Effect of band occupations in intermediate-band solar cells

César Tablero Crespo

ABSTRACT

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Intermediate band semiconductors represent an alternative to increasing the efficiency of solar energy converters. However, the experimental results obtained so far do not reflect the expectations. Many factors are unable to explain it. In this work we have removed some of the approximations used for the efficiency evaluation taking into account the occupation of the bands, the inter-band absorption coefficients, and the optical thickness simultaneously. In many cases the results lower the expectations of the maximum efficiencies.

1. Introduction

An intermediate-band (IB) semiconductor (Fig. 1) can be obtained by introducing one or more intermediate bands (IBs) into a wide single-gap semiconductor, with the usual valence band (VB) and conduction band (CB). The IB semiconductor is a single absorbent material (multi-gap semiconductor with three bands) and not to several layers of different absorbent materials (single-gap semiconductor with two bands) with different optical thicknesses connected in series. Therefore the optical thickness affects all inter-band transitions within the multi-gap semiconductor. The IB solar cells are known as one of the third generation solar cells (Luque and Martí, 2003; Green, 2003; Würfel, 2005; Nelson, 2003). The maximum efficiency of the an IB solar cell is larger than that of a tandem cell with two layers (Green, 2003; Luque and Martí, 2003, 1997; Nelson, 2003; Würfel, 2005) ($\sim 63\%$ versus $\sim 55\%$ with maximum sunlight concentration). The value $\sim 63\%$ is found in this work in the favorable cases of occupation of the IB.

With selective contacts to the VB and CB, holes and electrons respectively can be extracted to an external circuit. The contacts allow a selective exchange of carriers (electrons or holes). In conventional semiconductors is done by two different semiconductor-metal junctions. To extract electrons (holes) from the CB (VB) a junction is ohmic for the electrons (holes) and rectifier for the holes (electrons). This allows the flow of one type of carriers, avoiding or obstructing the flow of the other type of carriers. The semiconductor junction to extract electrons from the CB (holes from the VB) is usually a n^+ -type (p^+ -type) doped semiconductor.

If no carriers can be extracted from the IBs, i.e. the IB is electrically isolated, the photocurrents is increased with respect to the host single-gap semiconductor. This is because the optical $V \rightarrow I$ and $I \rightarrow C$ transitions generate additional carriers (holes in the VB and electrons in the

CB), that add to those generated by the usual $V \rightarrow C$ optical transitions. In this way, the photons with less energy than the energy bandgap of the host single-gap semiconductor, which were lost, are used to generate additional carriers. As the IB is electrically isolated from the contacts, the photovoltage is controlled by the wide bandgap. Therefore an increase in the photocurrent with the preservation of the photovoltage increases the efficiency of this type of solar converter.

The IB could also open the possibility of a further radiationless mechanism $CB \rightarrow IB \rightarrow VB$. But the behavior as centers of non-radiative recombination depends on whether the states are localized or delocalized making up an IB. These intermediate states can be inserted into the bandgap using impurities. This can lead, in some cases, to localized defect states at low concentration (impurity-doping) or an energy band at high doping concentration (impurity-alloying). For impurity-doping these localized defect states act as Shockley, Read and Hall non-radiative recombination centers (Hall, 1952; Shockley and Read, 1952). In this case the energy of an excited carrier is dissipated by multi-phonon emission (Lang and Henry, 1975). It reduces the efficiency of the solar cells. Nevertheless, for the impurity-alloying case, the states make up an IB with delocalized states and the negative non-radiative recombination effect is suppressed (Luque et al., 2006; Tablero, 2009, 2012a). In the latter case the impurity concentration must exceed the threshold set by the Mott's transition (Luque et al., 2006).

When evaluating the maximum efficiency of this type of device, several approximations are made (Brown and Green, 2002; Luque and Martí, 1997): the cell operates at 300 K, carrier mobilities are infinite (no ohmic losses), non-overlapping absorption coefficients, etc. Additionally, for the transitions involving the IB to generate more carriers, the IB must be partially occupied: it must have empty states for the $V \rightarrow I$ transition to take place, and full states for the $I \rightarrow C$ transition to take place. If not, the efficiency would decrease and the IB solar cell would behave as one single-gap solar cell.

Fig. 1. Simplified (a) band diagram and (b) total (α_T) and inter-band α_{AB} absorption coefficients of an IB solar cell. μ_A and f_A are the chemical potential and occupation factor associated with the A-band respectively. z_{AB} depends on the inter-band $A \rightarrow B$ transition probability, and on the density of states of the A and B bands.

The experimental results related to the operation of IB solar cell (Ramiro et al., 2014) have not yet led to the expected efficiencies for this type of solar cell. Among many factors that could explain it would be the IB occupation, the weakness of the absorption coefficients, and the optical thickness of the samples.

Despite the importance of the IB occupation and its dependence on the optical thickness, not much attention has been paid to this fact. In this work we have carried out a study on the impact of these factors on the efficiency of the IB solar cell. Experimentally, based on the original IB solar cell model (Luque and Martí, 1997), the coefficient of absorption, thickness, and mainly the band occupation are almost never considered. For this reason, absence of experimental data regarding band occupation, it is very difficult to contrast with experimental data. However, the results of this work could justify why some IB solar cells do not improve the performance of traditional single-gap solar cells or do not reach the expected efficiency.

2. Methodology

The photocurrent J resulting from A to B band transitions is the difference between the current due to the absorbed and emitted photons (Luque and Martí, 1997, 2003; Würfel, 2005; Green, 2003): $J_{AB} = J_{AB}^{(a)} - J_{AB}^{(e)}$, where $J_{AB}^{(x)} = q \int a(E, \alpha_T, w)(\alpha_{AB}/\alpha_T)\phi_x^{(AB)}(E)dE$ ($x = a, e$ for absorption and emission respectively). In this expression α_{AB} is the absorption coefficient for the $A \rightarrow B$ transitions, α_T is the total absorption coefficient ($\alpha_T = \sum_A \sum_{B > A} \alpha_{AB}$), $a(E, \alpha_T, w) \simeq 1 - e^{-\zeta \alpha_T w}$ is the absorptivity (ζ is 1, 2 both with and without the back reflector respectively), w the thickness of the absorbent material, q is the electron charge, and $\phi_a^{(AB)}$ and $\phi_e^{(AB)}$ are the incident and the emitted spectrum photon flux density respectively from the A to B band transitions. The 6000 K Black-body (BB) spectrum has been used as the incident spectrum ($\phi_a^{(AB)} \equiv \phi_a$). Because of the distance from the sun's surface to the earth, at a point just outside the Earth's atmosphere the sun's surface power density (62 MW m^{-2}) is reduced (on account of the reduced angular range of the sun) by 46,200 (Green, 2003; Nelson, 2003). It corresponds to the Black-body spectrum on earth without concentration, i.e. with a sunlight concentration factor $X = 1$. If the sunlight is concentrated then the incident spectrum will be multiplied by the sunlight concentration factor X ($1 \leq X \leq 46,200$). Therefore, at maximum concentration

($X_{\max} = 46,200$), the power density on earth is equal to that on the surface of a Black-body at 6000 K. For the emitted spectrum we have used the standard approach considering that the device emits radiation as a generalized Black-body (also known as Kirchhoff's and Planck's laws for non-black bodies (Green, 2003; Würfel, 2005)) at $T = 300 \text{ K}$ (Luque and Martí, 1997, 2003; Würfel, 2005; Green, 2003) ($\phi_e^{(AB)} = E^2(2\pi/h^3c^2)(\alpha_{AB}/\alpha_T) \sum_P \sum_{Q > P} (\alpha_{PQ}/\alpha_T) b_{PQ}(E, T, \mu_{QP})$ where $b_{BA}(E, T, \mu_{BA}) = [e^{(E-\mu_{BA})/kT} - 1]^{-1}$ is the Bose-Einstein factor, k is the Boltzmann constant and $\mu_{BA} = \mu_B - \mu_A$ is the chemical potential associated with the radiation emitted between the A and B bands (Luque and Martí, 1997, 2003; Würfel, 2005; Green, 2003)). Note that the Kirchhoff's or Planck's law describes both the emission of thermal radiation for $\mu_{QP} = \mu_Q - \mu_P = 0$ and the emission of luminescence radiation for $\mu_{QP} \neq 0$. With illumination, part of the electron population increase electrochemical potential energy because the $P \rightarrow Q$ transitions. Then the system develops inter-band chemical potentials μ_{QP} . As a consequence spontaneous emission is increased. The rate of emission depends upon μ_{QP} and the difference μ_{QP} of chemical potentials of the bands (or quasi-Fermi energies) is the chemical potential of the emitted photons.

The net current for the A band is $J_A = \sum_{B \neq A} J_{BA}$, with $J_{AB} = -J_{BA}$. For a IB semiconductor the carriers are extracted from the VB (hole current J_V) and CB (electron current $-J_C$), and no current is extracted from the IBs, i.e. $J_I = 0$ ($I \neq V, C$). Therefore, the current density-voltage (J - V) characteristic is obtained by solving the multi-variable non-linear problem simultaneously where the set of equations are $J = J_V = -J_C$, $J_I = 0$ ($I \neq V, C$), and the target magnitudes to be obtained are the chemical potentials μ_A , where $V = \mu_C - \mu_V$. This photovoltage V is lower than the energy gap (E_g) of the absorbent semiconductor ($V < E_g$). This is because part of the energy absorbed is reemitted by radiative recombination. Note also that the photon emission current depends on the voltage. In fact, for single-gap non-degenerate semiconductors with VB and CB, the Bose-Einstein factor b_{CV} of the emission current can be approximated by the classical Boltzmann statistics and then (Baruch et al., 1995; Green, 2003; Ross and Collins, 1980; Sze and Ng, 2007) where $qV = \mu_{CV}$. Other recombination mechanisms (non-radiative, superficial, etc) also cause voltage losses and can be modeled with the current expression (Baruch et al., 1995; Ross and Collins, 1980; Sze and Ng, 2007) $J_{\text{loss}}(V) \approx J_{\text{loss}}(0)e^{qV/kT}$ if $qV \gg kT$.

Note that the both the absorption coefficient (via $(f_A - f_B)$), where f_A are the Fermi-Dirac factors $f_A \equiv f_A(E, T, \mu_A) = [e^{(E-\mu_A)/kT} + 1]^{-1}$ and the emission current (via the Boltzmann factors $b_{BA} \equiv b_{BA}(E, T, \mu_{BA}) = [e^{(E-\mu_{BA})/kT} - 1]^{-1}$, depend on the target variables μ_A of the multi-variable non-linear problem.

The energy conversion efficiency η of a PVC is the relationship between the output power from the device ($P_{\text{out}} = JV$) and the power from the incident (sun) spectrum P_{sun} ($\eta = P_{\text{out}}/P_{\text{sun}}$). Therefore, in order to obtain the maximum efficiencies for an IB semiconductor it is necessary to solve a multi-variable non-linear optimization problem where the position of the IB within the energy bandgap is optimized simultaneously in order to obtain the maximum efficiency. For this the absorption coefficient is necessary.

The absorption coefficient depends on the occupation factors f_A , energies E_A , and density of states g_A of the A-bands, and the square of the momentum matrix elements p_{AB} between the A and B bands. If the band structure is isotropic then the absorption coefficient can be expressed as (Casey and Panish, 1978; Nelson, 2003):

$$\alpha_{AB}(E) \sim (1/E) \int [f_A(x) - f_B(x+E)] |p_{AB}|^2 g_A(x) g_B(x+E) dx \quad (1)$$

Usually in semiconductor physics and in solar cells the bands are considered isotropic (in most cases parabolic near the band edges). If the bands are not isotropic for the absorption coefficient should be used the general equation (Bassani, 1975):

$$\alpha_{AB}(E) \sim (1/E) \iint [f_A(E_A) - f_B(E_B)] |p_{AB}|^2 \delta(E_B(\mathbf{k}_B) - E_A(\mathbf{k}_A) - E) d\mathbf{k}_A d\mathbf{k}_B \quad (2)$$

where δ is the Dirac delta function and $\mathbf{k}$ represent points in the Brillouin zone, instead of Eq. (1) (Casey and Panish, 1978; Nelson, 2003). These equations can be applied to both bands and levels only considering that for N_A degenerate levels with energy E_A the density of states g_A is proportional to the Dirac delta function: $g_A(x) = N_A \delta(x - E_A)$.

For low enough excitation levels, the absorption coefficients can be split approximately as $\alpha_{AB}(E) \sim (f_A - f_B) \cdot z_{AB}$, i.e. on a function depending on the band occupations ($f_A - f_B$), often referred to as the *band-filling factor* (Haug, 2004), and on a term z_{AB} depending on the transition probability and the density of states ($z_{AB} = |p_{AB}|^2 g_A(E_A) g_B(E_B)$).

3. Results and discussion

In most evaluations of maximum efficiencies the absorptivity, and therefore the absorption coefficient α_{AB} , is considered as a step function (Luque and Martí, 2001; Nelson, 2003) with a value of not zero and constant only for energies above the energy bandgap $E_{AB} = E_B - E_A$, with $E_B > E_A$. The difference in occupation numbers ($f_A - f_B$) is considered constant and equal to one, i.e. $\alpha_{AB} \equiv z_{AB}$. This consideration is equivalent to assuming that the bands are carrier reservoirs.

We will relax this approximation to take into account the dependence on the band occupation factors f_A ($0 \leq f_A \leq 1$). To do so, as previously mentioned, the absorption coefficients are split into two terms, one dependent ($f_A - f_B$) and the other independent (z_{AB}) of the occupation factors, i.e. $\alpha_{AB} = (f_A - f_B) \cdot z_{AB}$. For z_{AB} we use the conventional step functions: zero if the photon energy is lower than the energy bandgap between the bands E_{AB} , and a constant value z_{AB} for $E_{AB} \geq 0$.

We consider a double-gap semiconductor with three bands, the usual VB and CB and, between them, an IB. In order to evaluate the dependence of the efficiencies on the IB occupation factor f_I we consider the VB and the CB, with occupation factors f_V and f_C , almost filled and empty respectively ($f_V \sim 1$ and $f_C \sim 0$), i.e. as electron and hole reservoirs respectively, and $z \equiv z_{VI} = z_{VC} = z_{IC}$.

In Fig. 2 the maximum efficiency is represented as a function of the energy band gap for several $p_I = f_I \cdot (zw)$ values. The set of values of zw , within the range $10^{+2} \leq zw \leq 10^{-1}$, include most of the possibilities for absorption coefficients and optical thicknesses of the solar cells. For example, considering an habitual average absorption coefficient (without taking into account the occupation factors) of $z = 10^{+4} \text{ cm}^{-1}$, then $10^{-2} \text{ cm} \leq w \leq 10^{-5} \text{ cm}$ ($10^{+2} \mu\text{m} \leq w \leq 10^{-1} \mu\text{m}$). In all cases: (i) when $p_I = f_I = 0$ the results correspond to a single-gap semiconductor; (ii) for $zw \geq 10^{+2}$ the efficiencies are equal, because the absorptivity $a \sim 1$. The case $zw = 10^{+2}$ is shown in panel a. The efficiencies for $zw > 10^{+2}$ are equal to the results shown in panel a. Also, for this reason, the results when the occupation numbers are not considered for $zw \geq 10^{+2}$ (labeled as REF in figure) and $zw \rightarrow \infty$ (labeled as REF1 in figure) match. Therefore the quotient η/a between the efficiency η and the absorptivity a is a constant that does not depend on zw for $zw \geq 10^{+2}$.

In Fig. 2b $p_I = f_I$ because $zw = 1$. In this case the values corresponding to p_I and $(1 - p_I)$ almost match. For example the results for the pairs of p_I values (0.0, 1.0), (0.2, 0.8), and (0.4, 0.6) are almost equal. The efficiencies are lower than those of the previous case ($zw \geq 10^{+2}$, panel a), because the absorption capacity is lower. For the same reason the maximum efficiencies for single-gap semiconductors ($p_I = f_I = 0$) and IB semiconductor (curve labeled as 'REF1') are lower than when $zw \geq 10^{+2}$ (or when $zw \rightarrow \infty$, curve labeled as 'REF'). Finally when the absorbent capacity zw is very poor, either because the absorption coefficient, the width, or both are very small, the efficiencies are very low (panel c in Fig. 2 for $zw = 10^{-1}$).

In order to evaluate the influence on the absorption capacity zw and on the occupation f_I we have fixed the semiconductor gap to $E_g = E_{VC} = 2 \text{ eV}$ next to the gap with maximum overall efficiency

Fig. 2. Maximum efficiency as an energy gap function for several $p_I = f_I \cdot (zw)$ values using the BB spectrum, with maximum sunlight concentration ($X_{\max} = 46,200$), and with (a) $zw \geq 10^{+2}$, (b) $zw = 10^0 = 1$, and (c) $zw = 10^{-1}$. The curve labeled 'REF1' corresponds to the maximum efficiency when the occupation factors are not considered, i.e. $(f_A - f_B) = 1$ for all transitions. The curve labeled 'REF' corresponds to the absolute maximum efficiency when $zw \rightarrow \infty$.

($\sim 1.9 \text{ eV}$). The maximum efficiency, in accordance with the IB occupation for several values of zw , is represented in Fig. 3a. With the choice of the x axis in the figure, the center corresponds to $f_I = 1/2$. To the left f_I decreases from $1/2$ to zero (empty IB), and to the right f_I increases from $1/2$ to one (full IB). In all cases: (i) the maximum efficiencies extend to an interval of around $f_I = 1/2$. This interval is larger when the absorption capacity zw is greater. When $zw \rightarrow \infty$ the interval would include all possible values of f_I occupation factors, except $f_I = 0$ and $f_I = 1$; (ii) only when $zw \geq 10^{+2}$, are the absolute maximum efficiencies (without considering the occupation factors and in the limit $zw \rightarrow \infty$) reached for $f_I \rightarrow 1/2$. In the scale of the figure, it seems that the maximum efficiencies are also reached when $zw = 10^{+1}$. However, they are slightly different (63.06% versus 62.86% for maximum sunlight concentration, and 45.22% versus 45.39% without sunlight concentration). This small difference cannot be appreciated in the scale of the figure; (iii) when the IB is completely full ($f_I = 1$) or empty ($f_I = 0$) (right- and left-hand limits of the horizontal axis in the figure respectively) the results coincide with the overall maximum efficiencies of a single-gap semiconductor with $E_g = 2 \text{ eV}$.

The output voltage does not vary significantly in all cases. It is between 1.874 V and 1.879 V. However, the IB position (Fig. 3b) varies considerably. For the limits $f_I \rightarrow 0$ (or $f_I \rightarrow 1$) the IB semiconductor behaves like a single-gap semiconductor. Then the IB approaches the

Fig. 3. (a) Maximum efficiency η , and (b) the energy position of the IB with respect to the VB ($E_{VI} = E_i - E_V$) as a function of the occupation factor f_I for several zw values of an IB semiconductor with an energy bandgap $E_g = E_{VC} = 2.0$ eV. The thin and thick curves correspond to the BB spectrum without concentration ($X = 1$) and with maximum concentration ($X_{\max} = 46,200$) respectively. The function on the x-axis is: $F_2(f_I) = +\log(f_I)$ if $0 \leq f_I < 1/2$, $F_2(1/2) = 0$, and $F_2(f_I) = -\log(1 - f_I)$ if $1/2 < f_I \leq 1$. With this definition, the center of the figure corresponds to the IB full up to the middle, to the left the occupation decreases towards zero (empty IB), and to the right it increases towards one (full IB).

VB (or the CB). On the other hand, when $f_I \rightarrow 1/2$ and the absorption capacity zw is large, the semiconductor efficiencies tend toward the maximum for an IB semiconductor.

So far we have obtained the overall maximum efficiencies by also optimizing the energy position of the IB in the bandgap (Fig. 3b). For this reason, when $f_I \rightarrow 0$ or 1 the IB tends towards the VB or CB, and the IB semiconductor works like a single-gap semiconductor. The results could be very different if the IB energetic position is not optimized, i.e. it has a constant value for all f_I . Fig. 4 details the efficiency results for two IB semiconductors with $E_{VC} = 2$ eV (Fig. 4a) and $E_{VC} = 3$ eV (Fig. 4b) using the BB spectrum and $X = 1$. The first is very close to the optimal value. The second will illustrate better the latter conclusions. In this figure we have analyzed three different cases with respect to the IB position: (1) the position is optimized to reach the maximum efficiency for each value of f_I ; the position is kept fixed (2) at the optimal value ($E_{VI} \sim 0.7$ eV and 1.2 eV respectively) or (3) at a non-optimal value ($E_{VI} = 0.9$ eV and 1.0 eV respectively). Cases 2 and 3 reflect the expected behavior of an IB semiconductor more accurately. Obviously, for case (3), with non-optimal E_{VI} , the efficiency is lower than in the other cases. Several other conclusions can be drawn: (i) the efficiencies for cases (1) and (2) are similar. There is a slight narrowing of the flat area of maximum efficiencies, and a decrease in the efficiencies in case (2) with respect to the optimum case (1) in the rest of the f_I values. This confers certain strength to the optimal E_{VI} values; (ii) in all cases by reducing or increasing the IB occupation f_I with respect to the IB half-full, the

Fig. 4. Maximum efficiency η as a function of the occupation factor f_I for $zw = 10^+4$, $X = 1$, and (a) $E_{VC} = 2.0$ eV and (b) $E_{VC} = 3$ eV. $F_2(f_I)$ is defined in the caption of Fig. 2. The three curves in the figure correspond to different cases: (1) E_{VI} is optimized for each f_I ; (2) E_{VI} is fixed to the optimum for $f_I = 1/2$ ($E_{VI} \sim 0.7$ eV and 1.2 eV for $E_{VC} = 2.0$ eV and 3.0 eV respectively) for all f_I values; and (3) E_{VI} is fixed to non-optimal values ($E_{VI} = 0.9$ eV and 1.0 eV for $E_{VC} = 2.0$ eV and 3.0 eV respectively) for all f_I values.

efficiency tends towards that of a single-gap semiconductor with an energy bandgap E_{VC} independently of the sub-bandgaps E_{VI} and E_{IC} , i.e. of the position of the IB in the gap. This is reflected more clearly for $E_{VC} = 3$ eV (Fig. 4b), where all the maximum efficiencies of single-gap solar cells for all sub-gaps (the optimal $E_{VI} \sim 1.2$ eV and $E_{IC} \sim 1.8$ eV, and the non-optimal $E_{VI} \sim 1.0$ eV and $E_{IC} \sim 2.0$ eV) are greater than 24% (30.7, 27.2, 28.8 and 24.4% respectively), and larger than the E_{VC} single-gap efficiency ($\eta \sim 10.6\%$). This fact, in principle, is non-intuitive. In the limits $f_I \rightarrow 0$ ($f_I \rightarrow 1$) we might think that the IB semiconductor behaves like a conventional single-gap semiconductor with a gap E_{VI} (E_{IC}), and not with a gap E_{VC} . However this is because the contacts through which the carriers are extracted are to the VB and CB. Therefore the IB net current must be zero and the voltage is determined by E_{VC} .

In this study we have taken $z \equiv z_{VI} = z_{VC} = z_{IC}$ in order to focus exclusively on the IB occupation. As z_{AB} depends on the A $\rightarrow$ B transition probability and on the density of states of the A and B bands, it implicitly implies that: (i) the IB has a density of states similar to the VB and CB. Then, as it is mentioned in the introduction, the non-radiative recombination is suppressed; (ii) all inter-band transitions have a similar probability but occurs at different rates because the absorption coefficients are different because they depends on the occupation: $\alpha_{VC} = z$, $\alpha_{VI} = (1 - f_I)z$, and $\alpha_{IC} = f_I z$.

From the results shown in the figures the overall maximum efficiencies of the original IB solar cell model (Luque and Martí, 1997) are obtained approximately when $f_I \cdot (zw) > 10$ with the constraint $0 \leq f_I \leq 1$. Else the efficiencies are lower than those predicted by

the original model. However the efficiency of the ideal multi-gap solar cell is always larger than or equal to the efficiency of the ideal single-gap solar cell. Then the photovoltage is controlled by the wide bandgap E_{VC} independently of the sub-bandgaps E_{VI} and E_{IC} . Only in the unfavorable cases the efficiency is equal. For example when the IB is completely full or empty. Of course, this is true as long as the IB is well isolated from contacts to the VB and to the CB. Otherwise, if the IB is not electrically isolated and one of the contacts is to the IB instead of to the VB or to the CB, it would not be a multi-gap solar cell. This case would correspond to the usual single-gap solar cell where the voltage would be determined by one of the smallest bandgaps (E_{IC} or E_{VI} respectively). Note also that the effect of absorption capacity zw on efficiencies affects all solar cells, with single- or multi-gap semiconductors. If the absorptivity is less than unity, all solar cells absorb less photons, thus decreasing the efficiency.

As previously mentioned, it is difficult to contrast with experimental results. In some cases, due to the absence of occupation factors, optical thickness, and/or because the absorption coefficients (or other optical properties) obtained experimentally are not absolute values. They depend explicitly on occupations: $\alpha_{VI} = (1 - f_I)z$, and $\alpha_{IC} = f_I z$. In the literature there are theoretical calculations of IB materials. In fact, this methodology to obtain efficiencies has previously been used with the absorption coefficients obtained from first-principles (Crespo, 2018; Tablero, 2016) as a photon energy function for the host semiconductor, and the habitual step absorption coefficients for modelling the $VB \rightarrow IB$ and $IB \rightarrow CB$ transitions. In these works the optimal occupation $f_I = 1/2$ is assumed, i.e. the effect of band occupations is not considered. Also some IB materials based on III-V, II-VI, and other semiconductors highly doped by a variety of transition elements have been described theoretically (Aguilera et al., 2010; Seminóvski et al., 2011; Tablero, 2012b, c; Tablero and Wahnón, 2003; Wahnón and Tablero, 2002). In most of these materials the IB occupation is $1/3$ or $2/3$. Therefore, as a consequence of the results in this work, they would be in the range of favorable f_I cases (close to $f_I = 1/2$) to obtain the maximum efficiencies when considering the band occupation and the usual thicknesses of solar cells.

Also, in the literature, there are some studies where optical thickness is considered. For example, according with results in Okada et al., 2015, the maximum efficiency is 52.8% for $w = 500$ nm InAs/GaAs QD-IBSCs under maximum concentration when $z_{IC}/z_{VI} = 0.2$ with $z_{IC} \geq 10^5$ cm⁻¹. Although we have $z \equiv z_{VI} = z_{VC} = z_{IC}$ in order to focus exclusively on the IB occupation, the previous parameters would be equivalent to take in our model $w = 500$ nm, $z = 10^5$ cm⁻¹ ($zw = 5$) and $f_I = 0.166$ (then $\alpha_{IC}/\alpha_{VI} = f_I/(1 - f_I) \sim 0.2$). With this parameters the maximum efficiency is 52%, similar to Okada et al., 2015.

4. Conclusions

We have carried out an evaluation of the variation of the main characteristics of an IB semiconductor according to the occupation of the IB and the optical thickness w , or more specifically with the absorption capacity zw . z corresponds to the part of the absorption coefficient independent of the band occupation factors. The main conclusions can be summarized as: (1) when the absorption capacity $zw \geq 10^{+2}$ the efficiencies are equal because the absorptivity $a \sim 1$; (2) the maximum efficiency is reached within an interval of around $f_I = 1/2$ because the results for f_I and $(1 - f_I)$ almost match. This interval is larger, the bigger the absorption capacity zw . Furthermore, only when $zw \geq 10^{+2}$ are the absolute maximum efficiencies (limit $zw \rightarrow \infty$, and without considering the occupation factors) reached; (3) The results correspond to a single-gap semiconductor with energy bandgap E_{VC} when $f_I = 0$ or 1 regardless of whether the IB is located in the optimal energy position or not.

In addition to the IB occupation, the efficiency depends on z which comes from the transition probability and the density of states. Therefore, to achieve high efficiencies, the IB density of states and the inter-band transition probabilities $VB \rightarrow IB$ and $IB \rightarrow CB$ must also be large.

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