman and Tom Feng, J. Appl. Phys. **51** (1980) 446

[3] D. de Noble. Philips Res. Rep. **14** (1959) 487

[4] D. P. Joshi and R. S. Srivastava, J. Appl. Phys. **56** (1984) 2375

[5] G. Agostinelli, D.L. Batzner and M. Burgelman , Thin Solid Films **431-432** (2003) 407

[6] Hyeson Jung, *Solar Cells Based on CdTe Thin Film and Composite of Organic and Inorganic Nano-Scale Materials*, Ph.D. Thesis, University of Illinois at Chicago, Illinois, U.S (2010)

[7] J. Martinez and J. Piqueras, Solid-St. Electron. **23(4)** (1980) 297

[8] J. N. Roy, S. Basu, and D. N. Bose, J. Appl. Phys. **54** (1983) 847

[9] John Y. W. Seto, J. Appl. Phys. **46** (1975) 5247

[10] M. S. Anjan and M. Z. Kabir, Phys. Status Solidi, **A 208** (2012) 1813

[11] Makoto Takahashi, Kohei Uosaki, Hideaki Kita and Shoji Yamaguchi, J. Appl. Phys. **60** (1986) 2046

[12] Mitsuru Imaizumi, Tadashi Ito and Masafumi Yamaguchi, J. Appl. Phys. **81** (1997) 7635

[13] R. B. Bergmann, Recent. Res. Devel. Crystal Growth Res. **1** (1999) 241

[14] R. Brendel and U. Rau, Solid State Phenom. **67–68** (1999) 81

[15] S. Hegedus, D. Desai and C. Thompson, Prog. Photovolt. Res. Appl. **15** (2007) 587

[16] Y. Bourezig, B. Bouabdallah, S. Mansouri and F. Gaffiot, Int. J. Nanoelectronics and Materials **2(1)** (2009) 63-74

APPENDIX

Device fabrication

The device were fabricated and tested by Prof. Mitra Dutta and Dr. Hyeson Jung in the Nano-engineering research laboratory, department of electrical and computer engineering in the University of Illinois at Chicago. The fabrication process is given below [16].

Transparent conducting oxide (TCO) coated glasses from Wooyang and Pilkington were used. Then CdS was deposited. The grain size of CdTe will depend upon the deposition temperature and in general higher the temperature, larger will be the grain size. Therefore CdTe deposition was carried out at different temperatures (from 400^0 C to 500^0 C) to get the maximum grain size. $CdCl_2$ vapor treatment was used to increase the efficiency of the cell. It was spin coated, followed by rinse and then annealed under $CdCl_2$ treatment for different temperatures and time durations so as to get the maximum grain size. The surface was etched followed by copper deposition and diffusion. Finally gold was deposited as the back contact. The experimental data were collected at temperature of 300K and $1000W/m^2$ of light intensity.

Irrespective of the growth process or deposition techniques, the grain size is the essential parameter that influences the performance of these films and that's why it was decided to propose a model to study the effect of grain size on the performance of the device.