Simulation of Current-Voltage Curves for CdS Cylinders Embedded in P3HT

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INTRODUCTION

In this paper, the current-voltage (I-V) curve of the heterojunction formed by cadmium sulphide (CdS) cylinder arrays embedded in the conductive polymer poly (3-hexylthiophene-2, 5-diyl) (P3HT) is modeled in light of its possible use in photovoltaic applications. CdS cylinders were grown by DC electrodeposition on a nanoporous template which is made by anodized aluminum layer on Indium Tin Oxide (ITO) coated glass substrate, then P3HT solution was put on the CdS nanowires template to form the CdS/P3HT heterojunction [1]. The Ag contact on top was formed by silver paint, and Ag/P3HT/CdS/ITO heterojunction was formed as shown in Figure 1.

THEORY

Some polymers are conductive since carriers can transport in overlap bonds. The overlapping carbon p orbitals in the successive units in a conjugated polymer produce two split energy levels. One is π bonding orbital and another is π^* anti-bonding orbital. A series of π bonds form a π energy band which is called the highest occupied molecular orbital (HOMO), and a series of π^* bonds form a π^* energy band which is called the lowest unoccupied molecular orbital (LUMO) in the energy band of the polymer. These two energy bands are similar to the valence band and conduction band of inorganic semiconductors [2][3]. The band diagrams of CdS/P3HT are shown in Figure 2. CdS is n-type semiconductor and P3HT is a p-type material. The equation of heterogeneous pn junction is used to build the simulation model. The I-V curve was measured from -2 eV to +2 eV and compared with simulation as shown in figure 3. The deviation is caused by lots of reasons such as defects from growth of CdS, polymer properties…etc. The one main cause is that defects cause some carriers recombine at the interface. The recombination could be presented by an activation energy (E_A) in the I-V equation [4].

$$I = I_0 * \left(e^{\left(\frac{qV_A}{kT}-\frac{E_A}{kT}\right)} - 1\right) \quad (1)$$

$$I_0 = A * q * \left[\left(\frac{D_n}{L_n}\right) * N_{p0} + \left(\frac{D_p}{L_p}\right) * P_{n0}\right] \quad (2)$$

I_0 is the saturation current and A is area of the heterojunction which is 0.25 cm^2. N_{p0} and P_{n0} are the initial minority carrier concentrations which are calculated by minority carrier equations.

$$N_{p0} = N_{cp} e^{\left(\frac{E_{F0}-E_{cp}}{kT}\right)} \quad (3)$$

$$P_{n0} = N_{vn} e^{\left(\frac{E_{vn}-E_{F0}}{kT}\right)} \quad (4)$$

and,

$$N_{cp} = 2 * \left[\frac{m_n * kT}{2*\pi*\hbar^2}\right]^{\frac{3}{2}} = 2.51 * 10^{19} * \left(\frac{m_n}{m_0}\right)^{\frac{3}{2}} \quad (5)$$

$$N_{vn} = 2 * \left[\frac{m_p * kT}{2*\pi*\hbar^2}\right]^{\frac{3}{2}} = 2.51 * 10^{19} * \left(\frac{m_p}{m_0}\right)^{\frac{3}{2}} \quad (6)$$

The diffusion constants - D_p and D_n - were calculated by Einstein equation.

$$D = \frac{kT}{q}\mu \quad (7)$$

where μ is mobility of minority carriers.

The diffusion length of electrons in P3HT (L_n) is 10^{-6} cm [5].

The diffusion length of holes in CdS is:

$$L_p = \sqrt{D_p * \gamma_p} \quad (8)$$

where γ_p is lifetime of holes in CdS.

DISCUSSION

The I-V curve was computed iteratively until the value of E_A provided for a simulation closest to measurement; this yielded the value of E_A to be $0.3*V_A^{1.88}$ as shown in figure 4. If the causes of the defects could be figured out and minimized, it is helpful for CdS/P3HT to be used in forming photovoltaic and other devices.

ACKNOWLEDGMENT

Work supported, in part, under AFOSR Grant FA9550-11-1-0271.

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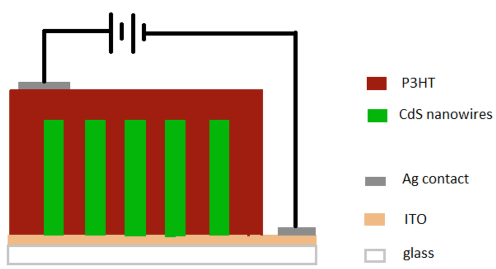

Fig.1. Brief schematic of CdS/P3HT circuit.

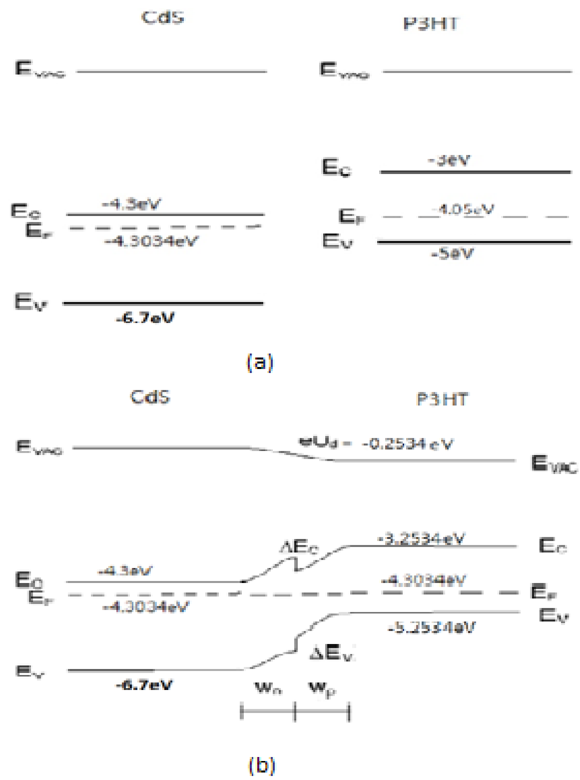

Fig.2. (a) Lineup band structure of CdS and P3HT before contact. (b) The band diagram of CdS/P3HT after contacted. The vacuum level of P3HT is lowered by 0.2534eV.

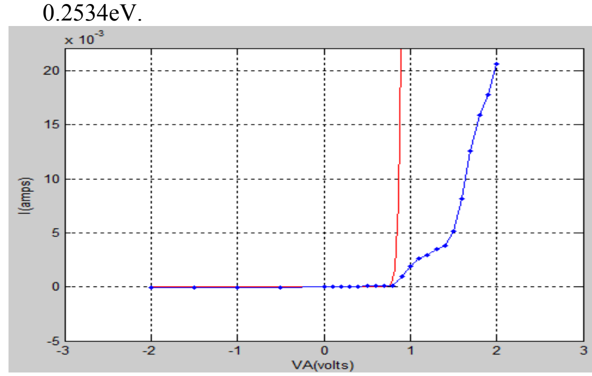

Fig.3. Comparison of measurement (blue) and simulation (red) CdS/P3HT I-V curves.

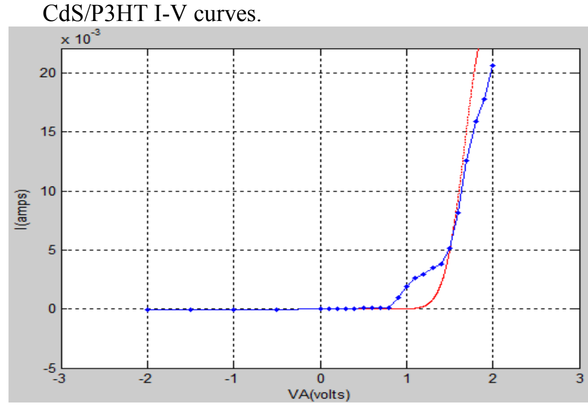

Fig.4. Comparison of measurement (blue) and simulation (red) CdS/P3HT I-V curves after E_A was added in simulation.