Gains in Activation Energy from Quasi Fermi Splitting, In Selectively Doped MQW Solar Cells

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Abstract: - Illumination of a Multiple Quantum Well (MQW) solar cell, affects the Fermi level position in the gap, directly under the conduction band of the narrow gap layer. In this communication, we explore Fermi level shifting and splitting in these structures. The neutrality condition is examined in terms of (a) availability of carriers (b) carrier confinement (c) escaping carriers (d) doping levels (e) layer width and (f) Fermi level dependence on doping and illumination. We conclude that short circuit currents and open circuit voltage are seriously affected.

Key Words: - Quantum wells, Fermi level, solar cells, open circuit voltage, short circuit current.

1 Introduction

Low dimensional optical devices are ideal probes for the study of excess carriers in quantum wells. The latter are regions where quantum size phenomena become important, because they are essentially traps of excess electrons.

Optical devices or optical heterostructures offer two advantages over their bulk counterparts: (a) they provide wider optical gaps, expanding the spectrum to shorter wavelengths and (b) they reduce recombination through mass separation: pre-existing electro-static separate electron-hole pairs (in the conduction band and the valence band respectively) This latter phenomenon is more accentuated in reduced dimensionality structures. Typical examples are GaAs and its Alloys: GaAs-AlGaAs (at several Al percentages). In solar cells; they provide higher short circuit currents (at least the III-V ones).

Nomenclature:

ΔE_c	=	conduction band difference
E_{c2}-E_{d2}	=	donor shallow levels
d_1, d_2	=	low and wide gap width
N_{d2}	=	donor concentration
N	=	number of periods
$\gamma_{0,1}$	=	miniband width
ΔE	=	minibands (from the bottom of the QW)
ΔE_{CF}	=	$E_c - E_F$ (activation)

2 The neutrality condition

The concentration of electrons bound in donor atoms can be estimated by ignoring electron-electron interactions. The mean number of electrons is [1,2,3]:

$$n_d = \frac{N_d}{1 + (1/2)\exp(E_d - E_F)} \quad (1)$$

Where, E_d is the donor level of energy in a sample with N_d (cm^{-3}) donor atoms and E_F is the "Fermi" energy or chemical potiental. For an n-type sample (N_d>N_a), electrons distribute themselves in such a way that overall charge neutrality is sustained.

$$n_c + n_d = (N_d - N_a) + p_v + p_a \quad (2)$$

The number of conduction and donor electrons at some temperature T increases over the T=0 state by the number of holes in the valence band (ρ_v). This is the neutrality condition, which allows one to locate the Fermi level at any temperature. In a multi-layered structure consisting of N repeatable periods, each of width (d) equal to the sum of the potential barrier width (d_1) and the quantum well width (d_2). Conduction carriers come from the donor sites in the gap of the layer doped with donor impurities. The role of such donor atoms is to raise the Fermi level closer to the conduction band of the lower gap material. More free electrons spill into neighboring quantum well sites increasing the electron population and reducing the gap between the conduction band and Fermi energy, and since conductivity $\sigma = \sigma_o \times \exp(-(E_c - E_F)/kT)$ the transport properties of solar cells are enhanced. While conduction is possible because of excess carriers from the donor sites, neutrality requires that the electrons (per volume) contributed by donor atoms be equal in numbers with the carriers left at the donor levels, plus the carriers that remain in the quantum wells, plus the conduction band free carriers. This is summarized in the following expression (2 refers to the wide gap and 1 to low gap layer):

$$
\begin{aligned}
& n_{d2}(NV_2) + n_w(NV_1) + \\
& V_T \int_{\Delta E_c}^{\infty} dE g_{3d}(E) f(E) \\
& = N_{d2}(NV_2)
\end{aligned}
\tag{3}
$$

Where n_{d2} is the electron concentration due to donor atoms, V_1 and V_2 are the volumes of layers 1 and 2, V_T is the total volume of the sample (the solar cell itself), N is the number of periods of the superlattice, and N_{d2} is the donor concentration in layer 2 (AlGaAs). ΔE_c is the conduction band discontinuity, g_{3d} is the bulk density of states (DOS), and f(E) is the probability distribution of the electrons (Fermi-Dirac or Maxwell-Boltzmann). Since $V_i/V_T = d_i/(Nd)$, expression (3) becomes:

$$
\begin{aligned}
& n_{d2}\left(\frac{d_2}{d}\right) + n_w\left(\frac{d_1}{d}\right) + \int_{\Delta E_c}^{\infty} dE f(E) g_{3d}(E) \\
& = N_{d2}\left(\frac{d_2}{d}\right)
\end{aligned}
\tag{4}
$$

3 Carriers in QW's

Carriers in the quantum wells are expressed via similar integrals as in (3):

$$n_w(T) = \int dE g_{2d}(E) f(E) \tag{5}$$

Where the DOS in (5) is 2-dimensional:

$$g_{2d} = \left(\frac{m^*}{\pi\hbar^2}\right)\sum_{k_z} \Theta(E - E(k_z)) \tag{6}$$

Where Theta is the step function, and k_z is the wave-vector of the III-V alloy in the growth direction according to the tight binding theory. The energy dispersion relation is then:

$$E(k_z) = E_n + 2\gamma_n \cos(k_z d) \tag{7}$$

Assuming a Maxwell-Boltzmann distribution function for the f(E) probability, and integrating (5) over the widths of the minibands in the quantum wells, we obtain:

$$
\begin{aligned}
& n_w(T) = \\
& 4\Gamma_o \exp\left(-\frac{\Delta E_F^0}{kT}\right)\exp\left(\frac{\gamma_o}{kT}\right)\sinh\left(\frac{\gamma_o}{kT}\right) \\
& -8\Gamma_o \exp\left(-\frac{\Delta E_F^0}{kT}\right)\exp\left(-\frac{\gamma_o}{kT}\right)\sinh\left(\frac{\gamma_o}{kT}\right) \\
& +10\Gamma_o \exp\left(-\frac{\Delta E_F^0}{kT}\right)\exp\left(\frac{\gamma_o}{kT}\right)\sinh\left(\frac{\gamma_o}{kT}\right) \\
& +\ldots\left[\text{Terms with the } 2^{\text{nd}} \text{ mini-band}\right]
\end{aligned}
\tag{8}
$$

Where $\Gamma_o = m^*(kT)/\pi\hbar^2 (cm^{-3})$, and ΔE_F^0 is the distance of the miniband from the Fermi level plus the activation energy:

$$E_0 - E_F = \Delta E_F^0 = \Delta E_0 + \Delta E_{CF}$$

All quantities in (8) are known parameters based on the geometry of the superlattice, and the exponential factors include the Fermi energy.

4 Carriers due to donors and carriers above E_{c2}

The number of carriers donated by shallow donor impurities is [4, 5, 6, 7]:

$$n_{d2} = N_{d2} \exp\left(-\frac{E_{c2} - E_F}{kT}\right) \tag{9}$$

Replacing the difference in (9) in terms of the band discontinuity:

$$n_{d2} = N_{d2} \exp\left(-\frac{\Delta E_{CF}}{kT}\right) \exp\left(-\frac{\Delta E_C}{kT}\right) \qquad (10)$$

On the other hand, free carriers above the conduction band of the wide gap layer, are simple carriers in the energy continuum in the bulk of both layers in a mqw-solar cell. Namely,

$$n_c = N_c \exp\left(-\frac{\Delta E_c}{kT}\right) \exp\left(-\frac{\Delta E_{CF}}{kT}\right) \qquad (11)$$

Where N_c is the effective DOS of the wide gap material.

5 Activation energy ΔE_{CF}

We solve for the activation energy from (4) via (5), (8), (10) and (11):

$$\Delta E_{CF} = kT \ln\left\{ \frac{\exp\left(-\frac{\Delta E_c}{kT}\right)}{\sinh\left(\frac{\Delta E_c}{2kT}\right)} \times F \right\} \qquad (12)$$

With

$$F = \left(\frac{d_1 A}{2 d_2 N_{d2}}\right) + \left(\frac{N_c d}{2 N_{d2} d_2}\right) \exp\left(-\frac{\Delta E_c}{kT}\right)$$

And where

$$A = 4\Gamma_0 \exp\left(-\frac{\Delta E_0}{kT}\right) \sinh\left(\frac{\gamma_0}{kT}\right)\left[3\sinh\left(\frac{\gamma_0}{kT}\right) - \cosh\left(\frac{\gamma_0}{kT}\right)\right] +5\left[\exp\left(-\frac{\Delta E_0 + 2\gamma_0}{kT}\right)\right]$$

6 QFL's and illumination

We consider a single quantum well between two layers of wide gap material (potential wells). Typically, this means a GaAs layer in contact with two layers of AlGaAs from left and right. An open-circuited solar cell, under illumination, develops a non-zero voltage in its output. This called the open circuit voltage, which is the most important solar cell parameter. It is because of this voltage, that the device will eventually sustain a current through a load, when applied for production of electricity. The question becomes: what is the effect on the Fermi levels on both sides of the solar p-n junction? Under zero illumination the Fermi levels coincide. This is because the number of carriers from left to right equals the number of carriers from right to left. Note that if $f_1(E)$, $f_2(E)$ are the Fermi functions in the two regions, $g_1(E)$, $g_2(E)$ the DOS of the two regions, then:

$$\begin{aligned} &g_1(E)(1-f_1(E))g_2(E)f_2(E) = \\ &g_1(E)f_1(E)g_2(E)(1-f_2(E)) \end{aligned} \qquad (13)$$

and therefore $f_1 = f_2$.

Also, under illumination, open circuit voltage develops, so that:

$$\begin{aligned} &g_1(E)(1-f_1(E))g_2(E+qV_{oc})f_2(E+qV_{oc}) = \\ &g_1(E)f_1(E)g_2(E+qV_{oc})(1-f_2(E+qV_{oc})) \end{aligned} \qquad (14)$$

From (14) it follows that

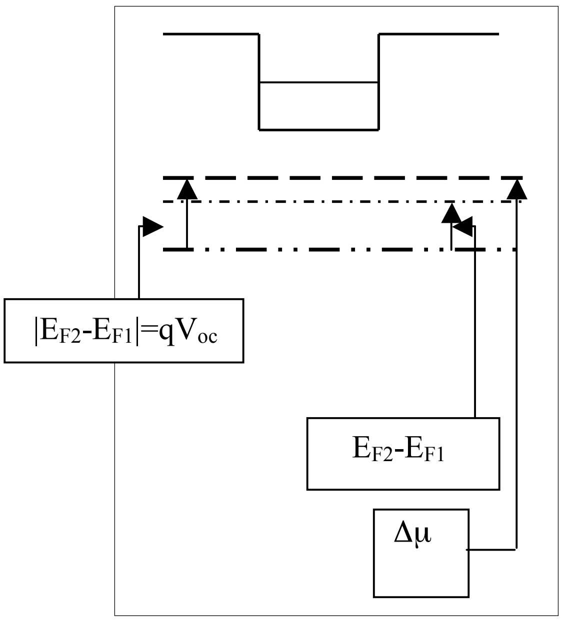
$$f_1(E) = f_2(E+qV_{oc})$$

Or that

$$E_{F2} - E_{F1} = qV_{oc} \qquad (15)$$

Expression (15) establishes the fact that under open-circuit condition and under illumination, the solar cell (any solar p-n junction) reacts within neutrality accordingly. First of all, due to open-circuit voltage, the device adjusts to zero currents by splitting the Fermi level into two quasi-Fermi level in regions 1 and 2. This exactly is the meaning of expression (15). On the other hand, illumination causes a further split in the quasi Fermi level of medium 1 (low gap medium). This is due to the fact that as carriers in the quantum wells increase in numbers, the mere quantum event of carrier confinement cause a re-adjustment of the quasi-Fermi level in medium one. Thus, under illumination (a) the Fermi levels split by qV_{oc} due to neutrality conditions and (b) the quasi Fermi level E_{F1} shifts upwards by an amount $\Delta\mu$ of the order of 12 meV. Thus the overall open circuit voltage will increase. Figure 1 below depicts the situation: a quantum well and Fermi level behavior.

Figure 1: Three quasi-Fermi levels in the vicinity of a quantum well with its eigen-energy. The total open circuit voltage and the excess Fermi level splitting are shown explicitly.



As seen from Fig. 1 above, the expected open circuit voltage increases by an amount Dm, due to quantum size effects. Thus an overall gain is expected as far as open circuit conditions are concerned.

7 Results

The goal in this communication is to show clear improvements in the activation energy of a solar cell with quantum wells in its intrinsic region. Activation energy is the difference in energy between the bottom of the quantum well (hence the conduction band E_{c1}) and the actual Fermi energy right beneath it. As seen in Fig. 1, the Fermi energy shifts and splits under illumination. Table 1 below depicts the gain on activation energy.

Table 1: Activation energy without and with Fermi level split due to quantum size effects, in the quantum wells.

d_2(A)	E_c-E_{F1} (eV) No split	E_c-E_{F1} (eV) With split
5	0.260	0.248
10	0.250	0.238
15	0.240	0.228
20	0.245	0.233
25	0.244	0.232
30	0.240	0.228
35	0.220	0.208

Table 2: Activation energy dependence on doping.

N_{d2} (cm^{-3})	E_{c1}-E_{F1} (eV) Without QF-split	E_{c1}-E_{F1} (eV) With QF- split
8.65×10^{16}	0.360	0.348
1.47×10^{17}	0.355	0.343
2.35×10^{17}	0.350	0.338
3.88×10^{17}	0.335	0.323
6.39×10^{17}	0.320	0.308
1.0×10^{18}	0.310	0.298

As seen from Table 2, high doping of the barrier region causes narrower activation energy. The third column of table 2 depicts the final position after the Fermi level split correction. We notice that the activation energy reduces by a net amount of the order of 12 meV. Such reductions cause an increase to conductivity by a factor exp ($\Delta\mu/kT$). Thus gains in the activation energy and in the open circuit voltage are expected when superlattices are incorporated in heterostructure solar cells.

8 Conclusions

When superlattices [8,9] are used in solar cells, the activation energy is the difference in energy between the bottom of the conduction band and the Fermi level (see Fig. 1). This study has shown that the Fermi level depends on (a) the geometry of the device (this means the layer characteristics and (b) on the doping levels, as seen from Table 2. In both cases (as in Table 1, 2) the activation energy reduces. Our general conclusion is that excessive doping of the wide gap layer and gradual increase of the of the width of the potential barrier produce a Fermi level split which is equal to the open circuit voltage. Furthermore, the open circuit voltage will increase by the amount of ~12 meV, which produces an even higher open circuit voltage. Losses are found from the fact that temperature increases cause a reduction in the activation energies. We attribute this fact to the role of high temperatures: the higher the temperatures the more scattering expected, and hence more losses.

9 References

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