Tunneling Assisted Photo-Conductivity For Novel High Efficiency p-i-n MQW Solar Cells

ARGYRIOS C. VARONIDES & ANDREW W. BERGER
Physics and Electrical Engineering E Department
University of Scranton
800 Linden Street, Scranton PA, 18510
United States

Abstract: - We propose a first principles method of calculating the photo-component of tunneling conductivity of a specific superlattice (SL) photovoltaic structure: an InP/InGaAs P-I(SL)-N solar cell. The method we follow is based on the generalized Greenwood-Kubo formulation and on the causal form of the Green's function. The vertical conductivity (along the growth direction of the device), under illumination, involves a group of parameters directly connected to the geometry of the device (hence it is on one's disposal) and the quantum size effects in the quantum wells of the superlattice. The latter is incorporated in the intrinsic region of p-i-n solar cells and bring along the advantage of carrier tunneling, which is possible if thin layers of wide-gap material (InP at 25A/layer) are grown successively on narrow bandgap material (lattice-matched $In_{0.53}Ga_{0.47}As$ at 70A/layer) to form a sequence of quantum wells. Appropriate doping of the barrier regions ensures Fermi level pinning inside the quantum wells (a great advantage, since the excitation energy of photo-generated electrons greatly reduces in this case) in the neighborhood of the ground state miniband. We propose a direct calculation of conductivity under illumination:

(a) we replace the intrinsic region of the *p-i-n* solar cell with an InP/InGaAs superlattice
(b) we explicitly derive the photoconductivity $\sigma(\omega,T)$ as a function of photon frequency and temperature T
(c) we explore the variations of photoconductivity for a large number of superlattice periods
(d) we examine the variation of photoconductivity for a range of incident photon energies from 1.4eV to 2.6eV
(e) we find that conductivity is greatly enhanced and may reach average maximum levels for superlattices with above 12 total periods
(f) we predict efficiency gains in excess of 24%, under moderate levels

Key-Words: - Superlattices, solar cells, conductivity, Green's functions

1 Introduction

The growth and properties of such heterojunction superlattices, under selective doping [1,2,3], are of great importance in the case of solar cells as well, where one is interested in improved carrier transport, that is, high carrier mobility, low scattering rates, low resistivity and thus high conductivity values. One important feature of selectively doped (or modulation doped) heterostructures is that all the mobile carriers (trapper int he

quantum wells, due to mainly moderate doping levels of "donor" impurities) are spatially separated from their parent donor impurities in a permanent and irreversible manner [1]. Typically this is the case for GaAs/A1GaAs structures. Superlattices in solar cells have been proposed [4] as a new means for better solar cell performance. One of the transport properties that is greatly improved is conductivity. Superlattices incorporated in solar cells are responsible for quantum effects that are generally expected to improve device performance. Transport of carriers is enhanced via tunneling through thin potential barriers. These carriers will be trapped in minibands within quantum wells of sufficient widths. It is to be understood that layers of wide band-gap material (as is the case of interest in InP/lattice matched alloys here) are grown on top of narrow gap material in order to form quantum wells. In the present case, InP layers would play the role of the wide gap semiconductor and its lattice matched [5] alloy $In_{(0.53)}$ $Ga_{(0.47)}$ as is the narrow gap layer that is incorporated in the n-region as well.

Quantum wells and superlattices are known to (a) improve solar cell performance [6], in the sense that they provide traps for the electrons within specific eigen-energies (minibands) (b) these carriers are capable of tunneling through thin barriers (i.e. along the growth direction), while they are essentially free along the transverse direction and (c) they are known to pin the Fermi level toward the conduction band edge and even in the quantum well [7]. If the Fermi level can be shifted in the quantum well and coincide with an energy miniband, it will cause an uninhibited flow of carriers through the potential barriers making them almost transparent. It is this last advantage that is to be explored in this communication: to study the conductivity under illumination for a p-i-n solar cell, where the Fermi level coincides with a miniband in the quantum wells of the superlattice. A specific geometry is to be picked, namely: (i) well and barrier widths (d_1,d_2, respectively) at preselected values (ii) moderate doping to pin the Fermi level along with the ground state. A formula is derived from first principles and in the weak scattering limit. Section 2 outlines the mathematical model used in the Kubo-Greenwood general formula for conductivity and in terms of the Green's function [8]. Section 3 deals with the results of the calculations, and discusses the plots. The method provides the means for conductivity and resistivity calculations of devices that include superlattices. In section 4 we conclude our discussion with improvements predicted and future designs where the same formalism can be applied directly. The method can be extended to FET structures and diode lasers as well.

2 Computations

The real part of the conductivity given by the Kubo-Greenwood formula is

$$\sigma = \frac{e^2\hbar}{\pi m^2 \Omega} \int dE \, \frac{f(E) - f(E+\hbar\omega)}{\omega\hbar} Tr\left[P_\alpha \; Im\, G(E+\hbar\omega) P_\alpha \; Im\, G(E)\right] \tag{1}$$

Where m represents the effective mass of the carriers in InP, f (E) is the Fermi-Dirac distribution function, P_a is the momentum operator, with α = x, y, z. The integral in (1) is performed over the narrow band from E_0- (1/2 bandwidth of E_0) to E_0+ (1/2 bandwidth of E_0). E_0 is the ground state in the quantum well which is taken to be coinciding with E_F. The Green's function is:

$$G(E,k_z) = \frac{1}{E - \Sigma_1 + i\Sigma_2 - E(k_z)} \tag{2}$$

In (2), E (k_z) is the superlattice dispersion relation with k_z being the superlattice wave-vector confined in the superlattice Brillouin zone [10], and where the rest of the denominator includes the electronic self-energy. The DC case may be derived from (1) as photon frequency approaches zero values (not studied here). Here we are presenting the AC case for a range of incident photons. We want to apply the (1) by means of (2) in a superlattice structure embedded in the n-region of the p-I-n solar cell. It turns out the conductivity is a function of (i) the superlattice parameters (repeat distance, miniband width, number N of periods) (ii) the temperature T (iii) the volume of the device (as seen in (1). Inserting (2) in (1), one obtains a final result that describes the conductivity along the growth direction of the superlattice structure. We impose the following condition: *we want the Fermi level to coincide with the ground state in the quantum wells.* From (1) and (2) we obtain that:

$$\sigma(\omega,T) = \frac{2e^2(\Sigma_2\gamma_n d)^2}{\hbar\ \omega\pi\Omega} \sum \int \frac{e^{-(E_n - E)/kT}\ \sin^2(k_z d)}{g(E,\omega,\gamma_n,N)^2} dE \tag{3}$$

Where the summation is over the superlattice wave number k_z, in the tight-binding approximation over the bandwidth of the minibands, and where the function g in the denominator of (3) is:

$$g = \left[E + \hbar\omega - E_n + \gamma_n \cos(2\pi n/N)\right]^2 \left[E - E_n + \gamma_n \cos(2\pi n/N)\right]^2 \tag{4}$$

N is the number of periods, E_n is the sub-band energy, and Σ_2 [8,9] is the self-energy of the carriers in InP. InGaAs layers are of lower gap and thus the quantum wells are formed

within the gap of the InP layers. This means that the Fermi level can easily be pinned at the ground state level *with moderate doping levels.* Once ground state channeling is established, the carriers are expected to overlap with neighboring ones thus settling the tunneling process. By insertion of (2) and (1) and after some manipulation, one is led to a third relation where the conductivity becomes an explicit function of all superlattice parameters (period number (N), layer widths (in nm), miniband widths (meV), dimensions of solar cell, doping levels).

3 Results

The superlattice region is the n-side of the device where multi-quantum wells (MQW's) are formed of InP and InGaAs layers. The selected geometry is as follows: well width d_1 = 50A, barrier width d_2 = 25A. The overall period of the superlattice is d=75A, while as energy dispersion relation is the one of the tight-binding approximation [10,11]. The conduction band discontinuity is at 0.210 eV and supports two minibands at ~71meV and 208meV (very close to the edge of the discontinuity) respectively. Tight binding calculations [12] give a miniband width, at least for the ground state (which is the case here), of ~10 to 14meV. Under moderate doping levels (N_d ~10^{18} cm^{-3} in the In-barrier regions) and under weak scattering conditions, the integral in (3) can be computed. Ground state based tunneling conductivity is taken into account, at 300K, and $\sigma(\omega, T)$ is computed against number of superlattice periods N at three difference incident photon energies: 1.4, 2.2 and 2.6 eV respectively. Computations show that:

(a) Conductivity as a function of superlattice period-number devices, with 20 superlattice periods (total width 0.15 μm) reach conductivity values above 2,000 S/cm at 2.6eV (λ = 0.477 μm), and T= 77 ^oK; a clear improvement over bulk cases (~300 S/cm [10,13]).
(b) At room temperature, photoconductivity is found to exceed 3,000 S/cm.
(c) Shifting to longer wavelengths, corresponding to photon energies of the order of the energy gap of InP, photoconductivity exceeds 10,000S/cm at room temperature and 6,000 S/cm at 80 ^oK.
(d) For length of superlattice region ~0.3 μm (~40 periods), conductivity decreases with increasing photon energy range from 1.4 to 2.6 eV ($E_{g,\ InP}$ = 1.35eV) from (less than) 3,000 to 900 S/cm (wavelengths varying from 0.477 μm to 0.88 μm). At 80^oK, photoconductivity drops from a maximum value in excess of 1500 S/cm to 500 S/cm in the same energy range or wavelength interval as before.
(e) Photoconductivity maximum values (see above results) seem to be very sensitive to the number of superlattice periods: its predicted value decreases consistently with increasing number of periods N. We attribute this reduction of transport quality to increased losses due to further scattering, as the extent of device increases drastically (e.g. at 300^oK, for N=40 periods, conductivity drops to 2,500 S/cm (down from 10,000 S/cm), while for space conditions photoconductivity

values drop to ~1,500 S/cm (from 3,000 S/cm). The latter is not so dramatic an effect, because of less scattering, taking place at low temperatures.

(f) Negligible conductivity is predicted at incident photon entries below the energy gap of InP (<1.35eV), abiding by the fact that no (or negligible) absorption would be expected to be succeeded by the material.

(g) For photovoltaic use, and for space applications, it seems likely that, photons near the band gap of InP will cause maximum absorption and hence highest device performance. The latter, is to be explored further and in terms of open circuit voltage and short circuit current.

(h) Computations were based on the following fact: the fermi energy was taken to be coinciding with the ground state (miniband) in the quantum wells. This maximizes the probability of escaping electrons from the quantum wells into neighboring wells, via tunneling, essentially making the potential barriers transparent to electrons.

Similar calculations-computations can be repeated for other III-V / Alloy material candidates, especially for space applications of solar cells. At the moment, terrestrial advantages of these devices are overcome by production costs, which are much higher compared to competing materials (especially silicon). On the other hand, III-V / Alloy materials offer much higher conductivity values, therefore the exhibit excellent transport properties via quantum size effects (tunneling), and they are already known to have higher collection efficiencies compared to silicon devices (in excess of 20% for space-related applications as opposed to 10-15% for silicon-based solar cells).
Low temperatures are of interest here for two reasons:

(i) InP and its lattice matched alloys are known to be resistive to radiation when exposed as devices in space applications and

(ii) Computation results show a clear possibility of Superlattice-based InP/Alloy solar cells for space applications.

4 Conclusions

Tunneling assisted photoconductivity in III-V/Alloy devices is shown to be superior to that of bulk "main stream" devices. When quantum wells are incorporated into p-i-n photovoltaic devices, improvement of transport properties in general and of photoconductivity specifically, is found. Such devices may be designed for various purposes, namely, solar cells, photoconductors, LED's etc. Special interest in this paper is focusing around possible photovoltaic use of these multi-layered materials.

In this communication we propose a method of predicting the transport properties of InP/Alloy superlattice heterostructures, in terms of photoconductivity. We explore the situation of carrier *tunneling* in solar cells made out of InP and lattice-matched alloys. We find that the conductivity is expected to increase far above 300 S/cm, which is the nominal value for bulk InP solar cells. In fact, we observe an increase of conductivity in excess of 2600 S/cm at room temperature and at 1.4eV illumination of incident photons. Overall

conductivity response of InP/InGaAs solar cells under illumination from 1.4 eV to 2.6 eV gives encouraging results, namely, conductivity values from 900 S/cm to 2600 S/cm for incident light spectrum from 0.477 μm to 0.88μm. Such improvements in transport properties indicate that InP/Alloy solar cells are very good candidates for wide-scale applications. The design considered here includes a superlattice structure of thickness 0.3 μm (~40 periods at 75A each). The p-i-n (SL) device is assumed to have the appropriate moderate donor doping to guarantee coincidence of the Fermi level with the ground state in the quantum well. As it is shown from the discussion in section 3 above, the conductivity of the device is highly increased and hence such structures may lead to low resistivity (~3.8 X 10^{-4} Ohm cm) solar cells. Note of course, that photovoltaic devices (illuminated over a wide range of incident photon energies) will essentially compromise their photoconductivity response accordingly, but as it has been shown here, (lattice-matched) InP related devices seem to have an advantage over similar counterparts (Si, Si-Ge), for succeeding very high conductivity values. Complete solar analysis of these structures, such as open circuit voltage, short circuit current, fill factors, and efficiency calculations are currently under study.

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