Tunneling Conductivity of III-V Multiquantum Well P-I-N Photovoltaic Heterostructures by Means of the Causal Green's Function

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Abstract: - The generalized Kubo-Greenwood formula for conductivity is used for an explicit calculation of the perpendicular conductivity of GaAs-AlGaAs (crystalline III-V) heterostructures. Two cases are discussed (a) evaluation of DC conductivity at low temperatures and (b) AC conductivity at any temperature T. The method involves the causal Green's function and relates the conductivity with superlattice (multilayer) parameters such as repeat distance, miniband energies and their corresponding widths, and the Fermi level. Analytical results are derived that are applicable to III-V photovoltaic structures with multiple layers and non-zero tunneling.

Key-Words: - Green's function, Photoconductivity, Superlattices, Solar cells

1 Introduction

AC and DC conductivity is a fundamental transport parameter for any device that produces free conducting carriers under illumination, and in the dark respectively. Such carriers are expected to tunnel through the potential barriers, thus contributing to appreciable conductivity values along the growth direction of these devices. Illuminated heterostructures exhibit improved AC photoconductivity when exposed to different wavelengths (either single or multiple). More specifically, illuminated photovoltaic ***p-i-n*** heterostructures are of high interest, because they provide (a) wide gap front window for more effective incident photon collection and (b) high drift velocities leading to higher current collection efficiencies. Improved design proposals include superlattices in the intrinsic regions with an overall effect of decreasing recombination losses. Thus, the transport properties of the superlattice p-i-n photovoltaic structures are of interest, and this is exactly what is proposed in this communication: an explicit method of derivation of the AC-conductivity, as a general function of the incident solar photons. When the intrinsic multi-layer region of a heterostructure solar cell is illuminated by an incident photon flux $G(\lambda)$, electrons are faced with two choices: (a) they may thermally escape to the uppermost conduction band (wide gap material) and (b) they may tunnel through the thin potential barriers. It is a known fact that tunneling prevails at low temperatures, while thermal escape dominates at relatively high temperature. In either case the Fermi level is positioned accordingly, and plays a crucial role in the evaluations of the photoconductivity. Photoconductivity is treated as a complex quantity of which the real part is provided from the generalized Kubo-Greenwood formula which includes (a) the Green's function (b) Fermi level and (c) the incident photon energy.

2 Theory

In any superlattice structure there is a certain number of energy solutions that are associated with certain miniband widths. Carriers are expected to tunnel through potential barriers, thus producing non-zero (photo)-conductivity along the growth direction of the device. In this communication the Kubo-Greenwood formula is used for the case of a superlattice structure. The real part of the conductivity is given from the Kubo-Greenwood formula [1,2] by:

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

where f(E) is the probability function distribution of the carriers, m is the effective mass of the carriers, e is the electronic charge, hω/2π is the energy of the electronic jump from state to state, photons at frequencies f = ω/2π, h is Planck's constant, the sub-index of the momentum operator α = x,y,z, Ω is a normalization volume and $G^+(E, k_z)$ is the causal Green's function in the weak scattering limit (no self-energy of electrons) [2]:

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

where k_z is the wave vector of the superlattice Brillouin zone, and $E(k_z)$ is the energy of a carrier in the superlattice $E(k_z) = E_o + g_n \cos(k_z d)$, g_n is the miniband width, d is the period of the superlattice, E_o is the miniband solution in the quantum well, and in the tight-binding approximation. In the k-representation [1,4], the momentum operator and the Green's function are both diagonal and thus (1) becomes as follows:

$$\sigma_{zz}(\omega) = \frac{2e^2\hbar}{\pi\Omega} \int dE \frac{f(E) - f(E+\hbar\omega)}{\hbar\omega} \sum_k \left| \left\langle k_z / \frac{P_z}{m} / k_z \right\rangle \right|^2 \left| Im\, G^+(E, k_z) \right|^2 \tag{3}$$

Since the momentum matrix element in (3) is just

$$\frac{1}{\hbar} \frac{\partial E(k_z)}{\partial k_z}$$

And since the probability at DC conditions becomes:

$$-\frac{\partial f(E)}{\partial E}$$

Expression (3) simplifies as follows:

$$\sigma(0)=\frac{2e^2\hbar}{\pi\Omega}\int dE(-\frac{\partial f(E)}{\partial E})\sum\left(\frac{1}{\hbar}\frac{\partial E(k)}{\partial k}\right)^2\frac{1}{(E-E(k))^2} \tag{4}$$

Where the factor 2 is for the two spin orientations of the electrons, and where for simplicity k_z (along the growth direction has been replaced by k). For Maxwellian probability distributions, and therefore at any temperature T, the perpendicular tunneling conductivity (by means of the tight binding energy dispersion relation mentioned above) becomes:

$$\sigma(0)=\frac{2e^2g^2{}_nd^2}{\pi\Omega\hbar(kT)}\sum_k e^{(E(k)-E_F)}\int_E dEe^{-(E-E_F)/kT}\left(\frac{1-(\frac{E-E(k)}{g_n})^2}{(E-E(k))^2}\right) \tag{5}$$

The summation in (5) is over all k-values of the superlattice and the integration scans all available energy values in the quantum wells, starting from the lowest miniband. In realistic devices, the summations runs over a finite number of k (= k_z), which in most cases are not more than two (for ~10nm and less, quantum well widths). A preliminary advantage of (5) is the explicit relation (difference) between superlattice energy dispersion and the fermi level. Changing variables: y= (E-E(k))/kT, the conductivity is found to depend on y as follows:

$$\sigma(0)=\frac{e^2g_nd^2}{\pi\hbar(kT)^2\Omega}\sum_k\int_y dy(\frac{e^{-y}}{y^2})-\frac{e^2d^2}{\pi\hbar\Omega}\sum_k e^{-y_k} \tag{6}$$

Since in most cases of interest (in the context where thin quantum well layers cause pinning of the fermi level in-between the minibands, where the energy differences are less that kT) E – E(k_z) = g_n << kT, the exponentials in (6) can be linearized by a Taylor expansion with the first two terms kept (and neglecting second order terms). Thus (6) is simplified as follows:

$$\sigma(0) \cong \frac{e^2 g^2{}_n d^2}{\pi\hbar(kT)^2\Omega}\sum_k\left[-(\frac{1}{y_k}+\ln y_k)\right]-\frac{e^2d^2}{\pi\hbar\Omega}\sum_k(1-y_k) \tag{7}$$

Or

$$\sigma(0)=\frac{(ed)^2}{(kT)\pi\hbar\Omega}\sum_k(E-E(k))-\frac{(eg_nd)^2}{(kT)^2\hbar\Omega}\sum_k \ln\left(\frac{E-E(k)}{kT}\right)$$
$$-\frac{(eg_nd)^2}{(kT)\pi\hbar\Omega}\sum_k\left(\frac{1}{E-E(k)}\right)-\frac{(ed)^2}{\pi\hbar^2\Omega}\sum_k\delta\big(E-E(k)\big) \tag{8}$$

Expression (8) provides an analytic result for the tunneling conductivity of a multiple quantum well heterostructure at DC conditions. Tunneling is due carriers trapped in quantum wells, of which the corresponding wavefunctions overlap (for nearest neighbors) in the multi-structure. As it is seen from (8), the dark conductivity is a strong function of temperature, miniband width, superlattice repeat distance, and carrier energy E relative to superlattice dispersion energy $E(k_z)$. The superlattice wave-vector is confined in the 1st Brillouin zone:

$$-\frac{\pi}{d}\le k_z \le \frac{\pi}{d}$$

And is given by the Born von Karman cyclic boundary conditions [3]:

$$k_{z,n}=-\frac{\pi}{d}+\frac{2\pi n}{N\cdot d}, n=0,1,2,..,N$$

Where N is the number of repeat distances of the superlattice.

3 AC Conditions for Conductivity

Information can be extracted about light induced conductivity directly from (1), at any frequency ω: by splitting (1) in a difference of two integrals I_1, I_2,

$$I_1=\frac{e^2}{\pi m^2\omega\Omega}\int dEf(E)Tr\left\{P_z \, Im\, G^+(E+\hbar\omega)P_z \, Im\, G^+(E)\right\}$$

And

$$I_2 = \frac{e^2}{\pi m^2 \omega\Omega} \int dEf(E+\hbar\omega) Tr\left\{P_z \, Im\, G^+(E+\hbar\omega) P_z \, Im\, G^+(E)\right\} \tag{9}$$

Where now:

$$G^+ = \frac{1}{(E+\hbar\omega-\Sigma(E)-E(k_z))} \tag{10}$$

$\Sigma(E) = \Sigma_1 - i\Sigma_2$ is the electronic self-energy, to be used in the following for expressing carrier scattering under illumination. Substitution of (10) in (9) leads to the following explicit form of integrals I_1, I_2:

$$I_1(\omega) = \frac{e^2\Sigma^2{}_2}{\pi\omega\Omega} \sum_k \int_E \frac{dEv^2{}_z(k_z) f(E)}{\left\{(E-\Sigma_1-E(k_z))^2+\Sigma^2{}_2\right\}^2+\left\{(E+\hbar\omega-\Sigma_1-E(k_z))^2+\Sigma_2{}^2\right\}^2} \tag{11}$$

and

$$I_2(\omega) = \frac{e^2\Sigma^2{}_2}{\pi\omega\Omega} \sum_k \int_E \frac{dEv^2{}_z(k_z) f(E+\hbar\omega)}{\left\{(E-\Sigma_1-E(k_z))^2+\Sigma^2{}_2\right\}^2+\left\{(E+\hbar\omega-\Sigma_1-E(k_z))^2+\Sigma_2{}^2\right\}^2} \tag{12}$$

The difference of (12) from (11) will express photoconductivity of a multilayer III-V heterostructure, at any temperature. The quantity $v_z(k_z)$ is the electronic velocity along the tunneling direction. In the weak scattering limit, the real part of the self-energy (Σ_1) can be neglected in an absolute energy scale. For Maxwellian probability distributions, the second integral in (12) becomes a fraction of I_1 because of the fact that:

$$f(E+\hbar\omega) = e^{-(E+\hbar\omega-E_F)/kT} = e^{-\hbar\omega/kT} e^{-(E-E_F)/kT} \tag{13}$$

And therefore:

$$I_2(\omega) = e^{-\hbar\omega/kT} \times I_1(\omega) \tag{14}$$

The photoconductivity, after subtracting (12) from (11), via (13), (14) is:

$$\sigma_1(\omega) = I_1(\omega)\left[1 - e^{-\hbar\omega / kT}\right] \qquad (15)$$

Which at high temperatures (kT>>hν) simplifies to

$$\sigma_1(\omega) = \frac{\hbar\omega}{kT} I_1(\omega) \qquad (16)$$

At any other T, the photoconductivity is:

$$\sigma_1(\omega) = 2I_1(\omega)\, sinh(\frac{\hbar\omega}{2kT)}\, e^{-\hbar\omega / kT} \qquad (17)$$

4 Conclusion

The present work is an effort toward the evaluation of dark and photoconductivity (a fundamental transport property) of III-V multi-layered structures. The method is based on the Kubo-Greenwood formula and uses the Green's function for a direct evaluation of DC and AC conductivity. Under DC conditions ($\omega \rightarrow 0$), an explicit result is obtained, that expresses conductivity explicitly as a function of superlattice parameters, miniband width, and superlattice dispersion (via the superlattice wave number). At AC conditions, the photoconductivity is expressed explicitly as a function of incident light frequency. For a range of incident wavelengths, an integration of (17) would lead to the total frequency response of a superlattice-based photovoltaic structure.

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