Tunneling vs. Thermionic Currents in Multi-Quantum Well Photovoltaic Structures

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Abstract: - Photogeneration in the intrinsic region of a p-i-n device excites carriers in the conduction bands with non-zero currents. A special class of multi-quantum well photovoltaic structures (mqw-PV) is p-i-n PV structures where photo-generation may cause tunneling and or thermionic escape, from the intrinsic region. In this communication, we propose a formalism of tunneling versus thermal escape in p-i-n mqw-PV structures. The concept is a superlattice embedded in the intrinsic region of a p-i-n solar cell, which under illumination generates free carriers for current collection. We show that quantum size effects do matter in these devices and we compute the corresponding short circuit currents. We conclude that thermal and tunneling currents behave almost in a complimentary way: tunneling dominates at low temperatures and that thermal escape dominates at high temperatures. We report results at temperature levels (two extremes at -10and 100^{o}C) and predict total current density values near an average of 60mA/cm^2. We finally conclude that the main drawback of these devices is their compromised open circuit voltage.

Key – Words: Microelectronics, Solar cells, superlattices, quantum wells, tunneling

1 Introduction

Periodic heterostructures (superlattices) offer immediate advantages over their counterparts, especially in the area of solar cells. The existence of a superlattice in the intrinsic region of a p-i-n solar cell ensures (a) photo-carrier acceptance and (b) higher rate of carrier escape than rate of carrier losses (via recombination mechanisms). Excited carriers from the valence bands of the materials involved may gain sufficient energy from incident photons, and they may escape to the conduction bands. The latter are of two types; wide gap and low gap. Such an existence leads to the formation of quantum wells, where discrete energy levels are susceptible to carrier trapping at the eigen-energies. In realistic devices today, the maximum number of discrete levels is no more than two (III-V alloys of GaAs/AlGaAs). Appropriate choice of quantum well width may lead to only one energy level in each quantum well. The same picture is true for holes generated in the valence bands: they do get captured in their respective wells (for holes) and they abide by their own mini-band energies. The result of carrier photo-generation is the widening of the optical gap, in other words, the energy gap allows more incident wavelengths (shorter) to be absorbed by the device. This is a direct advantage of superlattice design, since multi-gaps offer wider acceptance of wavelengths. On the other hand, electrons may escape to the conduction band and become useful current, mainly due to pre-existing electrostatic fields that span the totality of the intrinsic region. Thus electrons, once free above the mid-region, are free to travel to the n-side of the device. In the process, they may encounter minimized collisions, simply because of the absence of impurity scattering (due to low doping). The aim of this work is to examine the two main current components and depict their behavior with temperature.

Tunneling currents are possible only via the potential barriers formed between neighboring cells. A cell is a complete superlattice period that includes, a quantum well confined between two adjacent potential barriers (wide gap material). A cell could be seen as a well and a barrier unit successively (periodically) repeated along the span of the intrinsic region. As long as the wide gap layers are thin, electrons may tunnel through the “walls” and thus may travel through the total intrinsic region. At high temperatures, electrons accumulate more kinetic energy and thus they are prone to escape from the wells, rather than to tunnel. On the other hand, for thick potential barriers, thermal escape becomes the only way out of the wells, particularly at high temperatures. Another advantage of superlattice in the intrinsic region of p-i-n solar cells is the effective mass separation. Once a carrier is in the quantum well, it has a finite probability either to recombine (lost) or to escape.

However, even in the case of escape, there is a chance for the carriers to recombine when they are above the wells, in the conduction band. In this situation, effective mass separation occurs. Electrons and holes with different mobility values in the crystal separate immediately. This is a further advantage, because electron-hole pair separation contributes to current increases.

2 Tunneling Currents

Transport along the growth direction is feasible. This is so because confined electrons in the quantum wells have a finite probability to tunnel through the potential barriers. Thus, *perpendicular* transport is possible in these structures. In addition, quantization of energy levels in the wells leads to mini-band formation and optical gap widening, by greater wavelength absorption. In other words, shorter wavelengths are absorbed, and thus a wider spectrum of photons is possible. One may evaluate tunneling current densities through potential barriers via a first principles method. Under photon illumination levels (with absorption coefficient α) G_{ph}, the net tunneling currents are the difference of carrier transport from left to right and from right to left. Thus, the tunneling current is [1]:

$$J_{TU} = \left(\frac{qA\tau}{L_w L_i}\right)\iint dx\, dE\, G_{ph}(\lambda) e^{-\alpha x} g(E) P(E) \times \left[f(E) - f(E + qV_{oc})\right] v(E) \tag{1}$$

Where g(E) is the density of states available for confined carriers in the quantum wells in units of $eV^{-1}\,cm^{-2}$ (2D-DOS), P(E) is the tunneling probability (assuming no inter-band hopping). $f(E-E_{FL})$ is the Fermi-Dirac distribution, by which the carriers are abiding in any system with quantum size effects (with explicit dependence on the quasi-Fermi level of the left side of the device), $f\left(E + qV_{oc} - E_{FR}\right)$ is the Fermi probability at the right side of the device (at the edge of the n-region). At the right side, the energy increases by the open-circuit voltage energy qV_{oc}. The last term in the above integral is the velocity of carriers $v(E) = \left\{2\left(\Delta E_c - E\right)/m^*\right\}^{1/2}$ as a function of conduction band discontinuity, eigen-energy and carrier effective mass.

The tunneling probability is:

$$P(E) = 16\left(1 - E/\Delta E_c\right) e^{\left\{-k_b\left[1 - E/\Delta E_c\right]\right\}^{1/2}} \tag{2}$$

Where the unit-less factor k_b is the barrier-related wave number

$$k_b = 2L_b\left\{4\pi m^* \Delta E_c / h\right\}^{1/2} \tag{3}$$

and L_b is the potential barrier width.

The Fermi-Dirac probability includes the quasi Fermi level of the left side of the device (at the end of the p-region). In (1), A is the cross section of the device, τ is the relaxation time of the carriers, and L_i is the intrinsic region length. The first integration in (1) covers the intrinsic region (from 0 to L_i), and the second integration allows for possible trapped energies in the quantum wells. The energy integration includes energy values within the bandwidth of the minibands in the quantum wells. Typically, III-V photovoltaic devices with quantum wells in the intrinsic region contain at most two energy levels. Under an appropriate choice of width of the quantum wells, these energy levels may reduce to only one in the well and the second one at the edge of the quantum well and conduction band continuum. The Fermi factor, after some manipulation, becomes:

$$f(E) - f(E + qV_{oc}) = \frac{\sinh\left(qV_{oc}/2kT\right)}{4\cosh\left(\frac{E - E_{FL}}{2kT}\right)\cosh\left(\frac{E - E_{FL} + qV_{oc}}{2kT}\right)} \tag{4}$$

Note also that, the Fermi levels split by an amount equal to the open circuit voltage. Via (2) and (4), (1) leads to the following explicit tunneling current formula [1, 2, 3]:

$$J_{TU} = J_{SC} =$$
$$32\pi(qA\tau/L_i)G_{ph}\left(1-e^{-\alpha L_i}\right) \times\left[\left(2m^*\Delta E_c\right)^{1/2}/h^2\right]\sinh(qV_{oc}/2kT) \tag{5}$$

Note in (5) the term qV_{oc}. This is the open circuit voltage and is equal to the difference between the quasi-Fermi levels in the device. Under dark conditions the quasi Fermi levels coincide along the structure due to the fact there is no net carrier population drifting across the device. However, under illumination with absorbable wavelengths, excess carriers do develop that cross the device along both directions (left to right and in reverse). If the solar cell is open-circuited, a non-zero voltage develops at the external leads of the cell: the open circuit voltage. For any solar cell, the total current is simply a diode current of the type:

$$J = J_s\left(e^{(qV/kT)}-1\right)-J_{sc} \tag{6}$$

Where the last term is the short-circuit current density. Under open-circuit conditions (ideality factor equal to one) the total current of the cell is simply zero, hence:

$$0 = J_s\left(e^{(qV_{oc}/kT)}-1\right)-J_{sc} \tag{7}$$

From (6), a dependance of the short circuit current on open circuit voltage is clear:

$$J_s\left(e^{(qV_{oc}/kT)}-1\right)=J_{sc} \tag{8}$$

The total current contribution is the superposition of all current components in the cell. These are the tunneling currents, the thermal currents and the excess-carrier currents. Evaluation of all three components may lead to computations via (8) of the open circuit voltage of any p-i-n cell with a superlattice in the mid-region.

3 Thermionic Currents

Thermal currents due to electrons escaping from the quantum wells are:

$$J_{TH} = q\frac{A\tau}{L_i}G_{ph}\left(1-e^{-\alpha L_i}\right)\times \int dEv(E)g(E)f(E+qV_{oc})(1-P(E)) \tag{9}$$

The last term in the integral ensures non-tunneling (recall that P(E) is the tunneling probability). The limits of the integration are from the lowest miniband to infinity (deep in the conduction bands of both layers involved). Expression (9) becomes as follows:

$$J_{TH} = J_{oo}T^{3/2}e^{-(qV_{oc}+E_1-E_F)/kT} \tag{10}$$

Where the pre-factor is:

$$J_{oo} = q\frac{A\tau}{L_i}G_{ph}\left(1-e^{-aL_i}\right)\left(2\pi m^* k^3\right)^{1/2}\left(\frac{4\pi}{h^2}\right) \tag{11}$$

The energy difference in (10) is $E_1 - E_F = \Delta E_1 + (E_{c2} - E_{FL}) - \Delta E_c$, where the first is the eigen-energy from the bottom of the quantum well (E_{c1}). Hence, the thermal currents will become explicitly dependent on the position of the Fermi levels relative to the wide gap layer and the conduction band discontinuity as follows:

$$J_{TH} = J_{oo}T^{3/2}e^{-\left\{\left(E_{g2}+qV_{oc}+\Delta E_1-\Delta E_c\right)/kT\right\}}e^{\left\{\left(E_{FL}-E_{v2}\right)/kT\right\}} = J_{oo}T^{3/2}e^{-\left\{\left(E_{g2}+qV_{oc}+\Delta E_1-\Delta E_c\right)/kT\right\}}\left(\frac{N_v}{p}\right) \tag{12}$$

Where, the last term is the ratio of the effective density of states and the doping of the wide gap layer, and where E_{g2} is the energy gap of the wide-gap material (AlGaAs).

4 Excess Carriers

Collection of carriers (during illumination) occurs in the n-region of the device as well. Minority holes are generated in the n-region, and hence minority hole-currents will develop from there as well. Thus, if δp_n

is the density of excess holes *diffusing* in the n-region, then [5]:

$$\delta p_n'' - \left(\frac{\delta p_n}{L_p^2}\right) + \left(\frac{G_{ph}}{D_p L_i}\right) e^{-\alpha\left(x + L_i\right)} = 0 \qquad (13)$$

Expression (13) is the diffusion equation for excess holes in the n-region of the device. L_p is the diffusion length of these holes. The double prime indicates the second derivative of the excess holes in the region; the exponential factor includes all values of x in the n region and beyond the i-region respectively (the point x = 0 is at considered to be at the interface between the p- and i-regions). The corresponding hole-current is found from (13):

$$\begin{aligned} J_p &= -qD_p\left(\frac{d\delta p_n}{dx}\right) \\ &= qG_{ph}\left(\frac{aL_p}{1+\alpha L_p}\right)e^{-\alpha L_i} \end{aligned} \qquad (14)$$

The diffusion length for holes in GaAs systems vary from 2.96 to 3.6 μm at temperature ranges from -10^{o} C to 100^{o}C.

5 Total Current

The total short-circuit current density is the sum of the tunneling and thermal current densities, as found in the previous sections. Table 1 depicts the results for thin quantum well layers in a solar cell device at two temperatures, -10 ^{o}C and 100 ^{o}C.

Table 1: Short circuit current of a p-i-n cell. Three different contributions are depicted along with the total current density [1].

J_{sc} (mA/cm^2)	+100^{o}C	-10^{o}C
J_{TH}	52.78	14.20
J_{TU}	6.92	42.94
J_p	2.26	2.17
J_{Total}	61.96	59.31

Short circuit currents are depicted at Table 1 above. It becomes clear that thermal currents are dominating at high temperatures, and tunneling currents are dominating at low temperatures. Total currents seem to be in the same order (given that numerical instabilities are unpredictable). From the same Table, one may conclude that tunneling currents are dominant at low temperature environments (as in outer space applications), while they are rather insignificant at relatively high temperatures (hot summer days at ~40^{0}C). Minority hole-currents do not seem to be seriously affected by temperature, as seen in the same Table. Their level remains the same (2.26 and 2.17 mA/cm^2). Notice also that the tunneling current increases almost by a factor of seven from low to high temperature, while the thermal component reduces by a factor of almost four. It seems (as seen from the results of Table 1) that superlattices in the intrinsic region of p-i-n devices offer the obvious advantage of really high short circuit currents. The likely values of the open circuit voltage can be obtained from expression (8):

$$V_{oc} = \left(\frac{kT}{q}\right)\ln\left[1 + \left(J_{sc}/J_s\right)\right] \qquad (8')$$

For short circuit currents at 60mA/cm^2, reverse saturation currents 10^{-7} mA/cm^2 (a cell 1x1cm^2 is considered), expression (8) at 100^{0}C yields open circuit values equal to 0.646V, and at -10^{0}C, the voltage values are at 0.460V. It becomes obvious then that superlattices do cause high short circuit currents but their response is rather compromised on the output voltage. A more comprehensive study of explicit current dependence on temperature is under way.

6 Recombination Issues

What is the role of recombination in the process of photogeneration? In thermal equilibrium, generation rates are equal to recombination rates. When thermal equilibrium is disturbed, direct recombination rates R may be expressed as follows:

$$R = (\text{constant}) \times np \qquad (15)$$

Where, n and p are the total electron and hole concentrations (including the equilibrium and the excess concentrations). At thermal equilibrium, recombination rates are:

$$R_o = (\text{constant}) \times n_o p_o = n_i^2 \qquad (16)$$

Thus,

$$R = R_o\left(pn/n_i^2\right) \tag{17}$$

R_o is found to be of the order of 10^{-5} cm^{-2} s^{-1} and the concentration of electrons in the quantum wells is of the order of 10^{12} to 10^{14} cm^{-2}, so that the total recombination does not seem to exceed 10^{12} cm^{-2} s^{-1}, and has no real effect on photo-generation under incident flux levels at 10^{17} photons per area per time (cm^{-2} s^{-1}).

7 Conclusions

Superlattices in the intrinsic region of p-i-n solar cells are promising probes for better cell performance [6, 7, 8, and 9]. This is clear from out calculations of short circuit currents. In this communication we propose incorporating a superlattice in the i-region of a solar cell. A superlattice provides a multiplicity of quantum wells where photogenerated carriers are trapped and subsequently escape via two routes: (a) tunneling and (b) thermionic escape. Both of these processes of escape are found to compete in carrier escape and final current collection. The first one (tunneling) dominates at the low temperature limit, while the second current component dominates at the high temperature limit. We attribute this split in roles to the fact that at high temperatures the photo-excited carriers have high thermal velocities and hence higher kinetics (kinetic energy). This provides a lead to thermal currents. With the same token, at low temperatures, the kinetic energy of the carriers reduces dramatically, and tunneling is more likely to happen. On the other hand, under low doping levels, phonon scattering (and impurity scattering) inhibit tunneling dramatically. We compute the contributions of both currents and find that the total current of the cell (short circuit current) finalizes in the neighborhood of $60mA/cm^2$ (see Table 1). We find that thermal currents reduce by a factor of seven from the high to the low limit of temperature, while the tunneling current increases by a factor of four from low to high temperature. We also find that these structures lack in voltage: the generated mediocre open circuit voltages, a rather serious flaw in their overall performance.

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