Exploitation of density of states and mobility difference between holes and electrons for high efficiency solar cells

AKEED AHMED PAVEL*, M. REZWAN KHAN**
*Department of Computer Science and Engineering
East West University, Dhaka, Bangladesh

**Department of Electrical and Electronic Engineering
Bangladesh University of Engineering and Technology, Dhaka, Bangladesh

ABSTRACT : The main inherent reason behind the low efficiency of a p-n junction solar cell has been studied analytically. Prevention of internal recombination of electron hole pairs under illuminated condition seems to be a solution towards the enhancement of the cell efficiency. The mechanism of electron-hole recombination in an illuminated p-n homo-junction solar cell has been studied, with special reference to the mobility of the carriers and the density of states, to visualize the actual mechanism of carrier diffusion across the junction. Accordingly, potential structures that can effectively prevent the high rate of charge carrier diffusion across the junction have been proposed. Results presented here indicate that there can be significant enhancement in the cell efficiency for the proposed structures.

Key words : solar cell, efficiency, mobility, density of states, hetero-structure

1. Introduction

Enhancement of solar cell efficiency is a topic of on going research and attempts have been made to achieve higher efficiency using different materials and structures. In case of homo-junction solar cells, increased energy band gap of the solar cell materials results in increased open circuit voltage with reduced short circuit current. On the other hand, decrease in the energy band gap increases the short circuit current reducing the open circuit voltage. Theoretically, the highest efficiency for such a solar cell under concentration of 1 sun is 31% for an energy band gap of about 1.35 eV [1]. Experimentally, the maximum conversion efficiency of a solar cell made from a single material under of 1 sun condition, has been reported to be around 25% [2]-[3]. The efficiency of commercially available solar cells is still much lower, around 15% [3]. Stacking of different band gap materials in multi-junction cells can achieve a maximum efficiencies of 37%, 50%, 56% and 72% for 1, 2, 3 and 36 different energy gaps respectively, at a concentration of 1000 sun [4]. But too many practical problems, including difficulty in fabrication and mismatch in the cascaded cells, intervene with such cells and the ultimate efficiency of 72% is virtually impossible to achieve in reality. However, there are many proposed hetero-junction solar cells, which show considerable promise for enhanced cell efficiency. In this paper, single junction solar cell properties are first studied to identify the main mechanisms responsible for low cell efficiency. The reported works mainly concentrate on the band gap of the p-n junction structures without giving due consideration to the fact that density of states, and significant difference between the mobility of the electrons and holes can play an important role in determining the overall efficiency of a solar cell. This paper makes focused study on the behavior of the above mentioned parameters and suggests potential structures for solar cells that can exploit them for higher conversion efficiency.

2. p-n junction under illumination

Inherent potential barrier in a p-n junction is the main driving force behind the operation of a solar cell. Incidence of photons having quantum energy more than the energy band gap of the cell material generates electron hole pairs, which get separated due to the junction potential. Thus when illuminated, the junction becomes forward biased and it's potential barrier is reduced. Assuming the holes and electrons in quasi-thermal equilibrium, there is always significant number of electrons and holes that can cross over the potential hill and cause an internal current flow by drift-diffusion mechanism. Forward biased junction due to incidence of photons allows this flow of holes and electrons from p and n sides of the p-n junction respectively, to grow at an exponential rate like a usual forward biased p-n

junction diode [3]. The potential barrier cross over mechanism is depicted in Fig1. The dotted lines show the energy band diagram under illuminated

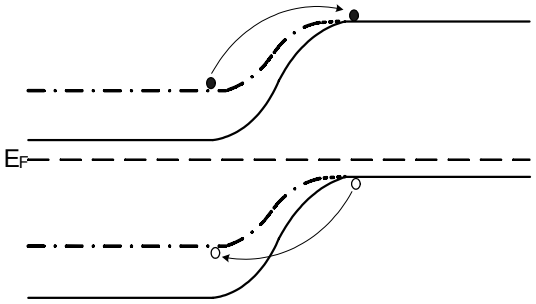

Fig. 1: Energy band diagram of a p-n junction solar cell in dark and under illumination

condition which indicates a forward biased junction. Under open circuit condition, optically generated electron and hole pairs keep on accumulating and the internal diode current starts flowing. The internal current keeps on increasing until the cell reaches its open circuit voltage when all the optically generated electrons and holes cross over the barrier and recombine. Any mechanism that can discourage such diffusion across the p-n junction would effectively reduce internal recombination and consequentially would increase open circuit voltage. Such a mechanism that can increase the open circuit voltage without causing any significant reduction in the short circuit current would increase the overall conversion efficiency. Practically, higher band gap p-n junctions make higher potential barriers with reduced short circuit current, as lesser number of photons in the solar spectrum have the corresponding high energy to generate electron hole pairs. Hence, any indefinite increase in the band gap ultimately causes reduced cell efficiency. On the other hand, reduction of the barrier increases the short circuit current but reduces the open circuit voltage. Hence, an optimum material band gap that produces maximum conversion efficiency for a homo-junction corresponds to 1.35eV [1].

Unlike a homo-junction, a hetero-junction solar cell has unequal potential barriers for holes and electrons. Two possible potential structures for hetero-junction are shown in Fig.2. In Fig.2a the potential barrier for holes are higher than the potential barrier for electrons. In Fig.2b, the situation is just the reverse. Choice between these two possible options is made based on the open circuit voltage for these two structures. Usually, mobility of the electrons are significantly higher than that of holes. Hence, structures having higher potential barrier for the electrons are expected to have higher open circuit voltage. However, there are other factors like density of states, which also play important role in determining the open circuit voltage and all these factors should be incorporated to reach a final conclusion. Detailed mathematical analysis is given in the following section.

3. Analysis of hetero-junction solar cell for higher open circuit voltage

Typical hetero-junction structures are shown in Fig.2. Due to difference in the work function of two different materials, there appears some notch like potential discontinuities in the structure. For the sake of easy understanding and analysis, we have ignored the notch like discontinuity in the structure shown in Fig.2a and Fig.2b. This notch like discontinuity can be avoided practically by choosing materials with appropriate electron and hole affinity [5].

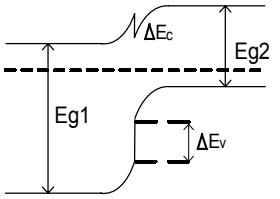

Fig 2a: Heterostructure with high band gap n type material

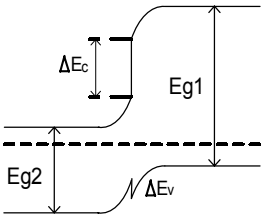

Fig 2b: Heterostructure with high band gap p type material

In following calculations for the a p-n junction the following assumptions are taken:

a. All the incident photon with energy higher than the smaller band gap is absorbed to produce the short circuit current
b. Potential notches and tunneling effects are ignored
c. Internal resistance are not considered in the calculation

The built in potential (V_D) for the structures shown in Fig.2a can be expressed as

$$qV_D = kT \ln \frac{N_{A2} N_{D1}}{N_{c1} N_{v2}} + E_{g2} \quad \text{.....(1a)}$$

Similarly, for structure Fig.2b, the final expression for the built in potential is

$$qV_D = kT \ln \frac{N_{A1} N_{D2}}{N_{c2} N_{v1}} + E_{g2} \quad \text{.....(1b)}$$

where q is the electronic charge, k is the Boltzmann constant, T is the absolute temperature, $N_{A,D}$ refer to acceptor of donor concentration, $N_{c,v}$ refer to the effective density of states at the conduction or valence band, subscript 1 and 2 refers to materials with high and low band gap respectively.

Looking at the above two equations it can be seen that built in potential can be different due to the variation in the values of N_c and N_v even if same doping densities are used for both p and n type materials. In case of the semiconductors like Ge or Si, value of N_c is higher than N_v. But the situations for many of the III-V compound semi-conductor materials are quite different; value of N_v is higher than N_c. Such variations should be taken into consideration while choosing materials for high efficiency solar cells. Table 1 shows theoretical values of V_D for some heterostructures composed of materials having different values of density of states .

Materials	Band gaps (eV)	Structure	V_D (V)
GaAs/Ge	1.42/0.66	p/n n/p	0.43 0.51
GaP/Si	2.26/1.12	p/n n/p	0.837 0.864
GaP/InP	2.26/1.34	p/n n/p	1.16 1.08
GaP/GaAs	2.26/1.42	p/n n/p	1.24 1.17

Table 1: Built in potentials for different heterostructures with $N_A=N_D=10^{17}$ cm^{-3}. ($N_{C,}N_V$) values in per cm^3 for Ge, Si, GaAs, InP and GaP are (1.04×10^{19}, 6×10^{18}), (2.8×10^{19}, 1.04×10^{19}), (4.7×10^{17}, 7×10^{18}),(5.7×10^{17}, 1.1×10^{19}) and (1.8×10^{19}, 1.9×10^{19}) respectively.

In calculating the values of V_D in Table 1, effects like lattice mismatch has been ignored.

The current flow inside the p-n junction has three different components

i. The current generated due to the incident photon stream (I_{ph})
ii. Internal current due to the electrons crossing over from the n to p-type material (I_n)
iii. Internal current due to holes crossing over from the p to n-type material (I_p)

Under open circuit condition, there is no current flowing through the external circuit and all the electron-hole pair generated optically is recombined within the diode material. The expression for electron and hole current density flowing internally for the structure in Fig.2 can be expressed as

$$J_n = J_{ns}(e^{qV/kT} - 1) \quad \text{.....(2a)}$$

$$J_p = J_{ps}(e^{qV/kT} - 1) \quad \text{.....(2b)}$$

For Fig 2a saturation currents J_{ns} and J_{ps} are given by [6]

$$J_{ns} = \frac{qD_n}{L_n} N_D e^{-(qV_D - \Delta E_C)/kT} = \frac{qD_n}{L_n} \frac{N_{c1}N_{v2}}{N_A} e^{-E_{g2}/kT} \quad \text{.....(3a)}$$

$$J_{ps} = \frac{qD_p}{L_p} N_A e^{-(qV_D + \Delta E_V)/kT} = \frac{qD_p}{L_p} \frac{N_{c1}N_{v2}}{N_D} e^{-E_{g1}/kT} \quad \text{.....(3b)}$$

In the above expressions, the notch like potential discontinuity ΔE_c is assumed to be zero.

For the structure shown in Fig.2b, these saturation currents are

$$J_{ns} = \frac{qD_n}{L_n} N_D e^{-(qV_D + \Delta E_C)/kT} = \frac{qD_n}{L_n} \frac{N_{c2}N_{v1}}{N_A} e^{-E_{g1}/kT} \quad \text{.....(4a)}$$

$$J_{ps} = \frac{qD_p}{L_p} N_A e^{-(qV_D - \Delta E_V)/kT} = \frac{qD_p}{L_p} \frac{N_{c2}N_{v1}}{N_D} e^{-E_{g2}/kT} \quad \text{.....(4b)}$$

For expressions of 4a and 4b the notch like potential discontinuity ΔE_v is assumed to be zero.

In the above expressions for the current density, effect of mobility ($\mu_{n,p}$) is included in the diffusion constant $D_{n,p}$ according to the Einstein relationship for non-degenerate semiconductors

$$D_{n,p} = \frac{kT}{q} \mu_{n,p} \quad \text{.....(5)}$$

In case of the structure shown in Fig 2a, the barrier for hole is much greater than the barrier for electron. The situation is reversed in case of the structure shown in Fig 2b. So, in case of fig 2a electron current will be dominating where as in Fig 2b hole current will dominate. Substituting the expression of $D_{n,p}$ in Eqn. 3 and 4 the final expression for the dominating components of saturation currents become

$$J_{ns} = kT \frac{\mu_n}{L_n} \frac{N_{c1}N_{v2}}{N_A} e^{-E_{g2}/kT} \quad \text{for Fig.2a} \quad \text{.....(6a)}$$

$$J_{ps} = kT \frac{\mu_p}{L_p} \frac{N_{c2}N_{v1}}{N_D} e^{-E_{g2}/kT} \quad \text{for Fig.2b} \quad \text{.....(6b)}$$

As the target of this work is to obtain maximum possible open circuit voltage, the values of the mobility and the density of states should be such that they produce the minimum possible values of saturation current. Hence the product of the mobility,

density of state terms in eqn. 6a or 6b is to be chosen properly to achieve that condition.

4. Results and Discussions

A number of p-n hetero- junction solar cell structures are considered to visualize the impact of mobility and density of states on the open circuit voltage (V_{OC}). The shining of the junction has been simulated by calculating the short circuit current density (J_{SC}) using the Air Mass 1.5 (AM1.5) spectrum of the solar radiation [4] to produce a realistic result. The calculated values of open circuit voltage (V_{OC}), maximum power out put (P_{max}), conversion efficiency (η) for different p-n junction solar cells are presented in Table 2.

Material	Stru-cture	V_{OC} (V)	J_{SC}	P_{max}	η(%)
GaAs/Ge	p/n n/p	0.20 0.25	50.58	6.0 8.6	7.32 10.5
GaP/Si	p/n n/p	0.644 0.657	34.29	18.5 19.0	22.6 23.2
Gap/InP	p/n n/p	0.896 0.796	26.93	21.0 18.5	25.6 22.58
GaP/GaAs	p/n n/p	0.995 0.89	24.46	21.5 19	26.24 23.2

Table 2: Open circuit voltage, maximum power output and efficiency for different solar cell structures. J_{SC}, and P_{max} values are given in mA/cm^2 and mW/cm^2 respectively.

It is interesting to see that the open circuit voltage for the same pair of materials in a hetero junction is not same when p and n type materials are swapped. It is quite interesting to see that the open circuit voltage in case of III-V compound semiconductors is higher when the higher band-gap material is p-type. When the higher band-gap p-type material is used, the potential barrier is higher for electrons that that for the holes. Under shining condition, the internal electron current is insignificant compared to the hole current due to the high potential barrier for the diffusing electrons. However, the mobility of the holes are in general is much lower than that of the electrons which cause lower current flow at any given forward junction potential. So, for a given amount of optical current, higher open circuit voltage is achieved. The density of state has also considerable effect, which can be visualized if we look at the values of V_D in Table 1.

5. Conclusions

The results show that the open circuit for a pair of material in a hetero-junction is not same if the p and n type materials are interchanged. Generally speaking, value of N_v is higher than N_c and value of μ_n is much higher than that of μ_p for III-V compound semiconductor materials. When hetero-junction solar cell is made from such materials, higher band gap material should be chosen for the p-side of the cell that produces higher open circuit voltage and corresponding higher efficiency. It is noteworthy that the efficiency of a n-InP/p-GaP hetero-junction solar cell is higher than that of p-InP/n-GaP cell by more than 13%. Similar is the magnitude of improvement for GaP/GaAs hetero-structures.

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