Hindawi Publishing Corporation
International Journal of Photoenergy
Volume 2013, Article ID 513217, 4 pages
http://dx.doi.org/10.1155/2013/513217

Research Article

C-V Calculations in CdS/CdTe Thin Films Solar Cells with a $\mathrm{CdS}_x\mathrm{Te}_{1-x}$ Interlayer

A. Gonzalez-Cisneros, F. L. Castillo-Alvarado, J. Ortiz-Lopez, and G. Contreras-Puente

Escuela Superior de Física y Matemáticas-IPN, Edificio 9 U.P.A.L.M., 07738 México, DF, Mexico

Correspondence should be addressed to A. Gonzalez-Cisneros; omeyotl@gmail.com

Received 3 June 2013; Accepted 9 August 2013

Academic Editor: Francesco Bonaccorso

In CdS/CdTe solar cells, chemical interdiffusion at the interface gives rise to the formation of an interlayer of the ternary compound $\mathrm{CdS}_x\mathrm{CdTe}_{1-x}$. In this work, we evaluate the effects of this interlayer in CdS/CdTe photovoltaic cells in order to improve theoretical results describing experimental *C-V* (capacitance versus voltage) characteristics. We extended our previous theoretical methodology developed on the basis of three cardinal equations (Castillo-Alvarado et al., 2010). The present results provide a better fit to experimental data obtained from CdS/CdTe solar cells grown in our laboratory by the chemical bath deposition (for CdS film) and the close-spaced vapor transport (for CdTe film) techniques.

1. Introduction

Polycrystalline solar cells based on the thin films technology are outstanding candidates for an aggressive expansion of the photovoltaic industry. During the past few years, despite the world economic recession, the photovoltaic market has continued to grow. In Europe and Asia, the market has expanded from the Mega Watt (MW) to the Giga Watt (GW) scale. PV installations grew to 7.3 GW in 2009, which represents 20% from the previous year. The various forecast scenarios predict an increase in the demand from 15.4 to 37 GW in 2014, more than five times the size of the 2009 market [1, 2]. Today, there is much interest and research activity concerning second generation solar cells based on polycrystalline cadmium telluride CdTe thin films and cadmium sulfide CdS as "window" layer. Capacitance versus voltage is one of the most important techniques for the device characterization. In this work, we extend the theoretical model used in a previous paper [3] in order to take into account the formation of a layer of the ternary compound $\mathrm{CdS}_x\mathrm{Te}_{1-x}$ (x, the concentration) at the CdS/CdTe interface generated by interdiffusion processes [4]. During manufacturing of these solar cells, the CdTe/CdS interface is subjected to relatively high temperatures giving rise to atomic interdiffusion and the formation of an interfacial region of composition $\mathrm{Cd}_x\mathrm{Te}_{1-x}$. The understanding of this ternary $\mathrm{CdS}_x\mathrm{Te}_{1-x}$ interlayer will help to conceive improvements in the efficiency of the photovoltaic cell. In this work, we use a *C-V* theoretical method for the determination of the interface charge density σ in the CdS/ternary/CdTe heterojunction and the band discontinuity ΔE_v simultaneously. The methodology is based on three cardinal equations as discussed in the theory below. For comparison with our calculations, we used solar cells of maximum efficiency (12.4%) fabricated in our group [5].

2. Theoretical Method

We present the methodology for the simultaneous calculations of the valence band offset ΔE_v and the interface charge density σ. It is assumed that these two quantities are independent of the bias voltage. This assumption is justified because we are interested in heterojunctions with fixed defect densities.

The clue for obtaining the energy bands at both sides of the interfaces are (a) the two interfacial potentials (φ_{s1}, φ_{s2}

which give the band bending at each side of the interface), (b) the energy increment of the valence band, and (c) the interface charge density. In addition to these, three cardinal equations originating from the displacement of the band line-up equation, charge neutrality, and the total capacitance of the interface are necessary. This method makes no use of any approximations and provides simultaneous determination of the discontinuities of the valence band and the interfacial charge density.

Assuming that the heterojunction is like a parallel plate capacitor, the capacitance-voltage characteristics for low bias voltages V_a are given by

$$C = \left[\frac{q\varepsilon_{S1}\varepsilon_{S2}N_d N_a}{2(\varepsilon_{S1}N_a + \varepsilon_{S2}N_d)}\right]^{1/2} * \left(V_d - V_a\right)^{-1/2}, \tag{1}$$

where V_d is the potential well in the heterojunction, V_a is the bias voltage, q is the electron charge, N_a is the acceptor concentration, N_d is the donor concentration, and ε_{S1} and ε_{S2} are the dielectric constants of n-type and p-type semiconductor [6]. Therefore, in our case, we have a linear dependence of $1/C^2$ versus V_a close to $V_a = 0$. We solve numerically the band energy in any site of the heterojunction using the interface according to the experimental data [7]; the spectral response of champion CdS/CdTe solar cells has an increase in a photon energy close to the band gap CdS. Thus, we have assumed in our equations that the physical properties of the ternary compound are closer to those of CdS for each part of the ternary compound, which are the total bending on each side of the two heterojunction (CdTe/CdS$_x$Te$_{1-x}$).

We note that the total band curvature at each side of the interface depends on the bias voltage V_a, that is, $\varphi_{S1}(V_a)$ and $\varphi_{S2}(V_a)$. We assume that the discontinuities of the valence band and the charge density at the interface are independent of the applied voltage, which is a usual assumption for low voltages. Validity of this assumption is validated by a good agreement with experiment.

Because there are a fixed equal number of separated positive and negative charges at the interface between different materials, we consider that the region of spatial charge behaves like a parallel plate capacitor.

2.1. Cardinal Equations for the CdTe/CdS$_x$Te$_{1-x}$ Interface (C-V Matching Method).

The band line-up equation in this case is (Figure 1)

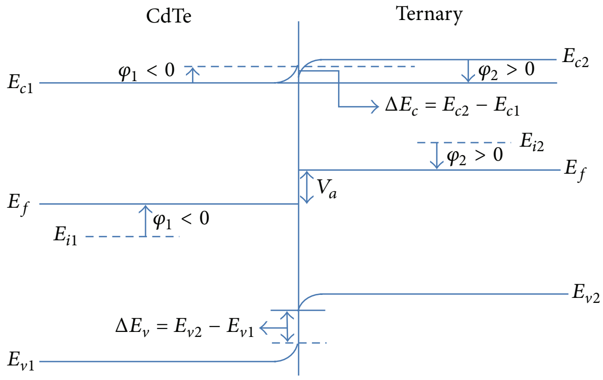


Figure 1: Energy band (band lineup) diagram of two n-p heterojunctions under reversible bias. The reference level for the potential of each semiconductor is at the intrinsic energy level. We assume that the ternary behaves like an n-type semiconductor for union with CdTe.

$$E_{FV1} - E_{FV2} - \Delta E_{V(\text{ternary})} - qV_a = q\left[\varphi_{S2}\left(V_a\right) - \varphi_{S1}\left(V_a\right)\right], \tag{2}$$

where "x" is the ternary concentration and E_{FV1} and E_{FV2} are the differences between the quasi-Fermi energy levels with subscripts 1 and 2 corresponding to CdTe and CdS$_x$Te$_{1-x}$, respectively. The valence band offset $\Delta E_{V(\text{ternary})}$ and the respective bulk valence band levels are given by

$$\begin{aligned} E_{FV1} &= E_{Fn1} - E_{V1} = \frac{E_{g1}}{2} + \frac{3}{4}kT\ln\left(\frac{m_{h1}^*}{m_{e1}^*}\right) - q\varphi_{F1}, \\ E_{FV2} &= E_{Fp2} - E_{V2} = \frac{E_{g2}}{2} + \frac{3}{4}kT\ln\left(\frac{m_{h2}^*}{m_{e2}^*}\right) - q\varphi_{F2}. \end{aligned} \tag{3}$$

The separation between the quasi-Fermi energy levels is determined for the bias voltage:

$$E_{Fn1} = E_{Fp2} + qV_a, \tag{4}$$

where V_a is the bias voltage in the p-n junction.

The charge neutrality equation under nonequilibrium is given by

$$Q_1\left[\varphi_{S1}\left(V_a\right)\right] + Q_2\left[\varphi_{S2}\left(V_a\right)\right] + q\sigma = 0, \tag{5}$$

where the expressions for the semiconductor charge under nonequilibrium, Q_1 and Q_2, are the half semiconductor charges (per unit area) which are given by [8]

$$\begin{aligned} Q_1 = {} & \operatorname{sign}\left[\varphi_{S1}\left(V_a\right)\right] \cdot \frac{\sqrt{2}\varepsilon_0\varepsilon_{S1}}{\beta L_{D1}} \cdot e^{\Delta u1/2} \\ & \times \left\{\varphi_{S1}\left(V_a\right) \cdot \sinh\left(u_1^*\right) + \cosh\left[u_1^* - u_{S1}\left(V_a\right)\right] \right. \\ & \left. - \cosh\left(u_1^*\right)\right\}^{1/2}, \\ Q_2 = {} & \operatorname{sign}\left[\varphi_{S2}\left(V_a\right)\right] \cdot \frac{\sqrt{2}\varepsilon_0\varepsilon_{S2}}{\beta L_{D2}} \cdot e^{\Delta u2/2} \\ & \times \left\{\varphi_{S2}\left(V_a\right) \cdot \sinh\left(u_2^*\right) + \cosh\left[u_2^* - u_{S2}\left(V_a\right)\right] \right. \\ & \left. - \cosh\left(u_2^*\right)\right\}^{1/2}, \end{aligned} \tag{6}$$

where

$$\operatorname{sign} = \begin{cases} +1, & u < 0 \\ -1, & u > 0. \end{cases} \tag{7}$$

Here, $u^* = \beta((\varphi_{F1} + \varphi_{F2})/2)$ and $\beta = q/kT$.

The third cardinal equation is obtained from the expression of the half capacitance per unit area of the device:

$$\frac{1}{C_{\text{CdTe-ter}}} = \frac{1}{C_1\left[\varphi_{S1}\left(V_a\right)\right]} + \frac{1}{C_2\left[\varphi_{S2}\left(V_a\right)\right]}, \quad (8)$$

where

$$\begin{aligned} C_1 &= \frac{\left(\varepsilon_0\varepsilon_{S1}\right)^2}{\beta L_{D1}^2 \cdot Q_1} \\ &\quad \cdot e^{\triangle u1/2} \cdot \left\{\sinh\left(u_1^*\right) - \sinh\left[u_1^* - u_{S1}\left(V_a\right)\right]\right\} \\ &= \frac{q\varepsilon_0\varepsilon_{S1}}{Q_1}\left\{N_1 + 2n_{i1} \cdot e^{\triangle u1/2} \cdot \sinh\left[u_1^* - u_{S1}\left(V_a\right)\right]\right\}, \\ C_2 &= \frac{\left(\varepsilon_0\varepsilon_{S2}\right)^2}{\beta L_{D2}^2 \cdot Q_2} \\ &\quad \cdot e^{\triangle u2/2} \cdot \left\{\sinh\left(u_2^*\right) - \sinh\left[u_2^* - u_{S2}\left(V_a\right)\right]\right\} \\ &= \frac{q\varepsilon_0\varepsilon_{S2}}{Q_2}\left\{N_2 + 2n_{i2} \cdot e^{\triangle u2/2} \cdot \sinh\left[u_2^* - u_{S2}\left(V_a\right)\right]\right\} \end{aligned} \quad (9)$$

$$\frac{1}{C_{\text{Total}}} \approx \frac{1}{C_{\text{CdTe-ter}}}. \quad (10)$$

It is important to note that the energy gap of the ternary is not a simple linear combination but a more complex function of x [9]:

$$E_g(x) = (1-x)E_g(\text{CdS}) + xE_g(\text{CdTe}) - bx(1-x), \quad (11)$$

where b is the "optical bowing coefficient" given by 1.69 eV and the valence band offset ΔE_V.

3. Results

We find the ternary concentration value of 0.75 with the best fitting of the curve, which is in good agreement with the results described by Cediel et al. [10]. The various quantities or constants in the cardinal equations were taken from the previous paper [3]. We show the result of the C-V fitting method in Figure 2 for a voltage range from 0 to 0.5 V. A much better fit is obtained by assuming the formation of a ternary compound at the CdTe/CdS interface.

In addition, we have also obtained the values of the valence band offset and the interface charge density simultaneously, namely,

$$\begin{aligned} \Delta E_V &= 0.99\ \text{eV}, \\ \sigma &= 1 \times 10^{13}\ \text{cm}^{-2}, \end{aligned} \quad (12)$$

which are in good agreement with the reported values [9, 11, 12].

4. Conclusions

In summary, we have calculated the capacitance versus applied voltage of CdS/CdTe thin film solar cells considering the formation of a $\text{CdS}_x\text{Te}_{1-x}$ interlayer using the C-V matching method. Our results are in better agreement with experimental data than our previous theoretical results that did not assume the presence of the $\text{CdS}_x\text{Te}_{1-x}$ interlayer. We may also say that the ternary layer acquires the properties of CdS and behaves like the type n semiconductor instead of the CdS itself. This could be taken as evidence of the existence of a ternary compound that plays an important role in solar cell devices. This can be taken as evidence of the existence of the ternary interlayer which plays an important role in the solar cell.

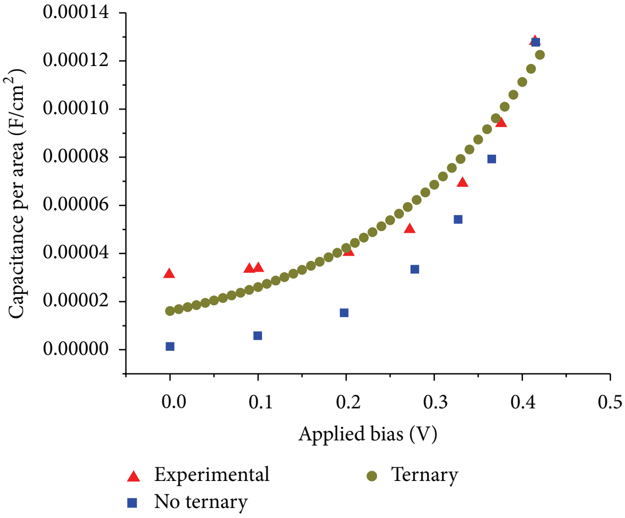


Figure 2: Calculated C-V characteristics of a CdTe/CdS PV cell assuming the formation of a ternary compound at the CdTe/CdS interface. Comparison is made with C-V measurements of a 12.4% efficient PV cell [5] and with calculated results within a model without the assumption of the ternary compound at the interface [3].

Acknowledgments

F. L. Castillo-Alvarado, J. Ortiz-Lopez, and G. Contreras-Puente gratefully acknowledge fellowships granted by COFAA-IPN, EDI-IPN, and EDD-IPN. This work was partially supported by CONACyT (Mexico).

References

[1] Manufacturing cost per watt at First Solar falls to US$0.76cents: Module Faults Hit Earnings, 2011, http://www.pv-tech.org/news/.

[2] M. Osborne, First Solar First to 1GW Annual Production, Photovoltaics, 2009, http://www.pv-tech.org/.

[3] F. L. Castillo-Alvarado, J. A. Inoue-Chávez, O. Vigil-Galán, E. Sánchez-Meza, E. López-Chávez, and G. Contreras-Puente, "C-V calculations in CdS/CdTe thin films solar cells," *Thin Solid Films*, vol. 518, no. 7, pp. 1796–1798, 2010.

[4] M. M. Aliyu, S. Hossain, M. A. Islam et al., "Evaluation of the effects and impacts of the CdSTe interlayer in CdS/CdTe solar cells through modeling and simulations," in *Proceedings of the*

2nd International Conference on the Developments in Renewable Energy Technology (ICDRET '12), pp. 248–251, January 2012.

[5] O. Vigil-Galán, A. Arias-Carbajal, and R. Mendoza-Pérez, "Improving the efficiency of CdS/CdTe solar cells by varying the thiourea/$CdCl_2$ ratio in the CdS chemical bath," *Semiconductor Science and Technology*, vol. 20, no. 8, p. 819, 2005.

[6] B. L. Sharma and R. K. Purohit, *Semiconductor Heterojunctions*, Pergamon Press.

[7] First Solar New Releases, 2011, http://www.firstsolar.com.

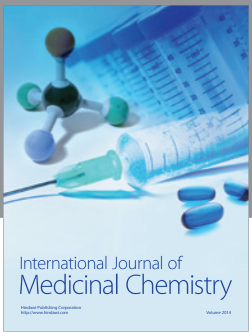
[8] R. S. C. Cobbolt, *Theory and Applications of Field Effect Transistors*, Willey, London, UK, 1970.

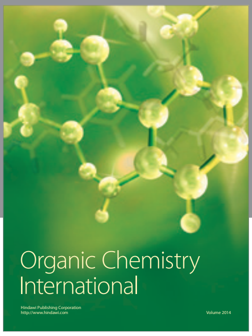
[9] S.-H. Wei, S. B. Zhang, and A. Zunger, "First-principles calculation of band offsets, optical bowings, and defects in CdS, CdSe, CdTe, and their alloys," *Journal of Applied Physics*, vol. 87, no. 3, pp. 1304–1311, 2000.

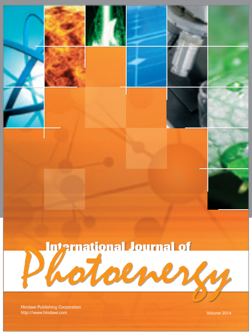
[10] G. Cediel, F. Rojas, H. L. Infante, and G. Gordillo, "Determinación de constantes ópticas y simulación teórica del espectro de transmitancia de pelóculas delgadas de CdS, CdTe y Cd(S,Te) depositadas por evaporación," *Revista Colombiana de Fisica*, vol. 34, no. 1, 2002.

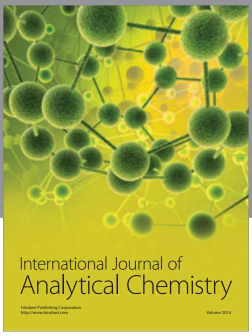
[11] A. Balcioglu, F. Hasoon, D. Levi, and R. K. Ahceukiel, "Investigation of deep impurity levels in CdTe/CdS solar cells (2000) (NCPV) program review meeting," in *N Spu Program Review Meeting Proceeding*, p. 279, 2006.

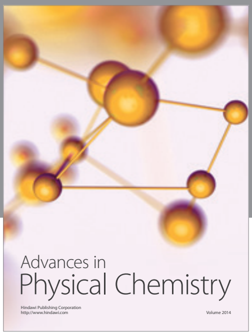
[12] S. Vatana, I. Caraman, G. Rasu, V. Fedorov, and P. Gasin, "The study of the nonequilibrium charge carrier transport mechanism through the interface of CdS/CdTe heterojunctions," *Chalcogenide Letters*, vol. 13, p. 9, 2006.

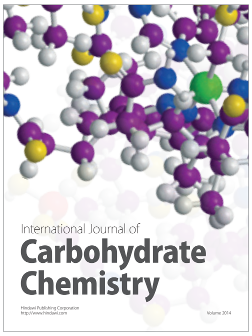

International Journal of
Medicinal Chemistry

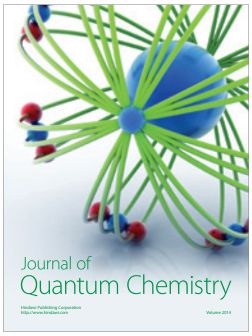

Organic Chemistry
International


International Journal of
Photoenergy

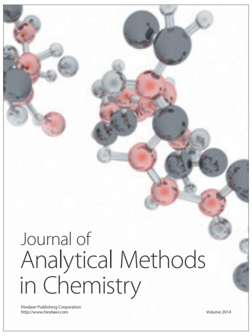

International Journal of
Analytical Chemistry


Advances in
Physical Chemistry

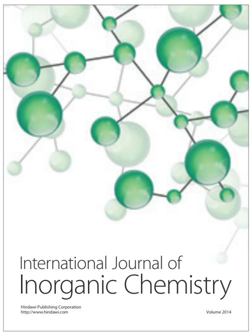

International Journal of
Carbohydrate
Chemistry


Journal of
Quantum Chemistry

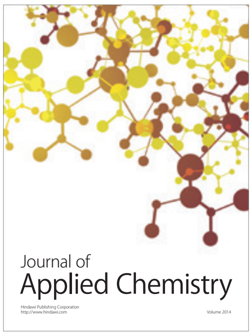

The Scientific
World Journal

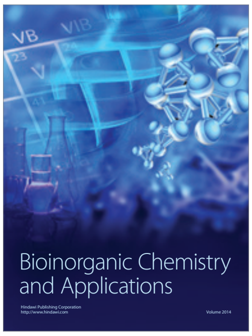

Journal of
Analytical Methods
in Chemistry


Journal of
Spectroscopy

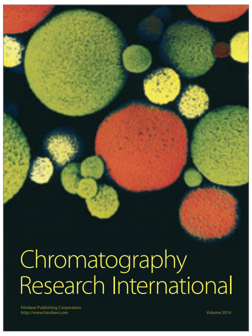

International Journal of
Inorganic Chemistry


International Journal of
Electrochemistry


Journal of
Applied Chemistry


Bioinorganic Chemistry
and Applications


Journal of
Theoretical Chemistry


Chromatography
Research International


Journal of
Catalysts


Journal of
Chemistry


International Journal of
Spectroscopy