Exact Solution for Excess Electrons in Quantum Mechanically Operating Solar Cells, under Cumulative Auger Effects

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Abstract: – We derive excess carrier populations in quantum wells, embedded in the intrinsic region of p-i-n solar cells. In the process of the analysis, we (a) solve for photo-generated carriers in quantum wells and (b) determine explicit dependence on incident solar wavelength. We include in the computations the existence of optical gaps near 1eV or wavelengths in the near infrared, so that our complete device design covers both visible and IR spectra simultaneously: a clear advantage over bulk and nitride-base solar currently studied solar cells. In the process of derivations, we include the effect of recombination losses via *cumulative Auger* recombination coefficients c_n on photo-excited carriers in intrinsic quantum wells n_{ph}, as found in the middle region of p-i-n solar cells, leading to an explicit new result of the form: $\boldsymbol{n_{ph} \sim c_n^{-1/3}}$.We find the total carrier concentration to be the sum of photo-excited and background carriers, namely, $\boldsymbol{n_{total} = n_{ph} + n_o}$. Our approach is general and can be applied to different semiconducting layers, while as a concrete application, we select lattice-matched germanium and gallium arsenide layers forming quantum wells. Excess carrier concentrations of the order of 10^{18} per unit volume are predicted for thin GaAs-Ge quantum wells, under steady solar photon incidence, while the background dark carrier concentration is near 10^{14} carriers per unit volume.

Key-Words: quantum wells, solar cells, solar spectrum, Auger recombination, material growth, quantum photovoltaics

1 Introduction

Low gap materials on top of wide gap materials, grown via MBE (molecular beam epitaxy) or MOCVD (metal-organic chemical vapor deposition) current techniques have been shown to be valuable additions for better solar cell performance. Major advantages of multi-gap solid state devices include (a) excess trapping in quantum wells and in discrete energy levels (b) subsequent carrier escape to the conduction band (c) effective mass separation and reduction of recombination of free electrons and holes, and (d) simultaneous absorption of both short and long wavelengths. Germanium (Ge) based quantum traps in gallium arsenide (GaAs) hosting background environment provide excess carrier concentration in the intrinsic region of a solar cell, where most of carrier excitation occurs. For a solar cell to operate in the full solar spectrum, suitable hosts need to be chosen, to ensure absorption of both short and long wavelengths. The latter (case (d) above) is one of the major advantages for a device that includes more than one layer, since it offers the chance for photon collection of both low and high energy. As it is well understood from semiconductor theory, incident photons on semiconductor samples get absorbed as long as their energy is higher than the energy gap that characterizes the specific semiconducting sample. Permanent

problem of traditional solar cell design is the use of bulk (single-layer) media, where a certain class of wavelengths is absorbed either from a long threshold or from a short wavelength threshold. Quantum wells in the mid-region of solar cells open the acceptance window of solar wavelengths, and thus an appropriate choice of (otherwise) matching media may provide the needed environment for a wide range of solar photons collection.

2 Device topography

The structure in mind is p-n (qw)-n^+ solar cell, where p, n are its p and n- regions respectively (the latter one heavily doped), while the mid region is lightly doped area with a sequential layer arrangement with low and wide energy gaps (see Fig. 1). GaAs and Ge constitute two lattice matched media with high and low band gaps (1.42 and 0.67 eV respectively). Germanium grown on top of GaAs and in succession, forms quantum traps, where electrons from the valence. The p-region is selected to be a double layer of aluminum arsenide and gallium arsenide (AlAs and GaAs at 2.4 and 1.42 eV respectively), where short wavelengths are expected to be collected (from 515 μm to 877 μm respectively). The end layer is of germanium at 0.67 eV or at 1.79 μm (short infrared). In the middle, quantum well formations between GaAs and Ge matched layers provide optical gaps of the order of 1eV (or 1.24 μm). The latter is a major advantage of quantum well devices: selection of the optical gap is on the designer's disposal (1 eV or different), by suitable selection of quantum well width (see Fig. 2). Typically, one selects width ranges so that only one eigen-state might be involved in electron capturing, while the second quantized level is the very top of the quantum well, where trapped carriers are essentially free to move along the conduction band edge. As seen in Figures 1 & 2, different band gaps introduce optical gaps at different values, so that most of the visible and the near infrared solar spectrum could be absorbed. The clear advantage of the devices as a whole will be discussed in a different communication paper. For the time being it is sufficient to emphasize the effect of Auger effects in the quantum well regions. The next section mathematically models the situation of an illuminated GaAs-Ge quantum well, anywhere in the intrinsic region of a p-i-(quantum well)-n- solar cell.

3 Theory and computations

We proceed as follows: first we develop and solve the diffusion equation in the intrinsic region and for any quantum well, secondly we determine the concentration of photo-carriers in the wells after recombination losses. The latter are taken to be of *Auger* type via an appropriate coefficient $\boldsymbol{c_n}$, which is included explicitly in the diffusion equation, shown below. In absence of tunneling, and under illumination, excess photocarriers per unit volume δn(x) depend on distance *x* in quantum wells, and diffuse accordingly. The latter event is usually treated via continuity between excited and lost carriers in GaAs-Ge quantum wells. Loss mechanisms are typically of radiation and non-radiation form, with the dominant one being the Auger recombination (a recombining electron gives off its excess energy to a neighboring one or to a hole in the valence band):

$$D_n \delta n''(x) + g(x) = \delta n(x)/\tau \qquad (1)$$

In equation (1), double prime indicates second derivative with respect to x, the coefficient D_n is the diffusivity of electrons, δn(x) is the excess electron concentration in a quantum well, g(x) is the generation rate of electrons, and the last term is the recombination rate number of carriers per volume per time). Loss mechanisms are "hidden" in the last term of (1). Expression (1) is subject to boundary conditions suitable at the two interfaces of the quantum well:

$$\delta n'(0) = -\frac{s_1}{D_n}\delta n(0) = s_{10}(cm^{-4})$$
$$\delta n'(L_w) = -\frac{s_2}{D_n}\delta n(L_w) = s_{2w}(cm^{-4}) \qquad (1')$$

Where the single primes indicate first derivatives of excess carriers, $s_{1,\ 2}$ are

recombination velocities at the two interfaces, all grouped as $s_{10,\,2w}$.
The generation rate depends on incident wavelength and it is meant to be as follows:

$$G_{ph}(cm^{-3}s^{-1}) = F_{ph}(cm^{-2}s^{-1})\alpha(cm^{-1})(1-R)e^{-\alpha x} \equiv Ge^{-\alpha x} \quad (2)$$

Expression (2) includes photon flux F_{ph} as strong function of the optical gap, absorption coefficient, reflectivity and distance. In (1), we include only the cumulative *Auger* coefficient, as the dominant loss mechanism against radiation recombination (expressed via a separate coefficient for electrons c_n) [ ]. This is based on the fact that in reduced dimensional systems (quantum wells and quantum dots) Auger cooling (AC) is *the* dominant loss mechanism, against radiative and phonon scattering losses (on one hand Auger effects are proportional to n^2p factors in n-type media, where n and p are electrons and holes in the quantum well layer, and where the n^2 factor includes all the excess carriers during and after illumination. On the other hand, relaxation lifetimes in Auger, radiative and phonon scattering regimes are under the condition: $\tau_{AC} << \tau_{Rad}, \tau_{phonon}$. Due to the connection between diffusion coefficient and diffusion length and relaxation life times, we eliminate the latter via the relation $L = (D_n \tau)^{½}$, and since $c\tau\delta n^2 = 1$, we re-write (1) as follows:

$$\delta n''(x)-[\delta n/L^2] + [G_{ph}/L^2 c\delta n^2] = 0 \quad (3)$$

The differential equation (3) is solved via standard methods, and its solution is:

$$\delta n(x) = n_1 \exp(-x/L) + n_2 \exp(x/L) + n_3 \exp(-\alpha x/3) \quad (4)$$

Where the coefficients in (4) are appropriate functions of the device parameters involved, especially optical gap (via λ_{opt} and Auger coefficient). The total *net* carrier concentration in the quantum wells, are strong functions of six factors: (a) device parameter (quantum well width) (b) absorption coefficient (c) incident photon flux (d) incident wavelength (e) electronic diffusion length L (f) Recombination velocity (g) Auger recombination (via parameter c_n:

$$\delta n\ (cm^{-3}) = n_{ph}\ (x, \lambda_{opt}, c_n) + n_o(x) \quad (5)$$

Expression (5), in its simplicity, may be interpreted as follows: the solar cell is illuminated via incident photon flux (G as in (2)), and excess carrier concentration is found to depend (in addition material properties) on two components: $n(x, \lambda_{opt}, c_n)$ and $n_o(x)$. The first term in (5) depends on distance, optical gap and Auger recombination, while the second term is just a function of distance inside a quantum well. Note also in (5) that when the photon source is switched off ($n(x, \lambda_{opt}, c_n) = 0$), excess carrier concentration is just a dark-carrier component $n_o(x)$. Via (4) and the Appendix, expression (5) is turned into a more explicit form (suitable for computations) as follows:

$$\delta n = [\alpha F_{ph}/c_n]^{1/3} n(x) + n_o(x) \quad (6)$$

Where photo-carrier concentrations n_{ph} are as follows (with $\alpha L << 1$):

$$n_{ph}\ (x, \lambda_{opt}, c_n) = [\alpha G_{ph}/c_n]^{1/3} n(x) \quad (7)$$

We notice from ((6, 7) that excess carriers in quantum wells depend on incident light, absorption and Auger effects. The photon flux needs to be expressed explicitly, and is treated via standard "black-body at temperature T" radiation techniques: Incident wavelengths (λ) are expected to be absorbed from a threshold and (optical gap, determining the threshold wavelength λ_{opt}) infinity (see Appendix A). The total carrier concentration dependence includes (a) distance in the QW (quantum well) (b) wavelength and wavelength range (c) Auger loss cumulative coefficient (d) absorption of semiconducting sample. The photon flux is expressed via F_{ph}, through which all the details of the incident solar light

are included, namely, low limit (optical gap) to the upper limit (see Appendix).

$$\delta n = \left\{\left(\alpha F_{ph}\right)^{1/3} \times c_n^{-1/3}\right\} \times n(x) + n_o(x) \quad (8)$$

Note that the total number of solar photons per area per time is easily found from (A-5) to be near 5.77 x 10^{21}(/cm^2/sec), for a solar black body radiating at a surface temperature of the order of T_S = 5800 ^{o}K. In that case, the coefficient of n(x) in (8) is of the order of: 1.412 x 10^{18} cm^{-3}. Table 1 (Appendix A) includes typical values, needed for computations. For a selected gap of 1eV, this wavelength is λ_{opt} = 1.24μm, while the upper limit is taken at infinity. Total excess carrier accumulation as seen from (8) is a strong function of distance and Auger cooling via the c_n dependence**.** As also seen from (8), the excess carrier concentration in a quantum well is a strong function of distance x through the terms n(x) and n_o(x). In addition, there is explicit dependence on Auger coefficient c_n, source temperature T_S, and absorption coefficient. Note also that (8) is a new and a general result, meaning that it could be used for different media (e.g. Ge, InP, GaAs, etc) as long as these media play the role of the low gap material in a superlattice or multiquantum well configuration. Anywhere inside the quantum well, the term n(x) is very small: at the left edge of a quantum well, n (0) is about one (no units) and n_o(x) is near 10^{14} cm^{-3}. On the other hand, at the right edge of a quantum well, n (L_W) is of the order of 10^{-3}, while n_o is not changing significantly from its original value.

4 Conclusions

A recurring issue in modern photovoltaics is the degree of spectral absorption: how much incident light is really absorbed by a solar cell. Modern PV structures show particular strength in light absorption but they lag in transport properties (low mobility of free carriers). On the other hand, more than band gaps in one solar cell are of advantage in terms of collection efficiency. In this paper we propose a way of overcoming current mobility problems by introducing a superlattice in the intrinsic region of a solar cell. This ensures photo-excited carriers trapped in quantum wells (or quantum dots for the same reason) made out of germanium layers lattice-matched with gallium arsenide ones, ensuring (a) quantum trapping and (b) not compromising mobility problems (due to GaAs-Ge). However, the main loss mechanism (auger cooling) cannot be drastically inhibited. In superlattices, Auger cooling is the fastest loss process (faster than radiation and phonon losses). In this communication, we have derived a quantitative connection between gains and Auger losses in a superlattice solar cell, and we conclude that when superlattice-based devices are illuminated, excess carriers do arise in individual quantum wells, but within the regime of Auger dominating effects (over radiative recombination) as the dominant loss mechanism. We predict excess carrier concentration values in the order of 10^{18} per unit volume and under illumination, and 10^{14} excess carriers per volume under dark. We find that excess carrier populations depend on cumulative Auger processes, as shown via expression (8) above.

In summary, in this communication, we provide a new and explicit result on excess carriers in illuminated quantum wells, where Auger cooling (AC) is the dominant loss mechanism against radiative recombination and phonon scattering mechanisms. This is feasible in narrow quantum wells, where the mean lifetime of Auger losses is shorter than the corresponding lifetimes of the other two mechanisms mentioned above. We find dependence n ~ $AC^{-\nu}$, ν is 0.333. Our generalized result is then:

n= {absorption} x $(AC)^{-\nu}$ + {n_o}.

A major advantage of our approach is the fact that it can be used in different quantum PV structures, with lattice-matched semiconducting media. Immediate advantages are sought via III-V structures, where absence of impurities in the intrinsic region reduce carrier

scattering and a recombination due to quantum well effective mass separation.

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Appendix A

Two analytic expressions for carrier density:

$$n(x) = \exp(-\alpha x/3)-(\alpha L/3)\exp(-x/L) \quad \text{A-1}$$

$$n_o(x) = 10^{14}\,(1+\exp(-x/L)) \quad \text{A-2}$$

In the above, L is the diffusion length of the electrons in the device, α is the absorption coefficient. In A-1 there are no units and in A-2 the units are cm^{-3}.

Incident photon flux:

$$G_{ph}(\lambda_{opt})(cm^{-2}s^{-1}) =$$

$$(2\pi)^4 c \int_{\lambda_{OPT}} \frac{d\lambda}{\lambda^4\left(^{hc/\lambda kT_s}-1\right)} \quad \text{A-3}$$

List of values needed for the computations:
α = 10,000 cm^{-1}, L = 0.00001 cm, T_s = 6,000 ^oK, δn (0) = 10^{18} cm^{-3}, δn (L) = $10^{17} cm^{-3}$,

diffusion coefficient D_n = 80 cm^2/sec, Auger coefficient c_n = 10^{-31} cm^6/sec, recombination velocities 1,000 m/sec, quantum well width values in the order of 5 to 7 nm.

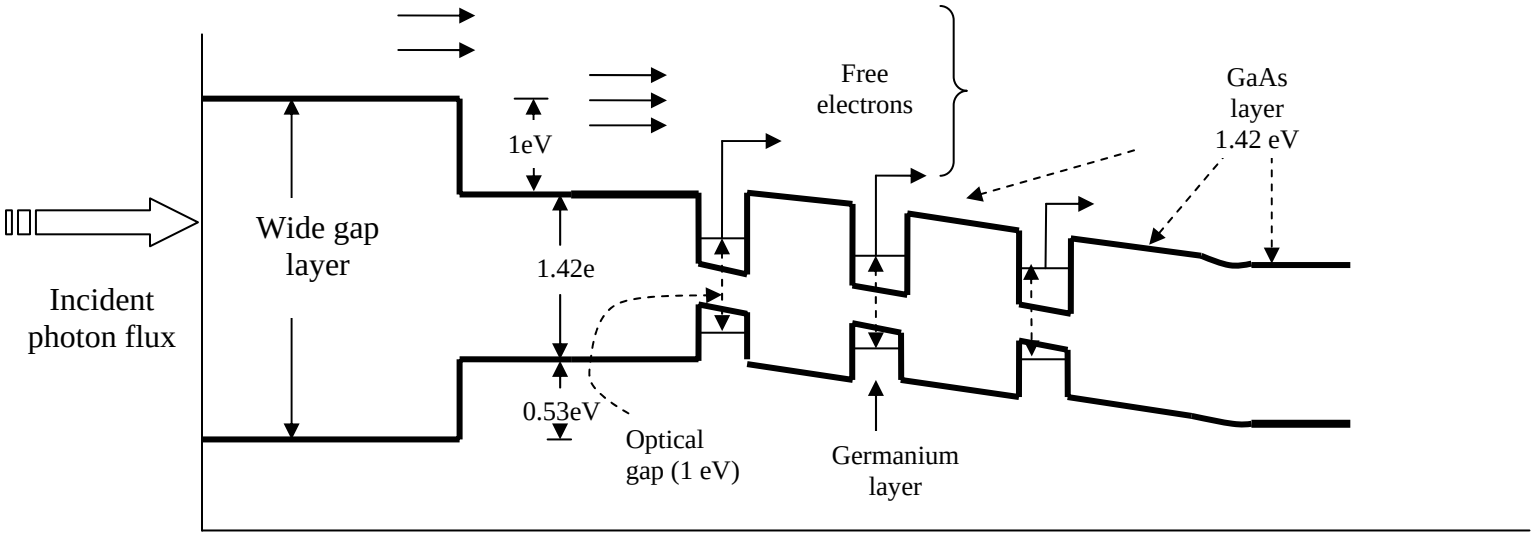

Figure 1: Quantum photovoltaic structure. Shown are (a) different gap layers (b) GaAs-Ge layers (c) optical gap and (d) conduction electrons. Excess carriers concentrate in the quantum well regions, from where they either escape and or recombine to the valence bands.