Intersubband Thermophotovoltaics

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Abstract. In this paper valence band designs that allow simple normal incidence in the TE mode as in a convention solar cell are studied and shown to be more efficient than conduction band-based TM structures in a range of the far infrared. The relevance of many-body corrections is further investigated numerically for III-V quantum well structures.

1. Introduction

Increasing the efficiency of photovoltaic (PV) materials and devices is one of the most important current challenges for optical sciences and technology [1]. One of the possible ways to improve the efficiency is by absorbing photons in the mid and far infrared for which conventional semiconductors are transparent. Different solutions have been proposed, e.g. up/down conversion layers [2] or introducing intermediate bands [3]. All of those have their own efficiency limitations and technological difficulties. One other solution, discussed in this paper is the concept of intersubband (ISB) thermophotovoltaic (TPV) devices, in which the transition energies leading to absorption of radiation do not depend on the band gap [4]. The present state-of-the-art in TPV [5] energy conversion from a thermal source at a temperature of 1300 K is about 0.8 W/cm\textsuperscript{2}, obtained with a 0.6-eV bandgap energy InGaAs interband photodetector grown lattice mismatched on InP with an InPAs buffer and the preliminary simulations of Ref. [6] indicate that at the same temperature the ISB TPV can generate 1.4W/cm\textsuperscript{2}. We can therefore conclude that the multiple-junction ISB device concept has the potential to provide a substantial improvement over existing technologies.

In this paper we analyze a different approach: valence-band based designs that lead to TE mode absorption and can directly absorb photons normal to the surface in contrast to usual conduction band based ISB devices that operate with TM incidence leading to additional complications like the requirement of prism and/or couplers. Furthermore, many body effects due to the electron-electron interaction that have a proven relevance in semiconductor lasers in both interband [7-14] and intersubband architectures [15-25]. Their relevance for TPV structures is made clear here and this may be particularly important for hot carrier architectures, where a large density of nonequilibrium carriers can be created [26].
2. Numerical Method and Applications

The photocurrent generation spectrum \([27]\) collected by each period \((n)\) with length \(d_n\), which here is the quantum well (QW) width, is given by

\[
J_n(\omega) = q \int_{z_n}^{z_n+d_n} G_n(\omega,z) dz,
\]

where the generation rate is

\[
G_n(\omega,z) = \alpha_n(\omega) Y(\omega) \left[ 1 - R(\omega) \right] \exp(-\alpha_n d_n).
\]

In Eq. (1), \(R(\omega)\) is the surface reflection coefficient, \(Y(\omega)\) is the photon flux incident on the sample surface, and \(z_n\) is the position of the QW along the device’s growth direction.

The absorption \(\alpha(\omega)\), or gain spectra \(g(\omega) = -\alpha(\omega)\) are calculated by means of a Keldysh nonequilibrium Green's functions approach in which the susceptibility \(\chi(\omega)\) is directly related to the carriers Green's functions \(G\), which satisfies a Dyson equation.

\[
\chi_0 = \frac{\pi \omega}{n_b c n_b} \text{Im}\{\chi(\omega)\}, \quad \chi(\omega) = \frac{Z}{V} \sum_{\mu \nu} \sum_{k} \sqrt{\frac{\epsilon_{\nu}}{\epsilon_{\mu}}} \phi_{\mu \nu}(k) \chi_{\mu \nu}(k).
\]

where \(n_b\) denotes the background refractive index, \(c\) is the speed of light, and \(\phi_{\mu \nu}\) is the transition dipole moment between subbands \(\nu\) and \(\mu\). The nonequilibrium steady-state susceptibility function in Eq. (3) stems from the carrier Keldysh Green’s function. The numerical scheme used here can be briefly summarized as follows. The first step is the solution of the 8×8 k·p Hamiltonian \([4, 17, 25, 28]\) describing the heterostructure without the Coulomb interaction. The Green’s functions and self-energies are expanded using eigenstates and eigenvalues of this Hamiltonian. Next, by assuming thermalized electrons or holes, the full NEGF scheme is simplified and reduces to the self-consistent evaluation of chemical potentials and self-energy matrix elements which lead to subband energy renormalizations, dephasing constants, and occupation functions. Only carrier-carrier scattering is considered here and details of the corresponding self-energy are given in Ref. 14. Finally, absorption and gain are given by the solution of the integrodifferential equation obtained from the carriers Green’s function by numerical matrix inversion \([17,18]\).

The numerical results presented next are for a single junction section composed of a 5 nm GaAs – Al0.3Ga0.7As quantum well. In all curves the valence band (for TE polarization) and conduction band (for TM polarization) electrons available due to doping are initially thermalized at 300K.

Figure 1 compares and contrasts the Photocurrent Generation Spectra with and without many body corrections at the same level as in Ref. [17].
Figure 1. TE Photocurrent generation spectra with (solid) and without manybody effects (dashed) for one section of a possible ISB device with a 5 nm quantum well active region. The electrons in the quantum well valence bands are thermalized at T=300K and the source is at T=750K. The carrier density is \( N = 3 \times 10^{12} / \text{cm}^2 \).

Figure 2 compares and contrasts the photocurrent for conduction band based (TM mode) and valence band based structures (TE mode). Even though in the mid infrared the much larger TM dipole moment more than compensates the losses due to the required prisms and/or couplers to bring TM polarized radiation to the active region, further in the infrared the TE mode dominates. This may be very useful to extract energy from thermal sources that emit strongly in that range.

Figure 2. Photocurrent generation spectra for the QW of Fig.1 under same conditions. The solid lines are for TE polarization and the dashed for TM at a maximum angle of incidence. The actual absorption would be smaller since a non-zero angle is required for TM absorption. Thus the contrast would be even better in practice. Note that for TM polarization we assume doping in the conduction bands and for TE in the valence bands.
At this point a few remarks are due related to the choice of materials and structures. The transition dipole moment is rigorously obtained through a commutator from the momentum matrix element. A general discussion has shown that for intervalence band transitions three terms contribute [28]. For example, in normal TE incidence (E, =O) and k=0, the last term couples light- and heavy-hole components of the initial and final states, with a strength proportional to the mixed derivatives (xz or yz) in the Hamiltonian. The second term is important only if the initial and final hole states have a significant mix of conduction-band states, which is possible in the 8x8 model as the light-hole bands are coupled to the conduction and spin-orbit bands even at k=0. For nonzero k, the first term allows transitions between same parity components of the initial and final states. For more details see the detailed discussion in Ref. [28]. This means that the second term leads to increased dipole moment for small bandgap materials, which might be an advantage in designing ISB TPVs based on TE mode operation. Larger well widths lead to larger dipoles even in the TM mode, dominated by interconduction band transitions that are not much sensitive to band coupling. In the TE mode a larger well width will further contribute by reducing the confined level separation between conduction and valence band states and thus increasing the dipole moment through bandcoupling in the same way that a reduced bandgap does. However, the Coulomb enhancement is reduced for larger well widths, so for a given target wavelength operation range a detailed analysis of the interplay between bandstructure and many body effects as a function of well width should be made.

In summary, this study demonstrates that inter-valence band absorption structures may lead to devices that can potentially convert thermal photons to current efficiently in the far infrared, which is a range that remains to be further exploited. Absorption due to valence band transitions allows simple perpendicular incidence in the TE mode without the need of prisms or other couplers that increase the complexity, cost, practicality and also the actual losses in a conduction-band-based TPV. Furthermore, the numerical analysis demonstrates the relevance of many body effects, which are now routinely considered in laser and optoelectronic device simulators, but have been essentially overlooked for photo and thermophotovoltaic simulation and design consideration.

References

[1] A. Feltrin and A. Freundlich, Renewable Energy 33, 180-185 (2008).
[2] T. Trupke et al, J. Appl. Phys. 92, 1668 (2007).
[3] S. Tomić, Phys. Rev. B 82, 195321 (2010).
[4] M.F. Pereira Jr, J. Opt. Soc. Am. B 28, 2014 (2011).
[5] B. Wernsman et al,” IEEE Trans. Electron. Dev. 51(3), 512 (2004).
[6] J. Yin and R. Paiella , Optics Express 18, 1618 (2010).
[7] W.W. Chow, M.F. Pereira Jr and S.W.Koch. Appl. Phys. Lett. 61, 758 (1992).
[8] M.F. Pereira Jr, R. Binder and S.W. Koch, Appl. Phys. Lett. 64, 279 (1994).
[9] M.F. Pereira Jr and K. Henneberger, phys. stat. sol. 202, 751 (1997).
[10] M.F. Pereira Jr and S.W.Koch. Appl. Phys. Lett. 61, 758 (1992).
[11] M.F. Pereira Jr, R. Binder and S.W. Koch, Appl. Phys. Lett. 64, 279 (1994).
[12] M.F. Pereira Jr and K. Henneberger, phys. stat. sol. 202, 751 (1997).
[13] M.F. Pereira Jr and K. Henneberger, phys. stat. sol. (b) 206, 477 (1998).
[14] M.F. Pereira Jr and K. Henneberger, phys. stat. sol. (b) 206, 477 (1998).
[15] G. Scalari et al, Phys. Rev. Lett. 93, 237403 (2004).
[16] J. Li and C.Z. Ning, Phys. Rev. B 70, 125309 (2004).
[17] M.F. Pereira Jr and H. Wenzel, Phys. Rev. B70, 205331 (2004).
[18] M.F. Pereira Jr., S.-C. Lee and A. Wacker, Phys. Rev. B69, 205310 (2004).
[19] R. Nelander et al, Journal of Applied Physics 102, 113104 (2007).
[20] M.F. Pereira Jr. et al, J. Mater Sci: Mater Electron 18, 689 (2007).
[21] M.F. Pereira Jr., Phys Rev B 75, 195301 (2007).
[22] M. F. Pereira Jr., Phys. Rev. B 78, 245305 (2008).
[23] T. Schmielau and M. F. Pereira Jr, Appl. Phys. Lett. 95, 231111 (2009).
[24] Thi Uyen-Khanh Dang et al, Phys. Rev. B 82, 045305 (2010).
[25] M. F. Pereira Jr. and S. Tomić, Appl. Phys. Lett. 98, 061101 (2011).
[26] A. Le Bris and J. F. Guillemoles, Appl. Phys. Lett. 97, 113506 (2010).
[27] V. Aroutiounian, et al. J. Appl. Phys. 89, 2268–2271 (2001).
[28] F. Szmulowicz, Phys. Rev. B51, 1613 (1995).