



Maximal Efficiencies in New Single GaAs_{1-x}Sb_x-Alloy Junction Solar Cells at 300 K

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Abstract:

In single n⁺(p⁺) – p(n) [X(x) ≡ GaAs_{1-x}Sb_x]-alloy junction solar cells at 300 K, 0 ≤ x ≤ 1, by basing on the same physical model and the same treatment method, as those used in our recent work (Van Cong et al., 2023; Van Cong, 2023), we will investigate the highest (or maximal) efficiencies, η_{I_{max}}(I_{I_{max}}), obtained at the open circuit voltage V_{oc}(= V_{ocI(ocII)}), according to highest hot reservoir temperatures T_H(K), obtained from the Carnot efficiency theorem, being proved by entropy law. Here, one first remarks that,

with increasing x=(0, 0.5, 1), (i)- from Table 3, for the single n⁺ – p X(x)-alloy junction solar cell and for given r_{Sn(Cd)}-radius, for example, η_{I_{max}}(∞)= 31.14%, 28.72%, 25.36%, according to T_H(K) = 435.7, 420.9, 401.9, at V_{ocI}(V) = 1.07, 1.09, 1.17, respectively, while, (ii)- from Table 5, for the single p⁺ – n X(x)-alloy junction solar cell and for given r_{Cd(Sn)}-radius, for example, η_{I_{max}}(∞)= 33.04%, 34.26%, 35.47%, according to T_H(K) = 448.0, 456.3, 464.9, at V_{ocII}(V)[> V_{ocI}(V)] = 1.20, 1.27, 1.38, respectively, suggesting that such η_{I_{max}}(I_{I_{max}})-and-T_H variations depend on the V_{ocII}(V)[> V_{ocI}(V)] – values. (iii)-Then, as given in Table 3, for x = 0 and for r_{d(a)} = r_{Te(Mg)}, one gets: η_I = 23.48 % and 29.71 % at V_{oc} = 0.98 V and 1.1272 V, respectively, which can also be compared with the corresponding results, obtained by Moon et al. (2016) and Green et al. (2022) for the single-junction GaAs thin-film solar cell, 22.08 % and 29.1 %; that gives the relative deviations in absolute values, as: 6.34 % and 2.1 %. Further, for x = 1 and for r_{d(a)} = r_{Sn(Cd)}, one gets in Table 3: η_{I_{max}} = 25.36 % at V_{oc} = 1.17 V, and in Table 5, η_{I_{max}} = 35.47 % at V_{oc} = 1.38 V, which can also be compared with the corresponding results, obtained for the single-junction GaSb-solar cells by Van Cong (2023), 11.17 % (12.03 %) and 11.34 % (12.16 %), respectively. As a result, in order to obtain the highest efficiencies, the single GaAs_{1-x}Sb_x-alloy junction solar cells could be chosen rather than the single crystalline [GaAs, or GaSb]-junction solar cells.

Keywords: single GaAs_{1-x}Sb_x-alloy junction solar cell; single crystalline (GaAs, or GaSb)-junction solar cells; photovoltaic conversion factor; photovoltaic conversion efficiency

Introduction

In single n⁺(p⁺) – p(n) [X(x) ≡ GaAs_{1-x}Sb_x]-alloy junction solar cells at 300 K, 0 ≤ x ≤ 1, by basing on the same physical model and treatment method, as used in our recent work (Van Cong, 2023; Van Cong et al., 2023), and also other works (Green, 2022; Moon et al., 2016; Singh & Ravindra, 2012;



Van Cong & Debiais, 1997, 1993; Van Cong et al., 1984), we will investigate the highest (or maximal) efficiencies, $\eta_{I\max.}(I\max.)$, according to highest hot reservoir temperatures $T_H(K)$, obtained at the open circuit voltage: $V_{oc} = V_{ocI(ocII)}$ and from the Carnot- efficiency theorem, being proved by entropy law.

Some concluding remarks are discussed as follows.

(i)-As noted in Tables 2 and 4, the total (or dark) carrier-minority saturation current density $J_{oI(oII)}$ decreases slightly with increasing $r_{d(a)}$ -radius for given x , and it increases with increasing x for given $r_{d(a)}$ -radius. Then, as observed in Tables 3 and 5, at a same V_{oc} , the photovoltaic conversion factor, $\eta_{I(II)}(V_{oc})$, also decreases with increasing $r_{d(a)}$ -radius for given x , and it increases with increasing x for given $r_{d(a)}$ -radius. In other words, as discussed in Eq. (45), at a same V_{oc} , both $J_{oI(oII)}$ and $\eta_{I(II)}$ have the same variations for the same physical conditions. Further, it should be noted in the work by Singh & Ravindra (2012) that the maximal efficiency value $\eta_{max.}$ could not be obtained, since the “quality factor n ” was assumed to be equal to 1.

(ii)- Then, as observed in Tables 3 and 5, with such variations of $\eta_{I(II)}(V_{oc})$, the maximal values of $\eta_{I(II)}$, $\eta_{I(II)\max.}$, and the corresponding ones of the H-reservoir temperature, T_H , obtained at same corresponding $V_{oc} = V_{ocI(ocII)}$ -values, as marked in bold, increase slightly with increasing $r_{d(a)}$ -radius for a given x .

(iii)-Finally, as given in Table 3, for $x = 0$ and for $r_{d(a)} = r_{Te(Mg)}$, one gets: $\eta_I = 23.48\%$ and 29.71% at $V_{oc} = 0.98\text{ V}$ and 1.1272 V , respectively, which can also be compared with the corresponding results, obtained by Moon et al. (2016) and Green et al. (2022) for the single-junction GaAs thin-film solar cell, 22.08% and 29.1% ; that gives the relative deviations in absolute values, as: 6.34% and 2.1% . Further, for $x = 1$ and for $r_{d(a)} = r_{Sn(Cd)}$, one gets in Table 3: $\eta_{I\max.} = 25.36\%$ at $V_{oc} = 1.17\text{ V}$, and in Table 5, $\eta_{II\max.} = 35.47\%$ at $V_{oc} = 1.38\text{ V}$, which can also be compared with the corresponding results, obtained for the single-junction GaSb-solar cells by Van Cong (2023), 11.17% (12.03%) and 11.34% (12.16%), respectively. As a result, in order to obtain the highest efficiencies, the single $\text{GaAs}_{1-x}\text{Sb}_x$ -alloy junction solar cells could be chosen rather than the single crystalline [GaAs, or GaSb]-junction solar cells.

In the following, we will show that the energy-band-structure parameters, due to the effects of x -Sb concentration, size impurity, temperature T and heavy doping, affect strongly the dark (or total) minority-carrier saturation current density and the photovoltaic conversion effect. Finally, some numerical results and concluding remarks will be also presented.

Energy-Band-Structure Parameters and Dark Minority-Carrier Saturation Current Density, due to the Effects of x - Sb Concentration, Impurity Size, and Heavy Doping

First of all, in the single $n^+(p^+) - p(n)$ $X(x)$ - alloy junction solar cells, $X(\equiv \text{GaAs}_{1-x}\text{Sb}_x)$, we present the effects of x -Sb concentration, donor (acceptor) $[d(a)]$ -size, temperature T and heavy doping, affecting the energy-band-structure parameters, as those investigated in our previous works (Van Cong, 2023; Van Cong et al., 2023).

A. Effect of x -Sb Concentration

In the $n^+(p^+) - p(n)$ single $n^+(p^+) - p(n)$ $X(x)$ - alloy junction at $T=0\text{ K}$, the energy-band-structure parameters are expressed as functions of x , are given in the following.

(i)-The unperturbed relative effective electron (hole) mass in conduction (valence) bands are given by:

$$\begin{aligned} m_c(x)/m_o &= 0.047 \times x + 0.066 \times (1 - x), \text{ and} \\ m_v(x)/m_o &= 0.300 \times x + 0.291 \times (1 - x), \end{aligned} \quad (1)$$

so that one obtains: $m_c(x = 0)/m_o = m_{c(\text{GaAs})}/m_o = 0.066$, $m_v(x = 0)/m_o = m_{v(\text{GaAs})}/m_o = 0.291$, and $m_c(x = 1)/m_o = m_{c(\text{GaSb})}/m_o = 0.047$, $m_v(x = 1)/m_o = m_{v(\text{GaSb})}/m_o = 0.300$.

(ii)-The unperturbed relative dielectric constant of the intrinsic of the single crystalline X- alloy is found to be defined by:

$$\epsilon_o(x) = 15.69 \times x + 13.13 \times (1 - x), \quad (2)$$

which gives: $\epsilon_o(x = 0) = \epsilon_{\text{GaAs}} = 13.13 \approx 13.1$, and $\epsilon_o(x = 1) = \epsilon_{\text{GaSb}} = 15.69 \approx 15.7$.

(iii)-Finally, the unperturbed band gap at 0 K is found to be given by:

$$E_{go}(x) \text{ in eV} = 0.81 \times x + 1.52 \times (1 - x), \quad (3)$$

giving rise to: $E_{go}(x = 0) = E_{g\text{GaAs}} = 1.52 \text{ eV}$, and $E_{go}(x = 1) = E_{g\text{GaSb}} = 0.81 \text{ eV}$.

Therefore, we can define the effective donor (acceptor)-ionization energy at $r_{d(a)} = r_{do(ao)}$ in absolute values:

$$E_{do(ao)}(x) \equiv \frac{13600 \times [m_c(v)(x)/m_o]}{[\epsilon_o(x)]^2} \text{ meV}, \quad (4)$$

and then, the isothermal bulk modulus, by:

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{(4\pi/3) \times (r_{do(ao)})^3}. \quad (5)$$

B. Effects of Impurity-Size, with a Given x

Here, the effects of $r_{d(a)}$ and x-Sb concentration affect the changes in all the energy-band-structure parameters, being expressed in terms of the effective relative dielectric constant $\epsilon(r_{d(a)}, x)$, as follows.

At $r_{d(a)} = r_{do(ao)} = r_{As(Ga)} = 0.118 \text{ nm}$ (0.126 nm), respectively, the needed boundary conditions are found to be, for the impurity-atom volume $V = (4\pi/3) \times (r_{d(a)})^3$, $V_{do(ao)} = (4\pi/3) \times (r_{do(ao)})^3$, for the pressure p , $p_o = 0$, and for the deformation potential energy (or the strain energy) σ , $\sigma_o = 0$. Further, the two important equations (Van Cong et al., 1984), needed to determine the σ -variation $\Delta\sigma \equiv \sigma - \sigma_o = \sigma$, are defined by: $\frac{dp}{dV} = -\frac{B}{V}$ and $p = -\frac{d\sigma}{dV}$. giving: $\frac{d}{dV} \left(\frac{d\sigma}{dV} \right) = \frac{B}{V}$. Then, by an integration, one gets:

$$\begin{aligned} [\Delta\sigma(r_{d(a)}, x)]_{n(p)} = E_{do(ao)}(x) \times (V - V_{do(ao)}) \times \ln \left(\frac{V}{V_{do(ao)}} \right) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \\ \ln \left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 \geq 0. \end{aligned} \quad (6)$$

Furthermore, we also shown that, as $r_{d(a)} > r_{do(ao)}$ ($r_{d(a)} < r_{do(ao)}$), the compression (dilatation) gives rise to the increase (the decrease) in the energy gap $E_{gn(gp)}(r_{d(a)}, x)$, and in the effective donor (acceptor)-ionization energy $E_{d(a)}(r_{d(a)}, x)$ in absolute values, obtained from the effective Bohr model, and then such the compression (dilatation) is represented respectively by: $\pm [\Delta\sigma(r_{d(a)}, x)]_{n(p)}$, respectively,

$$\begin{aligned} E_{gn(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\epsilon_0(x)}{\epsilon(r_{d(a)})} \right)^2 - 1 \right] = \\ + [\Delta\sigma(r_{d(a)}, x)]_{n(p)}, \end{aligned}$$

for $r_{d(a)} \geq r_{do(ao)}$, and for $r_{d(a)} \leq r_{do(ao)}$,

$$\begin{aligned} E_{gn(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\epsilon_0(x)}{\epsilon(r_{d(a)})} \right)^2 - 1 \right] = \\ - [\Delta\sigma(r_{d(a)}, x)]_{n(p)}. \end{aligned} \quad (7)$$

Therefore, from Equations 6 and 7, one obtains the expressions for relative dielectric constant $\epsilon(r_{d(a)}, x)$ and energy band gap $E_{gn(gp)}(r_{d(a)}, x)$, as:

$$\text{(i)-for } r_{d(a)} \geq r_{do(ao)}, \text{ since } \epsilon(r_{d(a)}, x) = \frac{\epsilon_0(x)}{\sqrt{1 + \left[\left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3}} \leq \epsilon_0(x),$$

$$\begin{aligned} E_{gn(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \\ \ln \left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 \geq 0, \end{aligned} \quad (8a)$$

according to the increase in both $E_{gn(gp)}(r_{d(a)}, x)$ and $E_{d(a)}(r_{d(a)}, x)$, for a given x , and

$$\text{(ii)-for } r_{d(a)} \leq r_{do(ao)}, \text{ since } \epsilon(r_{d(a)}, x) = \frac{\epsilon_0(x)}{\sqrt{1 - \left[\left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3}} \geq \epsilon_0(x), \text{ with a condition, given}$$

$$\text{by: } \left[\left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 < 1,$$

$$E_{gn(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = -E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 \leq 0, \quad (8.b)$$

corresponding to the decrease in both $E_{gn(gp)}(r_{d(a)}, x)$ and $E_{d(a)}(r_{d(a)}, x)$, for a given x .

C. Effect of Temperature T, with Given x and $r_{d(a)}$

Here, the intrinsic band gap $E_{gin(gip)}(r_{d(a)}, x, T)$ at any T is given by (Van Cong, 2023; Van Cong et al., 2023):

$$E_{gin(gip)}(r_{d(a)}, x, T) \text{ in eV} = E_{gn(gp)}(r_{d(a)}, x) - 10^{-4} \times T^2 \times \left[\frac{3.6773 \times x}{T+94 \text{ K}} + \frac{5.405 \times (1-x)}{T+204 \text{ K}} \right], \quad (9)$$

which gives: $E_{gin(gip)}(r_{do(ao)}, x = 0, T = 0\text{K}) = 1.52 \text{ eV}$ and $E_{gin(gip)}(r_{do(ao)}, x = 1, T = 0\text{K}) = 0.81 \text{ eV}$, and $E_{gin(gip)}(r_{do(ao)}, x = 0, T = 300 \text{ K}) \simeq 1.42 \text{ eV}$ and $E_{gin(gip)}(r_{do(ao)}, x = 1, T = 300 \text{ K}) \simeq 0.73 \text{ eV}$,

suggesting that, for given x and $r_{d(a)}$, $E_{gin(gip)}$ decreases with an increasing T.

Furthermore, in the n(p)-type X(x)-alloy, one can define the intrinsic carrier concentration $n_{in(ip)}$ by:

$$n_{in(ip)}^2(T, r_{d(a)}, x) \equiv N_c(T, x) \times N_v(T, x) \times \exp \left(\frac{-E_{gin(p)}(T, r_{d(a)}, x)}{k_B T} \right), \quad (10)$$

where $N_{c(v)}(T, x)$ is the conduction (valence)-band density of states, being defined as:

$$N_{c(v)}(T, x) = 2 \times \left(\frac{m_{c(v)}(x) \times k_B T}{2\pi\hbar^2} \right)^{\frac{3}{2}} (\text{cm}^{-3}). \quad (11)$$

So, the numerical results of $E_{d(a)}(r_{d(a)}, x)$, $B_{do(ao)}(x)$, $\varepsilon(r_{d(a)}, x)$ and $E_{gin(gip)}(r_{d(a)}, x, T)$, calculated using Equations 4, 5, 8a (8b) and 9, are reported in following Table 1.

Table 1 in Appendix 1.

D. Heavy Doping Effect, with Given T, x and $r_{d(a)}$

Here, as given in our previous works (Van Cong, 2023; Van Cong & Debiais, 1993), the Fermi energy $E_{Fn}(-E_{Fp})$, band gap narrowing (BGN), and apparent band gap narrowing (ABGN), are reported in the following.

First, the Fermi energy $E_{Fn}(-E_{Fp})$, obtained for any T and any d(a)-density, $N_{d(a)}$, being investigated in our previous paper (Van Cong & Debiais, 1993), with a precision of the order of 2.11×10^{-4} , is found to be given by:

$$\frac{E_{Fn}(u)}{k_B T} \left(\frac{-E_{Fp}(u)}{k_B T} \right) = \frac{G(u) + Au^B F(u)}{1 + Au^B}, \quad A = 0.0005372 \text{ and } B = 4.82842262, \quad (12)$$

where u is the reduced electron density, $u(N_{d(a)}, T, x) \equiv \frac{N_{d(a)}}{N_{c(v)}(T, x)}$, $F(u) = au^{\frac{2}{3}} \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}} \right)^{-\frac{2}{3}}$, $a = \left[(3\sqrt{\pi}/4) \times u \right]^{2/3}$, $b = \frac{1}{8} \left(\frac{\pi}{a} \right)^2$, $c = \frac{62.3739855}{1920} \left(\frac{\pi}{a} \right)^4$, and $G(u) \simeq \ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2} \left[\frac{1}{\sqrt{27}} - \frac{3}{16} \right] > 0$.

Here, one notes that: (i) as $u \gg 1$, according to the HD [d(a)- X(x)- alloy] ER-case, or to the degenerate case, Eq. (12) is reduced to the function $F(u)$, and (ii) $\frac{E_{Fn}(u \ll 1)}{k_B T} \left(\frac{-E_{Fp}(u \ll 1)}{k_B T} \right) \ll -1$, to the LD [a(d)- CdS_{1-x}Se_x- alloy] BR-case, or to the non-degenerate case, Eq. (12) is reduced to the function $G(u)$.

Secondly, if denoting the effective Wigner-Seitz radius $r_{sn(sp)}$, characteristic of the interactions, by:

$$r_{sn(sp)}(N_{d(a)}, r_{d(a)}, x) = 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}}{N_{d(a)}} \right)^{1/3} \times \frac{m_{c(v)}(x)}{\varepsilon(r_{d(a)}, x)}, \quad g_{c(v)} = 1(1), \quad (13)$$

the correlation energy of an effective electron gas, $E_{cn(cp)}(N_{d(a)}, r_{d(a)}, x)$, is given as [4]:

$$E_{cn(cp)}(N_{d(a)}, r_{d(a)}, x) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908 + r_{sn(sp)}} + \left(\frac{2[1 - \ln(2)]}{\pi^2} \right) \times \ln(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67378876}}.$$

Now, taking into account various spin-polarized chemical potential-energy contributions such as [4]: exchange energy of an effective electron (hole) gas, majority-carrier correlation energy of an effective electron (hole) gas, minority hole (electron) correlation energy, majority electron (hole)-ionized d(a) interaction screened Coulomb potential energy, and finally minority hole (electron)-ionized d(a) interaction screened Coulomb potential energy, the band gap narrowing (BGN) are given as follows.

Then, in the n-type HD X(x)- alloy, the BGN is found to be given by (Van Cong, 2023):

$$\Delta E_{gn}(N_d, r_d, x) \simeq a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{3/4} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \right]^{5/4} \times \sqrt{\frac{m_v}{m_c}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \right]^{3/2} \times N_r^{1/6}, \quad N_r \equiv \left(\frac{N_d}{9.999 \times 10^{17} \text{ cm}^{-3}} \right), \quad (14n)$$

where $a_1 = 3.8 \times 10^{-3} \text{ (eV)}$, $a_2 = 6.5 \times 10^{-4} \text{ (eV)}$, $a_3 = 2.8 \times 10^{-3} \text{ (eV)}$, $a_4 = 5.597 \times 10^{-3} \text{ (eV)}$ and $a_5 = 8.1 \times 10^{-4} \text{ (eV)}$, and in the p-type HD X(x)- alloy, as:

$$\Delta E_{gp}(N_a, r_a, x) \simeq a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} \times (2.503 \times [-E_{cp}(r_{sp}) \times r_{sp}]) + a_3 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \right]^{5/4} \times \sqrt{\frac{m_c}{m_v}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \right]^{3/2} \times N_r^{1/6}, \quad N_r \equiv \left(\frac{N_a}{9.999 \times 10^{17} \text{ cm}^{-3}} \right), \quad (14p)$$

where $a_1 = 3.15 \times 10^{-3}(\text{eV})$, $a_2 = 5.41 \times 10^{-4}(\text{eV})$, $a_3 = 2.32 \times 10^{-3}(\text{eV})$, $a_4 = 4.12 \times 10^{-3}(\text{eV})$ and $a_5 = 9.80 \times 10^{-5}(\text{eV})$.

Therefore, in the HD[d(a)- X(x)- alloy] ER, we can define the effective extrinsic carrier concentration, $n_{en(ep)}^*$, by:

$$n_{en(ep)}^*(N_{d(a)}, T, r_{d(a)}, x) \equiv \sqrt{N_{d(a)} \times p_o(n_o)} = n_{in(ip)}(T, r_{d(a)}, x) \times \exp\left[\frac{\Delta E_{agn(aggp)}}{2k_B T}\right], \quad (15)$$

where the apparent band gap narrowing (ABGN), $\Delta E_{agn(aggp)}$, is defined by:

$$\Delta E_{agn}(N_d, T, r_d, x) \equiv \Delta E_{gn}(N_d, r_d, x) + k_B T \times \ln\left(\frac{N_d}{N_c(T, x)}\right) - E_{Fn}(N_d, T, x), \quad (16n)$$

$$\Delta E_{aggp}(N_a, T, r_a, x) \equiv \Delta E_{gp}(N_a, r_a, x) + k_B T \times \ln\left(\frac{N_a}{N_v(T, x)}\right) + E_{Fp}(N_a, T, x). \quad (16p)$$

Total Minority-Carrier Saturation Current Density

In the two $n^+(p^+) - p(n)$ X(x)- alloy -junction solar cells, denoted respectively by I(II), the total carrier-minority saturation current density is defined by:

$$J_{oI(oII)} \equiv J_{Eno(Epo)} + J_{Bpo(Bno)} \quad (17)$$

where $J_{Bpo(Bno)}$ is the minority-electron (hole) saturation current density injected into the LD[a(d)- X(x)- alloy] BR, and $J_{Eno(Epo)}$ is the minority-hole (electron) saturation-current density injected into the HD[d(a)- X(x)- alloy] ER.

$J_{Bpo(Bno)}$ in the LD[a(d)- X(x)- alloy]BR

Here, $J_{Bpo(Bno)}$ is determined by (Van Cong, 2023):

$$J_{Bpo(Bno)}(N_{a(d)}, T, r_{a(d)}, x) = \frac{e \times n_{ip(in)}^2(T, r_{a(d)}, x) \times \sqrt{\frac{D_{e(h)}(N_{a(d)}, T, r_{a(d)}, x)}{\tau_{eB(hB)}(N_{a(d)})}}}{N_{a(d)}}, \quad (18)$$

where $n_{ip(in)}^2(T, r_{d(a)}, x)$ is determined Eq. (10), $D_{e(h)}(N_{d(a)}, T, r_{d(a)}, x)$ is the minority electron (minority hole) diffusion coefficient:

$$D_e(N_a, T, r_a, x) = \frac{k_B T}{e} \times \left[200 + \frac{8300}{1 + \left(\frac{N_a}{1.3 \times 10^{17} \text{ cm}^{-3}} \right)^{0.91}} \right] \times \left(\frac{\varepsilon(r_a, x)}{\varepsilon_0(x)} \right)^2 \text{ (cm}^2 \text{ s}^{-1}), \quad (19a)$$

$$D_h(N_d, T, r_d, x) = \frac{k_B T}{e} \times \left[130 + \frac{270}{1 + \left(\frac{N_d}{8 \times 10^{17} \text{ cm}^{-3}} \right)^{1.25}} \right] \times \left(\frac{\varepsilon(r_d, x)}{\varepsilon_0(x)} \right)^2 \text{ (cm}^2 \text{ s}^{-1}), \quad (19b)$$

and $\tau_{eB(hB)}(N_{d(a)})$ is the minority electron (minority hole) lifetime in the BR:

$$\tau_{eB}(N_a)^{-1} = \frac{1}{10^{-7}} + 3 \times 10^{-13} \times N_a + 1.83 \times 10^{-31} \times N_a^2, \quad (20a)$$

$$\tau_{hB}(N_d)^{-1} = \frac{1}{10^{-7}} + 11.76 \times 10^{-13} \times N_d + 2.78 \times 10^{-31} \times N_d^2. \quad (20b)$$

J_{Eno(Epo)} in the HD[d(a)- X(x)- alloy]ER

In the non-uniformly and heavily doped emitter region of d(a)- X(x) devices, the effective Gaussian d(a)-density profile or the d(a) (majority-e(h)) density, is defined in such the HD[d(a)- X(x) alloy] ER-width W , as (Van Cong et al., 2023; Van Cong, 2023):

$$\rho_{d(a)}(y, N_{d(a)}, W) = N_{d(a)} \times \exp \left\{ - \left(\frac{y}{W} \right)^2 \times \ln \left[\frac{N_{d(a)}}{N_{do(ao)}(W)} \right] \right\} \equiv N_{d(a)} \times \left[\frac{N_{d(a)}}{N_{do(ao)}(W)} \right]^{- \left(\frac{y}{W} \right)^2}, \quad 0 \leq y \leq W,$$

$$N_{do(ao)}(W) \equiv 7.9 \times 10^{17} (2 \times 10^5) \times \exp \left\{ - \left(\frac{W}{184.2 (1) \times 10^{-7} \text{ cm}} \right)^{1.066 (0.5)} \right\} \text{ (cm}^{-3}), \quad (21)$$

where $\rho_{d(a)}(y = 0) = N_{d(a)}$ is the surface d(a)-density, and at the emitter-base junction, $\rho_{d(a)}(y = W) = N_{do(ao)}(W)$, which decreases with increasing W . Further, the “effective doping density” is defined by:

$$N_{d(a)}^*(y, N_{d(a)}, T, r_{d(a)}, x) \equiv \rho_{d(a)}(y) / \exp \left[\frac{\Delta E_{agn(agg)}(\rho_{d(a)}, T, r_{d(a)}, x)}{k_B T} \right],$$

$$N_{d(a)}^*(y = 0, N_{d(a)}, T, r_{d(a)}, x) \equiv \frac{N_{d(a)}}{\exp \left[\frac{\Delta E_{agn(agg)}(N_{d(a)}, T, r_{d(a)}, x)}{k_B T} \right]}, \text{ and}$$

$$N_{d(a)}^*(y = W, T, r_{d(a)}, x) \equiv \frac{N_{do(ao)}(W)}{\exp \left[\frac{\Delta E_{agn(agg)}(N_{do(ao)}(W), T, r_{d(a)}, x)}{k_B T} \right]}, \quad (22)$$

where the apparent band gap narrowing $\Delta E_{agn(aggp)}$ is determined in Eq. (16), replacing $N_{d(a)}$ by $\rho_{d(a)}(y, N_{d(a)}, W)$.

Now, we can define the minority hole (minority electron) transport parameter $F_{h(e)}$ as:

$$F_{h(e)}(y, N_{d(a)}, T, r_{d(a)}, x) \equiv \frac{n_{in(ip)}^2(T, r_{d(a)})}{p_o(n_o) \times D_{h(e)}} = \frac{N_{d(a)}^*}{D_{h(e)}} \equiv \frac{N_{d(a)}}{D_{h(e)}} \times \left(\frac{n_{in(ip)}}{n_{in(ip)}^*} \right)^2 \equiv \frac{N_{d(a)}}{D_{h(e)} \times \exp\left[\frac{\Delta E_{agn(aggp)}}{k_B T}\right]} (cm^{-5} \times s), \quad (23)$$

the minority hole (electron) diffusion length, $L_{h(e)}(y, N_{d(a)}, T, r_{d(a)}, x)$ by:

$$L_{h(e)}^{-2}(y, N_{d(a)}, T, r_{d(a)}, x) = [\tau_{hE(eE)} \times D_{h(e)}]^{-1} = (C \times F_{h(e)})^2 = \left(C \times \frac{N_{d(a)}^*}{D_{h(e)}} \right)^2 = \left(C \times \frac{n_{in(ip)}^2(T, r_{d(a)})}{p_o(n_o) \times D_{h(e)}} \right)^2,$$

where the constant C was chosen to be equal to: $2.0893 \times 10^{-30} (cm^4/s)$, and the minority hole (minority electron) lifetime $\tau_{hE(eE)}$ as:

$$\tau_{hE(eE)} \equiv \frac{1}{D_{h(e)} \times L_{h(e)}^{-2}} = \frac{1}{D_{h(e)} \times (C \times F_{h(e)})^2}. \quad (24)$$

Then, under low-level injection, in the absence of external generation, and for the steady-state case, we can define the minority-h(e) density by:

$$p_o(y)[n_o(y)] \equiv \frac{n_{in(ip)}^2}{N_{d(a)}^*(y=W, T, r_{d(a)}, x)}, \quad (25)$$

and a normalized excess minority-h(e) density $u(x)$ or a relative deviation between $p(y)[n(y)]$ and $p_o(y)[n_o(y)]$.

$$u(y) \equiv \frac{p(y)[n(y)] - p_o(y)[n_o(y)]}{p_o(y)[n_o(y)]}, \quad (26)$$

which must verify the two following boundary conditions as:

$$u(y = 0) \equiv \frac{-J_h(y=0)[J_e(y=0)]}{eS \times p_o(y=0)[n_o(y=0)]}$$

$$u(y = W) = \exp\left(\frac{V}{n_{I(I)}(V) \times V_T}\right) - 1.$$

Here, $n_{I(II)}(V)$ is the photovoltaic conversion factor, being determined later, S ($\frac{cm}{s}$) is the surface recombination velocity at the emitter contact, V is the applied voltage, $V_T \equiv (k_B T/e)$ is the thermal voltage, and the minority-hole (electron) current density $J_{h(e)}(y, r_{d(a)}, x)$.

Further, from the Fick's law for minority hole (electron)-diffusion equations, one has (Van Cong et al., 2023; Van Cong, 2023):

$$J_{h(e)}(y, r_{d(a)}, x) = \frac{-e(+e) \times n_{in(ip)}^2}{F_{h(e)}(y)} \times \frac{du(y)}{dy} = \frac{-e(+e)n_{in(ip)}^2 D_{h(e)}(N_{d(a)}, r_{d(a)}, x)}{N_{d(a)}^*(y, r_{d(a)}, x)} \times \frac{du(y)}{dy}, \quad (27)$$

where $N_{d(a)}^*(y, r_{d(a)}, x)$ is given in Eq. (22), $D_{h(e)}$ and $F_{h(e)}$ are determined respectively in Equations (19) and (23), and from the minority-hole (electron) continuity equation as:

$$\frac{dJ_{h(e)}(y, r_{d(a)}, x)}{dy} = -e(+e) \times n_{in(p)}^2 \times \frac{u(y)}{F_{h(e)}(y) \times L_{h(e)}^2(y)} = -e(+e) \times n_{in(p)}^2 \times \frac{u(y)}{N_{d(a)}^*(y, r_{d(a)}, x) \times \tau_{hE}(eE)}, \quad (28)$$

Therefore, the following second-order differential equation is obtained:

$$\frac{d^2 u(y)}{dy^2} - \frac{dF_{h(e)}(y)}{dy} \times \frac{du(y)}{dy} - \frac{u(y)}{L_{h(e)}^2(y)} = 0, \quad (29)$$

Then, taking into account the two above boundary conditions given in Eq. (22), one thus gets the general solution of this Eq. (29), as:

$$u(y) = \frac{\sinh(P(y)) + I(W, S) \times \cosh(P(y))}{\sinh(P(W)) + I(W, S) \times \cosh(P(W))} \times \left(\exp\left(\frac{V}{n_{I(II)}(V) \times V_T}\right) - 1 \right), \quad (30)$$

where the factor $I(W, S)$ is determined by: $D_{h(e)}(N_d, T, r_{d(a)}, x)$

$$I(T, r_{d(a)}, x, W, S) = \frac{D_{h(e)}(y=W, N_{do(ao)}(W), T, r_{d(a)}, x)}{S \times L_{h(e)}(y=W, N_{do(ao)}(W), T, r_{d(a)}, x)}. \quad (31)$$

Further, since $\frac{dP(y)}{dy} \equiv C \times F_{h(e)}(y) = \frac{1}{L_{h(e)}(x)}$, $C = 2.0893 \times 10^{-30}$ (cm^4/s), for the X(x)-alloy, being an empirical parameter, chosen for each crystalline semiconductor, $P(y)$ is thus found to be defined by:

$$P(y) \equiv \int_0^y \frac{dy}{L_{h(e)}(y)}, \quad 0 \leq y \leq W, \quad P(y=W) \equiv \left(\frac{1}{W} \times \int_0^W \frac{dy}{L_{h(e)}(y)}\right) \times W \equiv \frac{W}{L_{h(e)}^*(y)} = \frac{L_{h(e)}(y)}{L_{h(e)}^*(y)} \times \frac{W}{L_{h(e)}(y)}, \quad (32)$$

where $L_{h(e)}^*$ (y) is the effective minority hole (minority electron) diffusion length. Further, the minority-hole (electron) current density injected into the HD[d(a)- X(x) alloy] ER is found to be given by:

$$J_{h(e)}(y, W, N_{d(a)}, T, r_{d(a)}, x, S, V) = -J_{Eno}(y, W, N_d, T, r_d, x, S) [J_{Epo}(y, W, N_a, T, r_a, x, S)] \times \left(\exp\left(\frac{V}{n_{I(I)}(V) \times V_T}\right) - 1 \right), \quad (33)$$

where $J_{Eno(Epo)}$ is the saturation minority-hole (minority-electron) current density,

$$J_{Eno(Epo)}(y, W, N_{d(a)}, T, r_{d(a)}, x, S) = \frac{en_{in(ip)}^2 \times D_{h(e)}}{N_{d(a)}^*(y, N_{d(a)}, T, r_{d(a)}, x) \times L_{h(e)}} \times \frac{\cosh(P(x)) + I(W, S) \times \sinh(P(x))}{\sinh(P(W)) + I(W, S) \times \cosh(P(W))}, \quad (34)$$

In the following, we will denote $P(W)$ and $I(W, S)$ by P and I , for a simplicity. So, Eq. (30) gives:

$$J_{Eno(Epo)}(y = 0, W, N_{d(a)}, T, r_{d(a)}, x, S) = \frac{en_{in(ip)}^2 \times D_{h(e)}}{N_{d(a)}^*(y, N_{d(a)}, T, r_{d(a)}, x) \times L_{h(e)}} \times \frac{1}{\sinh(P) + I \times \cosh(P)}, \quad (35)$$

$$J_{Eno(Epo)}(y = W, W, N_{d(a)}, T, r_{d(a)}, x, S) = \frac{en_{in(ip)}^2 \times D_{h(e)}}{N_{d(a)}^*(y=W, N_{d(a)}, T, r_{d(a)}, x) \times L_{h(e)}} \times \frac{\cosh(P) + I \times \sinh(P)}{\sinh(P) + I \times \cosh(P)}, \quad (36)$$

and then,

$$\frac{J_{h(e)}(y=0, W, N_{d(a)}, T, r_{d(a)}, x, S, V)}{J_{h(e)}(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S, V)} \equiv \frac{J_{Eno(Epo)}(y=0, W, N_{d(a)}, T, r_{d(a)}, x, S)}{J_{Eno(Epo)}(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S)} = \frac{1}{\cosh(P) + I \times \sinh(P)}. \quad (37)$$

Now, if defining the effective excess minority-hole (electron) charge storage in the emitter region by:

$$Q_{h(e)}^*(y = W, N_{d(a)}, T, r_{d(a)}, x) \equiv \int_0^W +e(-e) \times u(y) \times p_o(y) [n_o(y)] \times \frac{\tau_{hE(eE)}(N_{d(a)}, T, r_{d(a)}, x)}{\tau_{hE(eE)}(\rho_{d(a)}(x), T, r_{d(a)}, x)} dy,$$

and the effective minority hole (minority electron) transit time [htt(ett)] by: $\tau_{htt(ett)}^*(y = W, W, N_{d(a)}, r_{d(a)}, x, S) \equiv Q_{h(e)}^*(y = W, N_{d(a)}, T, r_{d(a)}, x) / J_{Eno(Epo)}(y = W, W, N_{d(a)}, T, r_{d(a)}, x, S)$, and from Equations (24, 31), one obtains:

$$\frac{\tau_{htt(ett)}^*(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S)}{\tau_{hE(eE)}} \equiv 1 - \frac{J_{Eno(Epo)}(y=0, W, N_{d(a)}, T, r_{d(a)}, x, S)}{J_{Eno(Epo)}(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S)} = 1 - \frac{1}{\cosh(P) + I \times \sinh(P)}. \quad (38)$$

Now, some important results can be obtained and discussed below.

As $P \ll 1$ (or $W \ll L_{h(e)}$) and $S \rightarrow \infty$, $I \equiv I(W, S) = \frac{D_{h(e)}(N_{do(ao)}(W), T, r_{d(a)}, x)}{S \times L_{h(e)}(N_{do(ao)}(W), T, r_{d(a)}, x)} \rightarrow 0$, from Eq. (38), one has: $\frac{\tau_{htt(ett)}^*(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S)}{\tau_{hE(eE)}} \rightarrow 0$, suggesting a completely transparent emitter region (CTER)-case, where, from Eq. (36), one obtains:

$$J_{Eno(Epo)}(y = W, N_{d(a)}, T, r_{d(a)}, x, S \rightarrow \infty) \rightarrow \frac{en_{in(ip)}^2 \times D_{h(e)}}{N_{d(a)}^*(y=W, N_{d(a)}, T, r_{d(a)}, x) \times L_{h(e)}} \times \frac{1}{P(W)}. \quad (39)$$

Further, as $P \gg 1$ (or $W \gg L_{h(e)}$) and $S \rightarrow 0$, $I \equiv I(y = W, r_{d(a)}, x, S) = \frac{D_{h(e)}(N_{do(ao)}(W), T, r_{d(a)}, x)}{S \times L_{h(e)}(N_{do(ao)}(W), T, r_{d(a)}, x)} \rightarrow \infty$, and from Eq. (38) one has: $\frac{\tau_{htt(ett)}^*(y=W, W, N_{d(a)}, T, r_{d(a)}, x, S)}{\tau_{hE(eE)}} \rightarrow 1$, suggesting a completely opaque emitter region (COER)-case, where, from Eq. (36), one gets:

$$J_{Eno(Epo)}(y = W, N_{d(a)}, T, r_{d(a)}, x, S \rightarrow 0) \rightarrow \frac{en_{in(ip)}^2 \times D_{h(e)}}{N_{d(a)}^*(y=W, N_{d(a)}, T, r_{d(a)}, x) \times L_{h(e)}} \times \tanh(P). \quad (40)$$

In summary, in the two $n^+(p^+) - p(n)$ X(x)-alloy junction solar cells, the dark carrier-minority saturation current density $J_{oI(oII)}$, defined in Eq. (17), is now rewritten as:

$$J_{oI(oII)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, r_{a(d)}, x) \equiv J_{Eno(Epo)}(W, N_{d(a)}, T, r_{d(a)}, x, S) + J_{Bpo(Bno)}(N_{a(d)}, T, r_{a(d)}, x), \quad (41)$$

where $J_{Eno(Epo)}$ and $J_{Bpo(Bno)}$ are determined respectively in Equations (36, 18).

Photovoltaic Conversion Effect at 300K

Here, in the $n^+(p^+) - p(n)$ X(x) -alloy junction solar cells at $T=300$ K, denoted respectively by I(II), and for physical conditions, respectively, as:

$$W = 15 \mu\text{m}, N_{d(a)} = 10^{19} \text{ cm}^{-3} (10^{20} \text{ cm}^{-3}), r_{d(a)}, x, S = 100 \left(\frac{\text{cm}}{\text{s}}\right); N_{a(d)} = 10^{17} \text{ cm}^{-3}, r_{a(d)}, x, \quad (42)$$

we propose, at given open circuit voltages: $V_{ocI1(ocI2)}$ and $V_{ocII1(ocII2)}$, the corresponding data of the short circuit current density $J_{scI(II)}$, in order to formulate our following treatment method of two fix points (Green, 2022; Moon et al., 2016), as:

$$\text{at } V_{ocI1(ocI2)}(V) = 0.980 (1.1272), J_{scI1(scI2)}(\text{mA/cm}^2) = 27.06 (29.76),$$

$$\text{at } V_{ocI1(ocI2)}(V) = 0.980 (1.03), J_{scI1(scI2)}(\text{mA/cm}^2) = 24.2 (29.84). \quad (43)$$

Now, we define the net current density J at $T=300$ K, obtained for the infinite shunt resistance, and expressed as a function of the applied voltage V , flowing through the $n^+(p^+) - p(n)$ X(x)-alloy junction of solar cells, as:

$$J(V) \equiv J_{ph.}(V) - J_{ol(oII)} \times (e^{X_{I(II)}(V)} - 1), \quad X_{I(II)}(V) \equiv \frac{V}{n_{I(II)}(V) \times V_T}, \quad V_T \equiv \frac{k_B T}{e} = 0.02585 \text{ V}, \quad (44)$$

where the function $n_{I(II)}(V)$ is the photovoltaic conversion factor (PVCF), noting that as $V = V_{oc}$, being the open circuit voltage, $J(V = V_{oc}) = 0$, the photocurrent density is defined by: $J_{ph.}(V = V_{oc}) \equiv J_{scI(scII)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc})$, for $V_{oc} \geq V_{ocI1(ocI1)}$.

Therefore, the photovoltaic conversion effect occurs, according to:

$$J_{scI(scII)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc}) \equiv J_{ol(oII)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x) \times (e^{X_{I(II)}(V_{oc})} - 1), \quad (45)$$

where $n_{I(II)}(V_{oc}) \equiv n_{I(II)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, r_{a(d)}, x, V_{oc})$, and $X_{I(II)}(V_{oc}) \equiv \frac{V_{oc}}{n_{I(II)}(V_{oc}) \times V_T}$.

Here, one remarks that (i) for a given V_{oc} , both $n_{I(II)}$ and $J_{ol(oII)}$ have the same variations, obtained in the same physical conditions, as observed in the following calculation, (ii) the function $(e^{X_{I(II)}(V_{oc})} - 1)$ or the PVCF, $n_{I(II)}$, representing the photovoltaic conversion effect, converts the light, represented by $J_{scI(scII)}$, into the electricity, by $J_{ol(oII)}$, and finally, for given $(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc})$ -values, $n_{I(II)}(V_{oc})$ is determined.

Now, for $V_{oc} \geq V_{ocI1(ocI1)}$, one can propose the general expressions for the PVCF, in order to get exactly the values of $n_{I1(I1)}(V_{ocI1(ocI1)})$ and $n_{I2(I2)}(V_{ocI2(ocI2)})$, as functions of V_{oc} , by:

$$n_{I(II)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc}) = n_{I1(I1)}(V_{ocI1(ocI1)}) + n_{I2(I2)}(V_{ocI2(ocI2)}) \times \left(\frac{V_{oc}}{V_{ocI1(ocI1)}} - 1 \right)^{\alpha(\beta)}, \quad (46)$$

where, for example, the values of $\alpha(\beta)$, obtained for $x = (0, 0.5, \text{ and } 1)$, will be reported in Tables 3 and 5, for $\text{GaAs}_{1-x}\text{Sb}_x$ alloy junctions. One also notes that those $\alpha(\beta)$ -values depend on $(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x)$ -ones.

So, one can determine the general expressions for the fill factors, as:

$$F_{I(II)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc}) = \frac{X_{I(II)}(V_{oc}) - \ln[X_{I(II)}(V_{oc}) + b]}{X_{I(II)}(V_{oc}) + a}, \quad a=1 \text{ and } b=0.72. \quad (47)$$

Finally, the efficiency $\eta_{I(II)}$ can be defined in the $n^+(p^+) - p(n)$ X(x) alloy-junction solar cells, by:

$$\eta_{I(II)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc}) \equiv \frac{J_{scI(scII)} \times V_{oc} \times F_{I(II)}}{P_{in.}}, \quad (48)$$

being assumed to be obtained at 1 sun illumination or at AM1.5G spectrum ($P_{in.} = 0.100 \frac{W}{cm^2}$).

It should be noted that the maximal values of $\eta_{I(II)}$, $\eta_{I(max.)(II(max.))}$, are obtained at the corresponding ones of $V_{oc} = V_{ocI(ocII)}$, at which $\frac{\partial \eta_{I(II)}(W, N_{d(a)}, T, r_{d(a)}, S, N_{a(d)}, T, r_{a(d)}, V_{oc})}{\partial V_{oc}} = 0$, as those given in next Tables 3 and 5, being marked in bold. Further, from the well-known Carnot's theorem, being obtained by the second principle in thermodynamics, or by the entropy law, the maximum efficiency of a heat engine operating between hot (**H**) and cold (**C**) reservoirs is the ratio of the temperature difference between the reservoirs, $T_H - T_C$, to the H-reservoir temperature, T_H , expressed as:

$$\frac{\eta_{I(max.)(II(max.))}(W, N_{d(a)}, T, r_{d(a)}, S, N_{a(d)}, T, r_{a(d)}, V_{ocI(ocII)})}{T_H(W, N_{d(a)}, T, r_{d(a)}, S, N_{a(d)}, T, r_{a(d)}, V_{ocI(ocII)})} = 1 - \frac{T_C=300 K}{T_H(W, N_{d(a)}, T, r_{d(a)}, S, N_{a(d)}, T, r_{a(d)}, V_{ocI(ocII)})} \quad (49)$$

Numerical Results and Concluding Remarks

We will respectively consider the two following cases of $n^+(p^+) - p(n)$ -junctions such as:

HD (Te ; Sb; Sn) X(x) alloy ER – LD (Mg ; In ; Cd) X(x) – alloy BR –case, according to: 3 (n^+p) – junctions denoted by: (Te^+Mg, Sb^+In, Sn^+Cd), and

HD (Mg ; In ; Cd) X(x) alloy ER – LD (Te; Sb; Sn) X(x) – alloy BR –case, according to: 3 (p^+n) – junctions denoted by: (Mg^+Te, In^+Sb, Cd^+Sn).

Now, by using the physical conditions, given in Eq. (42), then, if denoting: heavily doped (HD), lightly doped (LD), emitter region (ER), and base region (BR), we can determine various photovoltaic conversion coefficients, as follows.

Firs case: HD [Te; Sb; Sn] X(x) – Alloy ER – LD [Mg ; In ; Cd] X(x) – Alloy BR

Here, there are the 3 (n^+p) – X(x) junctions, being denoted by: (Te^+Mg, Sb^+In, Sn^+Cd).

Then, the numerical results of $\frac{\tau_{htt}^*}{\tau_{hE}}$, J_{Bpo} , J_{Eno} and J_{OI} , are calculated, using Equations (38), (18), (36) and (41), respectively, and reported in Table 2. Further, those of n_I , J_{scI} , F_I , η_I , and T_H , are computed, using Equations (46, 45, 47, 48, 49), respectively, and reported in Table 3.

Tables 2 and 3 in Appendix 1

Second case: HD [Mg ; In ; Cd] X(x) – Alloy ER – LD [Te; Sb, Sn] X(x) – Alloy BR

Here, there are 3 (p^+n) – X(x)-junctions, being denoted by: (Mg⁺Te, In⁺Sb, Cd⁺Sn).

Then, the numerical results of $\frac{\tau_{ett}^*}{\tau_{eE}}$, J_{Bno} , J_{Epo} and J_{oII} , are calculated using Equations (38), (18), (36) and (41), respectively, and reported in Table 4. Further, those of η_{II} , J_{scII} , F_{II} , η_{III} , and T_H , are computed, using Equations (46, 45, 47, 48, 49), respectively, and reported in Table 5.

Tables 4 and 5 in Appendix 1

Finally, some concluding remarks are obtained and discussed as follows.

(i)-First, with increasing $x=(0, 0.5, 1)$, from Table 3, obtained for the single $n^+ - p$ X(x)-alloy junction solar cells, and for given $r_{Sn(Cd)}$ -radius, for example, one obtains: $\eta_{I\max.}(\lambda) = 31.14\%$, 28.72% , **25.36%**, according to $T_H(K) = 435.7, 420.9, 401.9$, at $V_{ocI}(V) = 1.07, 1.09, 1.17$, respectively.

(ii)- Secondly, with increasing $x=(0, 0.5, 1)$, from Table 5, obtained for the single $p^+ - n$ X(x)-alloy junction solar cells, and for given $r_{Cd(Sn)}$ -radius, for example, one gets: $\eta_{II\max.}(\lambda) = 33.04\%$, 34.26% , 35.47% , according to $T_H(K) = 448.0, 456.3, 464.9$, at $V_{ocII}(V)[> V_{ocI}(V)] = 1.20, 1.27, 1.38$, respectively, suggesting that such $\eta_{I\max.}(II\max.)$ -and- T_H variations depend on $V_{ocII}(V)[> V_{ocI}(V)]$ – values.

Then, as given in Table 3, for $x = 0$ and $r_{d(a)} = r_{Te(Mg)}$, one gets: $\eta_I = 23.48\%$ and 29.71% at $V_{oc} = 0.98\text{ V}$ and 1.1272 V , respectively, which can also be compared with the corresponding results, obtained for the single-junction GaAs thin-film solar cell, 22.08% and 29.1% by Moon et al. (2016) and Green et al. (2022), respectively, with relative deviations in absolute values, 6.34% and 2.1% . Further, for $x = 1$ and for $r_{d(a)} = r_{Sn(Cd)}$, one gets in Table 3: $\eta_{I\max.} = 25.36\%$ at $V_{oc} = 1.17\text{ V}$, and in Table 5, $\eta_{II\max.} = 35.47\%$ at $V_{oc} = 1.38\text{ V}$, which can also be compared with the corresponding results, obtained for the single-junction GaSb-solar cells by Van Cong (2023), 11.17% (12.03%) and 11.34% (12.16%), respectively. As a result, in order to obtain the highest efficiencies, the single $\text{GaAs}_{1-x}\text{Sb}_x$ -alloy junction solar cells could be chosen rather than the single crystalline [GaAs, or GaSb]-junction solar cells.

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Appendix 1

Table 1. From Equations (5, 8a, 8b, 9) and in the n(p)-type $X(x)$ -alloy, the Numerical Results of the Energy-Band-Structure Parameters, Reported Below, Suggest that, with Increasing x and $r_{d(a)}$, both $B_{do(ao)}(x)$ and $\varepsilon(r_{d(a)}, x)$ Decrease, while the Other Ones Increase

Donor		As	Te	Sb	Sn
r_d (nm)	\nearrow	$r_{do}=0.118$	0.132	0.136	0.140
x	\nearrow	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2)	\searrow	1.21, 0.86, 0.60			
$\varepsilon(r_d, x)$	\searrow	13.1, 14.4, 15.7	12.3, 13.5, 14.7	11.8, 13.0, 14.2	11.3, 12.4, 13.5
$E_d(r_d, x)$ meV	\nearrow	5.21, 3.70, 2.60	5.91, 4.20, 2.94	6.38, 4.54, 3.18	6.99, 4.97, 3.49
$E_{gn}(r_d, x)$ eV	\nearrow	1.52, 1.16, 0.81	1.52, 1.16, 0.81	1.52, 1.16, 0.81	1.52, 1.17, 0.81
$E_{gin}(T = 300K, r_d, x)$ eV	\nearrow	1.42, 1.07, 0.73	1.42, 1.07, 0.73	1.42, 1.07, 0.73	1.42, 1.08, 0.73
Acceptor		Ga	Mg	In	Cd
r_a (nm)	\nearrow	$r_{ao}=0.126$	0.140	0.144	0.148
x	\nearrow	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2)	\searrow	4.39, 3.70, 3.17			
$\varepsilon(r_a, x)$	\searrow	13.1, 14.4, 15.7	12.4, 13.6, 14.8	12.0, 13.2, 14.3	11.5, 12.6, 13.8
$E_a(r_a, x)$ meV	\nearrow	23.0, 19.4, 16.6	25.7, 21.6, 18.5	27.5, 23.2, 19.8	29.8, 25.2, 21.5
$E_{gp}(r_a, x)$ eV	\nearrow	1.52, 1.16, 0.81	1.52, 1.17, 0.81	1.52, 1.17, 0.81	1.53, 1.17, 0.81
$E_{gip}(T = 300K, r_a, x)$ eV	\nearrow	1.42, 1.07, 0.73	1.43, 1.08, 0.73	1.43, 1.08, 0.73	1.43, 1.08, 0.73

Table 2. In the HD [(Te; Sb; Sn)- X(x)-alloy] ER-LD[(Mg; In; Cd)-X(x)-alloy] BR, for Physical Conditions Given in Eq. (42) and for a Given x, Our Numerical Results of $\frac{\tau_{htt}^*}{\tau_{hE}}$, J_{Bpo} , J_{Eno} and J_{ol} , are Computed, Using Equations (38), (18), (36) and (41), Respectively, Noting that J_{ol} Decreases Slightly with Increasing $r_{d(a)}$ -Radius for Given x, but it Increases Strongly with Increasing x for Given $r_{d(a)}$ -Radius, Being New Results

n+p		Te+Mg	Sb+In	Sn+Cd
Here, $\mathbf{x=0}$, and for the (Te+Mg, Sb+In, Sn+Cd)-junctions and from Eq. (34), one obtains: $\frac{\tau_{htt}^*}{\tau_{hE}} = (0, 0, 0)$ suggesting a completely transparent condition.				
J_{Bpo} in 10^{-19} (A/cm ²)	↘	1.0315	0.9965	0.9565
J_{Eno} in 10^{-23} (A/cm ²)	↘	1.7830	1.7258	1.6624
J_{ol} in 10^{-19} (A/cm ²)	↘	1.0317	0.9967	0.9567
Here, $\mathbf{x=0.5}$, and for the (Te+Mg, Sb+In, Sn+Cd)-junctions and from Eq. (34), one obtains: $\frac{\tau_{htt}^*}{\tau_{hE}} = (0, 0, 0)$ suggesting a completely transparent condition.				
J_{Bpo} in 10^{-14} (A/cm ²)	↘	6.1514	5.9426	5.7041
J_{Eno} in 10^{-18} (A/cm ²)	↘	2.9271	2.8551	2.7771
J_{ol} in 10^{-14} (A/cm ²)	↘	6.1517	5.9429	5.7044
Here, $\mathbf{x=1}$, and for the (Te+Mg, Sb+In, Sn+Cd)junctions and from Eq. (34), one obtains: $\frac{\tau_{htt}^*}{\tau_{hE}} = (0, 0, 0)$ suggesting a completely transparent condition.				
J_{Bpo} in 10^{-8} (A/cm ²)	↘	3.4940	3.3754	3.2399
J_{Eno} in 10^{-13} (A/cm ²)	↘	2.5023	2.4573	2.4108
J_{ol} in 10^{-8} (A/cm ²)	↘	3.4940	3.3755	3.2400

Table 3. In the HD [(Te; Sb; Sn)-X(x)-alloy] ER-LD[(Mg; In; Cd)-X(x)-alloy] BR, for Physical Conditions Given in Eq. (42) and for a Given x, Our Numerical Results of n_I , J_{scI} , F_I , η_I , and T_H , are Computed, Using Equations (46, 45, 47, 48, 49), Respectively, Noting that Both $\eta_{I_{max}}$ and T_H , Marked in Bold, Decrease with Increasing x for Given $r_{d(a)}$

$V_{oc}(V)$	n_I	$J_{scI}(\frac{mA}{cm^2})$	$F_I(\%)$	$\eta_I(\%)$
Here, $x=0$. For the (Te ⁺ Mg, Sb ⁺ In, Sn ⁺ Cd) junctions, the value of α given in Eq. (46) is 1.0822				
n^+p	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd
0.980	0.945; 0.944; 0.943	27.06; 27.06; 27.06	88.54; 88.55; 88.56	23.48; 23.48; 23.48
1.06	1.017; 1.016; 1.015	33.09; 33.09; 33.10	88.59; 88.59; 88.60	31.07; 31.08; 31.09
1.07	1.027; 1.026; 1.025	32.83; 32.84; 32.84	88.59; 88.59; 88.60	31.12; 31.13; 31.14
			$V_{ocI} = 1.07 V$	435.5; 435.6; 435.7=$T_H(K)$
1.08	1.084; 1.083; 1.082	32.47; 32.47; 32.48	88.59; 88.59; 88.60	31.06; 31.07; 31.08
1.1272	1.084; 1.083; 1.082	29.76; 29.76; 29.76	88.56; 88.57; 88.58	29.71; 29.71; 29.72
3	3.317; 3.314; 3.311	0.160; 0.160; 0.159	87.28; 87.29; 87.30	0.420; 0.418; 0.416
Here, $x=0.5$. For the (Te ⁺ Mg, Sb ⁺ In, Sn ⁺ Cd) junctions, the value of α given in Eq. (46) is 1.0866				
n^+p	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd
0.980	1.414; 1.412; 1.410	27.06; 27.06; 27.06	84.48; 84.50; 84.51	22.40; 22.41; 22.41
1.08	1.549; 1.547; 1.545	31.39; 31.39; 31.40	84.54; 84.56; 84.58	28.66; 28.67; 28.68
1.09	1.564; 1.562; 1.560	31.14; 31.15; 31.15	84.54; 84.56; 84.57	28.70; 28.70; 28.72
			$V_{ocI} = 1.09 V$	420.7; 420.7; 420.9=$T_H(K)$
1.10	1.579; 1.577; 1.575	30.84; 30.84; 30.85	84.54; 84.55; 84.57	28.68; 28.69; 28.70
1.1272	1.620; 1.618; 1.616	29.80; 29.80; 29.80	84.52; 84.54; 84.56	28.39; 28.40; 28.41
3	4.970; 4.963; 4.956	0.849; 0.845; 0.841	82.83; 82.84; 82.86	2.110; 2.101; 2.090
Here, $x=1$. For the (Te ⁺ Mg, Sb ⁺ In, Sn ⁺ Cd) junctions, the value of α given in Eq. (46) is 1.0992				
n^+p	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd	Te ⁺ Mg; Sb ⁺ In; Sn ⁺ Cd
0.980	2.795; 2.788; 2.780	27.06; 27.06; 27.06	74.87; 74.91; 74.96	19.85; 19.87; 19.88
1.1272	3.193; 3.185; 3.175	29.78; 29.78; 29.79	74.99; 75.03; 75.02	25.17; 25.19; 25.21
1.16	3.291; 3.283; 3.273	29.11; 29.12; 29.12	74.96; 75.00; 75.05	25.31; 25.33; 25.35
1.17	3.321; 3.313; 3.303	28.88; 28.88; 28.89	74.95; 74.99; 75.04	25.32; 25.34; 25.36
			$V_{ocI} = 1.17 V$	401.7; 401.8; 401.9=$T_H(K)$
1.18	3.352; 3.343; 3.333	28.63; 28.63; 28.64	74.94; 74.98; 75.03	25.31; 25.33; 25.35
3	9.866; 9.841; 9.811	4.480; 4.459; 4.434	72.38; 72.43; 72.48	9.928; 9.688; 9.641

Table 4. In the HD [(Mg; In; Cd)-X(x)-alloy] ER-LD[(Te; Sb; Sn)-X(x)-alloy] BR, for Physical Conditions Given in Eq. (42) and for a Given x, Our Numerical Results of $\frac{\tau_{ett}^*}{\tau_{eE}}$, J_{Bno} , J_{Epo} , and J_{oII} are Computed, Using Equations (38), (18), (36) and (41), Respectively, Noting that J_{oII} Decreases Slightly with Increasing $r_{a(d)}$ -Radius for Given x, but it Increases Strongly with Increasing x for Given $r_{a(d)}$ -Radius, Being New Results

p+n		Mg ⁺ Te	In ⁺ Sb	Cd ⁺ Sn
Here, $\mathbf{x=0}$, and for the (Mg ⁺ Te, In ⁺ Sb, Cd ⁺ Sn)-junctions and from Eq. (34), one obtains: $\frac{\tau_{ett}^*}{\tau_{eE}} = (0, 0, 0)$ suggesting a completely transparent condition.				
J_{Bno} in 10^{-20} (A/cm ²)	↘	3.0094	2.8418	2.6512
J_{Epo} in 10^{-23} (A/cm ²)	↘	1.1965	1.1298	1.0513
J_{oII} in 10^{-20} (A/cm ²)	↘	3.0106	2.8429	2.6522
Here, $\mathbf{x=0.5}$, and for the (Mg ⁺ Te, In ⁺ Sb, Cd ⁺ Sn)-junctions and from Eq. (34), one obtains: $\frac{\tau_{ett}^*}{\tau_{eE}} = (0, 0, 0)$ suggesting a completely transparent condition.				
J_{Bno} in 10^{-14} (A/cm ²)	↘	1.7729	1.6831	1.5810
J_{Epo} in 10^{-18} (A/cm ²)	↘	7.9283	7.5654	7.1346
J_{oII} in 10^{-14} (A/cm ²)	↘	1.7737	1.6839	1.5818
Here, $\mathbf{x=1}$, and for the (Mg ⁺ Te, In ⁺ Sb, Cd ⁺ Sn)-junctions and from Eq. (34), one obtains: $\frac{\tau_{ett}^*}{\tau_{eE}} = (0, 0, 0)$ suggesting a completely transparent condition.				
J_{Bno} in 10^{-8} (A/cm ²)	↘	9.9807	0.9512	0.8980
J_{Epo} in 10^{-12} (A/cm ²)	↘	4.9874	4.7968	4.5697
J_{oII} in 10^{-8} (A/cm ²)	↘	9.9857	0.9517	0.8985

Table 5. In the HD [(Mg; In; Cd)-X(x)-alloy] ER-LD[(Te; Sb; Sn)-X(x)-alloy] BR, for Physical Conditions Given in Eq. (42) and for a Given x, Our Numerical Results of n_{II} , J_{scII} , F_{II} , η_{II} , and T_H , are Computed, Using Equations (46, 45, 47, 48, 49), Respectively, Noting that Both η_{IImax} and T_H , Marked in Bold, Increase with Increasing x for Given $r_{a(d)}$.

$V_{oc}(V)$	n_{II}	$J_{scII}(\frac{mA}{cm^2})$	$F_{II}(\%)$	$\eta_{II}(\%)$
Here, $x=0$. For the (Mg ⁺ Te, In ⁺ Sb, Cd ⁺ Sn)-junctions, the value of β given in Eq. (46) is 1.052.				
p ⁺ n	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn
0.980	0.919; 0.918; 0.917	24.20; 24.20; 24.20	88.78; 88.79; 88.81	21.05; 21.06; 21.06
1.03	0.961; 0.960; 0.958	29.84; 29.85; 29.86	88.83; 88.84; 88.85	27.30; 27.31; 27.33
1.19	1.110; 1.108; 1.106	31.21; 31.22; 31.23	88.84; 88.85; 88.86	32.99; 33.02; 33.03
1.20	1.119; 1.117; 1.116	30.96; 30.97; 30.98	88.83; 88.85; 88.86	33.01; 33.03; 33.04
			$V_{ocII} = 1.20 V$	447.8; 447.9; 448.0=$T_H(K)$
1.21	1.129; 1.127; 1.125	30.70; 30.71; 30.72	88.83; 88.84; 88.86	32.99; 33.01; 33.03
3	2.977; 2.973; 2.968	2.545; 2.536; 2.526	88.29; 88.30; 88.32	6.740; 6.719; 6.693
Here, $x=0.5$. For the (Mg ⁺ Te, In ⁺ Sb, Cd ⁺ Sn)-junctions, the value of β given in Eq. (46) is 1.0698.				
p ⁺ n	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn
0.980	1.357; 1.354; 1.351	24.20; 24.20; 24.20	84.95; 84.97; 84.99	20.15; 20.15; 20.16
1.03	1.415; 1.413; 1.409	29.80; 29.81; 29.83	85.03; 85.05; 85.08	26.10; 26.12; 26.14
1.26	1.727; 1.724; 1.720	31.91; 31.92; 31.94	85.06; 85.08; 85.10	34.20; 34.22; 34.25
1.27	1.741; 1.738; 1.734	31.67; 31.68; 31.70	85.06; 85.08; 85.10	34.21; 34.23; 34.26
			$V_{ocII} = 1.27 V$	456.0; 456.1; 456.3=$T_H(K)$
1.28	1.755; 1.752; 1.748	31.42; 31.43; 31.44	85.05; 85.07; 85.10	34.20; 34.22; 34.25
3	4.425; 4.417; 4.407	4.344; 4.329; 4.311	84.23; 84.25; 84.27	10.98; 10.94; 10.90
Here, $x=1$. For the (Mg ⁺ Te, In ⁺ Sb, Cd ⁺ Sn)-junctions, the value of β given in Eq. (46) is 1.1261.				
p ⁺ n	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn	Mg ⁺ Te; In ⁺ Sb; Cd ⁺ Sn
0.980	2.578; 2.570; 2.560	24.20; 24.20; 24.20	76.20; 76.26; 76.32	18.07; 18.08; 18.10
1.03	2.672; 2.663; 2.653	29.80; 29.82; 29.85	76.43; 76.49; 76.55	23.46; 23.50; 23.53
1.37	3.525; 3.514; 3.500	33.69; 33.72; 33.76	76.56; 76.62; 76.68	35.34; 35.40; 35.46
1.38	3.553; 3.541; 3.527	33.46; 33.49; 33.52	76.56; 76.61; 76.67	35.35; 35.40; 35.47
			$V_{ocII} = 1.38$	464.0; 464.4; 464.9=$T_H(K)$
1.39	3.580; 3.568; 3.555	33.22; 33.24; 33.29	76.55; 76.60; 76.66	35.34; 35.40; 35.46
3	8.612; 8.584; 8.551	7.091; 7.059; 7.022	74.76; 74.82; 74.88	15.90; 15.84; 15.77