TUNNELING CONDUCTIVITY OF SUPERLATTICE GAAS/ALGAAS N-I-P SOLAR CELLS BY MEANS OF THE GENERALIZED KUBO-GREENWOOD FORMULA AND THE GREEN'S FUNCTION

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ABSTRACT

We derive, from first principles, an explicit result for the perpendicular conductivity of superlattice solar cells by means of the generalized Kubo-Greenwood formulas and the Green's function. The advantage of superlattice based solar cells, when compared to their bulk counterparts is that quantization of energy levels takes place within the quantum wells leading to enhancement of conductivity. These energy levels form minibands that allow the carriers to tunnel through the barriers.

I. Introduction

An analytic result for the perpendicular tunneling conductivity of multiquantum well solar cells by means of Green's functions is derived. In p-i-n structures, the p- and n- regions may be replaced by superlattice contacts to increase V_{oc} . The dark perpendicular conductivity depends on a number of parameters, such as the period of the superlattice, the energy eigensolutions and their widths, and the Fermi level location. Carriers are expected to tunnel through the potential barriers, thus contributing to conductivity along the growth direction. It is possible to derive an explicit result for the tunneling conductivity by generalizing the Kubo-Greenwood formula by means of the causal Green's function. $\sigma_{zz}(T)$ is a sum over the discrete spectrum of the superlattice wave number k_z and includes the repeat distance d_z (period), Fermi level E_F , and miniband widths γ_n .

In this paper, a method of calculating the perpendicular dc conductivity of superlattice (SL) n(SL)-i-p solar cells is proposed. The generalized Kubo-Greenwood formula for the conductivity is used and appropriately arranged for the dark perpendicular conductivity $\sigma_{zz}(T)$, along the growth direction of the device. σ_{zz} depends primarily on temperature T , after the device parameters have been fixed. The new feature in this case is the replacement of either n- or p- regions with superlattice contacts. The superlattice contacts provide new parameters that are direct results of the new band formation. These band formations are due to quantum wells and barriers, formed after depositing wide gap semiconductors on top of narrow gap ones, at appropriate widths. The widths need to be thin enough to ensure quantum size effects. The combination of a wide gap material with a narrow gap one, leads to quantum well formation, where carriers may be trapped and contribute to conductivity. This sort of band-gap device design makes the trapped carriers essentially free along the planes parallel to the interfaces, while tunneling becomes possible through the barriers [1]. This is possible, that is the tunneling probability, along the growth direction is non-zero, and hence the tunneling conductivity $\sigma_{zz}(T)$ will be affected by it. It is worth noticing that different geometries of the superlattice contact regions have a direct effect on the widths of the quantum wells. Typical widths are of the order of 20 to 80 Å (e.g., for GaAs/AlGaAs) and typically two eigensolutions (minibands) exist in the wells. Once the geometry has been selected, one may enhance carrier trapping by doping of the wider gap semiconductor. In the n-type region, the barrier regions may be doped with donor impurities. The overall effect is a Fermi level shift towards the conduction band edge and possibly even past the band edge, inside the bottom of the quantum wells. The Fermi level can be evaluated from the total neutrality

condition. It is already known [2] that Fermi level shifting leads to improvements of V_{oc} (open circuit voltages) and to overall efficiency gains. It is the goal of this paper to show that the dark conductivity can be calculated for n(SL)-i-p superlattices.

The materials selected are GaAs (narrow gap) and AlGaAs (wider gap) for the reason that these alloys have been extensively studied and for being crystalline (no defects in the gap).

II. The Kubo-Greenwood Formula of Conductivity

The real part of σ is given by [3] the generalized Kubo-Greenwood formula:

$$\sigma_1(\omega) = \frac{e^2 \hbar}{\pi m^2 \Omega} \int dE \frac{f(E) - f(E + \hbar\omega)}{\hbar\omega} \times \quad (1)$$

$$\text{Tr} \{ P_\alpha \text{Im} G^+(E + \hbar\omega) P_\alpha \text{Im} G^+(E) \}$$

where the subindex is $\alpha = x, y, z$. Ω is a normalization volume, $f(E)$ is the Fermi Dirac distribution function, and $G^+(E)$ is the causal Green's function:

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

$\Sigma = \Sigma_1 - \Sigma_2$ being the electron self energy, k_z the superlattice wave number, confined in the superlattice's Brillouin zone.

The perpendicular conductivity σ_{zz} ($Z =$ growth direction) is then:

$$\sigma_{zz}(\omega, T) = \frac{e^2 \hbar}{\pi m^2 \Omega} \int dE \frac{f(E) - f(E + \hbar\omega)}{\hbar\omega} \times \quad (3)$$

$$\text{Tr} \{ P_z \text{Im} G^+(E + \hbar\omega) P_z \text{Im} G^+(E) \}$$

the DC case ($\omega \rightarrow 0$) leads to:

$$\sigma_{zz}(T) = \frac{2e\hbar^2}{\pi\Omega} \int dE \left(-\frac{\partial f(E)}{\partial E} \right) \cdot \sum_{k_z} \left| \langle k_z | \frac{P_z}{m} | k_z \rangle \right|^2 \left| \text{Im} G^+(E, k_z) \right|^2 \quad (4)$$

The sum is over the discrete spectrum of k_z (with a superlattice period d), which is confined in the superlattice's Brillouin zone:

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

and is given by the Born-von Karman boundary combination [4]

$$k_z^{(j)} = -\frac{\pi}{d} + \frac{2\pi j}{N \cdot d}, \quad j = 0, 2, \dots, N \quad (5)$$

where N is the number of periods of the superlattice.

Referring to (4), we can show that

$$\langle k_z | \frac{P_z}{m} | k_z \rangle = \frac{1}{\hbar} \frac{\partial E(k_z)}{\partial k_z} = V_z(k_z) \quad (6)$$

where $V_z(k_z)$ is the group velocity. For moderate dopings

$$f(E) = \exp\left(-\frac{E - E_F}{kT}\right) \quad (7)$$

Equation (4) becomes

$$\sigma_{zz}(T) = \frac{2e^2 \hbar}{\pi \Omega} \int dE \left(-\frac{\partial f}{\partial E} \right) \sum_{k_z} \left(\frac{1}{\hbar} \frac{\partial E}{\partial k_z} \right)^2 \times \quad (8)$$

$|\text{Im} G^+|^2$
where

$$|\text{Im} G^+|^2 = \frac{\Sigma_2^2}{[(E - \Sigma_1 - E(k_z))^2 + \Sigma_2^2]^2} \quad (9)$$

Inserting (9) in (8) and evaluating $-\frac{\partial f}{\partial E}$ through (7), at the limit $\omega \rightarrow 0$ one obtains:

$$\sigma_{zz}(T) = \frac{2e^2 \hbar}{\pi \Omega} \int dE \left[(kT)^{-1} e^{-\frac{(E - E_F)}{kT}} \right] \times \quad (10)$$

$$\sum_{k_z} \frac{1}{\hbar^2} \left(\frac{\partial E}{\partial k_z} \right)^2 \frac{\Sigma_2^2}{[(E - \Sigma_1 - E(k_z))^2 + \Sigma_2^2]^2}$$

where

$$E(k_z) = E_0 + \gamma_n \cos k_z d \quad (11)$$

(11) is the superlattice dispersion relation, and γ_n is the width of the nth miniband.

Since

$$\left(\frac{\partial E}{\partial k_z}\right)^2 = d^2(\gamma_n^2 - (E(k_z) - E_0)^2) \quad (12)$$

(10) becomes

$$\sigma_{zz}(T) = \left(\frac{2e^2 d^2 \Sigma_2^2}{(kT) \hbar \pi \Omega}\right) \sum_{k_z} [\gamma_n^2 - (E(k_z) - E_0)^2] \times \quad (13)$$

$$\int \frac{dE \exp\left(-\frac{E - E_F}{kT}\right)}{[(E - E_F) + (E_F - \Sigma_1) - E(k_z)]^2 + \Sigma_2^2}$$

Neglecting Σ_2^2 in the denominator, and letting $E_F - \Sigma_1 \sim E_F$ (weak scattering limit) [3] the function to be integrated becomes

$$\frac{\exp\left(-\frac{E - E_F}{kT}\right)}{[(E - E_F) + E_F - E(k_z)]^4} \quad (14)$$

Carrying the integral in (13) through (14) leads to the following explicit result for $\sigma_{zz}(T)$:

$$\sigma_{zz}(T) = \left(\frac{2e^2 d^2 \Sigma_2^2}{(kT) \hbar \pi \Omega}\right) \times \sum_{k_z} [\gamma_n^2 - \gamma_n^2 \cos^2 k_z d] \times \quad (15)$$

$$\exp\left(-\frac{(E_0 - E_F)}{kT}\right) \Phi(\gamma_n, k_z, d, kT)$$

where

$$\begin{aligned} \Phi = & [- (6 (kT)^2 \gamma_n \cos k_z d)^{-1} \\ & - (6 kT \gamma_n^2 \cos^2 k_z d)^{-1} \\ & - (3 \gamma_n^2 \cos^3 k_z d)^{-1} \\ & + \frac{1}{6 (kT)^3} \exp\left(-\frac{\gamma_n \cos k_z d}{kT}\right) \end{aligned} \quad (16)$$

$$Ei\left(-\frac{\gamma_n \cos k_z d}{kT}\right)$$

where Ei is the exponential integral of

$$\left(-\frac{\gamma_n \cos k_z d}{kT}\right)$$

Notice that for (15) not to be zero, $\cos k_z d$ must not be ± 1 , which leads to the fact that j must not be either 0 or N (see (5)).

The index n refers to the nth miniband in the wells.

From the treatment above, it is found that the dark conductivity of a superlattice solar cell of the type n(SL)-i-p can be calculated in terms of the Fermi level position E_f , eigen-energies inside the quantum wells, their widths γ_n , the period d of the superlattice. The Fermi level in (15) is found with very good accuracy by means of the neutrality condition for composite superlattices [5,6] as shown in Fig. 1. As it is usually the case, the superlattice parameters are at the designer's disposal and the general formula (15) may lead to values of $\sigma_{zz}(T)$. The A.C. case ($\omega \neq 0$) (see (1)) is under study. GaAs/AlGaAs thin heterojunctions are good candidates, since these junctions have been studied extensively.

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Fig.-1. Proposed superlattice solar cell structure, typically AlGaAs/GaAs, for which the dark perpendicular conductivity is evaluated [1].