



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

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Abstract:

In single $n^+(p^+) - p(n)$ [$X(x) \equiv GaAs_{1-x}P_x$]-alloy junction solar cells at 300 K, $0 \leq x \leq 1$, by basing on the same physical model and the same treatment method, as those used in our recent works (Van Cong, 2024), we will also investigate the highest (or maximal) efficiencies, $\eta_{I\max.}(I\max.)$ 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, which was demonstrated by the use of the entropy law. Here, some concluding

remarks are given in the following. (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: $\eta_{I\max.}(\nearrow) = 31.18\%$, 33.495% , **35.99%**, according to $T_H(K) = 435.9, 451.1, 468.7$, at $V_{ocI}(V) = 1.07, 1.06, 1.05$, 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: $\eta_{II\max.}(\searrow) = 33.05\%$, 31.95% , 31.37% , according to $T_H(K) = 448.0, 440.9, 437.1$, at $V_{ocII}(V) [> V_{ocI}(V)] = 1.20, 1.15, 1.12$, respectively, suggesting that such $\eta_{I\max.}(I\max.)$ -and- T_H variations depend on $V_{ocII}(V) [> V_{ocI}(V)] - values$. Then, in particular, as given in Table 3, for $x = 0$ and $r_{d(a)} = r_{Te(Mg)}$, one gets: $\eta_I = 23.48\%$ and 29.76% at $V_{oc} = 0.98 V$ and $1.1272 V$, respectively, which can 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 29.71% , with relative deviations in absolute values, 6.34% and 0.17% . Finally, one notes that, in order to obtain the highest efficiencies, the single $GaAs_{1-x}P_x$ -alloy junction solar cells could be chosen rather than the single crystalline GaAs-junction solar cell.

Keywords: single $GaAs_{1-x}P_x$ -alloy junction solar cell; single crystalline GaAs-junction solar cell; photovoltaic conversion factor; photovoltaic conversion efficiency.

Introduction

In single $n^+(p^+) - p(n)$ $GaAs_{1-x}P_x$ -alloy junction solar cells at 300 K, $0 \leq x \leq 1$, by basing on the same physical model and treatment method, as used in our two recent works (Van Cong, 2024), and also on other ones (Green et al., 2022; Kittel, 1976; Moon et al., 2016; Singh & Ravindra, 2012; Van Cong, 2024, 2016, 1999, 1995, 1991, 1975; Van Cong & Debais, 1997, 1996, 1993; Van Cong & Doan Khanh, 1992; 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 from the Carnot- efficiency theorem, being proved by the entropy law.

In the following, we will show that the energy-band-structure parameters, due to the effects of x-P concentration, size impurity, temperature T and heavy doping, affect strongly the dark (or total) minority-carrier saturation current density and the photovoltaic conversion effect.

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

First of all, in the single $n^+(p^+) - p(n)$ $X(x)$ - alloy junction solar cells, $X(\equiv GaAs_{1-x}P_x)$, we present the effects of x-concentration, donor (acceptor) [d(a)]-size, temperature T and heavy doping, affecting the energy-band-structure parameters, as those investigated in our recent works (Van Cong, 2024).

A. Effect of x-P Concentration

In the $n^+(p^+) - p(n)$ single $n^+(p^+) - p(n)$ $X(x)$ - alloy junction at $T=0$ K, the energy-band-structure parameters (Kittel, 1976) 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:

$$\begin{aligned} m_c(x)/m_o &= 0.13 \times x + 0.066 \times (1 - x), \text{ and} \\ m_v(x)/m_o &= 0.500 \times x + 0.291 \times (1 - x), \end{aligned} \quad (1)$$

so that one obtains: $m_c(x = 0)/m_o = m_{c(GaAs)}/m_o = 0.066$, $m_v(x = 0)/m_o = m_{v(GaAs)}/m_o = 0.291$, and $m_c(x = 1)/m_o = m_{c(GaP)}/m_o = 0.13$, $m_v(x = 1)/m_o = m_{v(GaP)}/m_o = 0.5$.

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

$$\epsilon_o(x) = 11.1 \times x + 13.13 \times (1 - x), \quad (2)$$

which gives: $\epsilon_o(x = 0) = \epsilon_{GaAs} = 13.13 \approx 13.1$, and $\epsilon_o(x = 1) = \epsilon_{GaP} = 11.1$.

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

$$E_{go}(x) \text{ in eV} = 1.796 \times x + 1.52 \times (1 - x), \quad (3)$$

giving rise to: $E_{go}(x = 0) = E_{gGaAs} = 1.52$ eV, and $E_{go}(x = 1) = E_{gGaTe} = 1.796$ eV ≈ 1.80 eV.

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

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

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 -P concentration affect the changes in all the energy-band-structure parameters, expressed in terms of the effective relative dielectric constant $\epsilon(r_{d(a)}, x)$, in the following.

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), used 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: $\frac{d}{dV}(\frac{d\sigma}{dV}) = \frac{B}{V}$. Then, by an integration, one gets:

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

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: $\pm [\Delta\sigma(r_{d(a)}, x)]_{n(p)}$,

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

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

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

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:

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

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

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

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

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

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

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, 2024):

$$E_{gin(gip)}(r_{d(a)}, x, T) \text{ in eV} = E_{gn(gp)}(r_{d(a)}, x) - 10^{-4} \times T^2 \times \left[\frac{3.065 \times x}{T+94 \text{ K}} + \frac{5.405 \times (1-x)}{T+204 \text{ K}} \right], \quad (9)$$

which gives: $E_{gin(gip)}(r_{do(ao)}, x = 0, T = 0K) = 1.52 \text{ eV}$ and $E_{gin(gip)}(r_{do(ao)}, x = 1, T = 0K) = 2.32 \text{ eV}$, and $E_{gin(gip)}(r_{do(ao)}, x = 0, T = 300 \text{ K}) \simeq 1.42 \text{ eV}$ and $E_{gin(gip)}(r_{do(ao)}, x = 1, T = 300 \text{ K}) \simeq 2.25 \text{ eV}$,

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:

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

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

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

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 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, 2024; 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, $u(N_{d(a)}, T, x) \equiv \frac{N_{d(a)}}{N_{c(v)}(T, x)}$, $F(u) = au^{\frac{2}{3}} \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}} \right)^{-\frac{2}{3}}$, $a = [(3\sqrt{\pi}/4) \times u]^{2/3}$, $b = \frac{1}{8} \left(\frac{\pi}{a} \right)^2$, $c = \frac{62.3739855}{1920} \left(\frac{\pi}{a} \right)^4$, and $G(u) \simeq \text{Ln}(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2} \left[\frac{1}{\sqrt{27}} - \frac{3}{16} \right] > 0$.

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)- X(x)- alloy] BR-case, or to the non-degenerate case, Eq. (12) is reduced to the function G(u). Here, the notations: HD(LD) and ER(BR), mean: heavily doped (lightly doped)-cases and emitter (base)-regions, respectively.

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

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

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

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

Now, taking into account various spin-polarized chemical potential-energy contributions such as (Van Cong, 2024): 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.

Thus, in the n-type HD $X(x)$ - alloy, the BGN is found to be given by (Van Cong, 2024):

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

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}^* , by :

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

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, 2024):

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

where $n_{ip(in)}^2(T, r_{a(d)}, x)$ is determined Eq. (10), $D_{e(h)}(N_{a(d)}, T, r_{a(d)}, x)$ 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 $\tau_{eB(hB)}(N_{a(d)})$ 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, 2024):

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

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

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 $\Delta E_{agn(agg)}$ 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:

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

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: 2.0893×10^{-30} (cm^4/s), and the minority hole (minority electron) lifetime $\tau_{hE(eE)}$ as:

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

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:

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

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

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, 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:

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

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

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

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 $\frac{dP(y)}{dy} \equiv C \times F_{h(e)}(y) = \frac{1}{L_{h(e)}(x)}$, $C = 2.0893 \times 10^{-30} \text{ (cm}^4/\text{s)}$, 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:

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

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:

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

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 $J_{ol(oII)}$, defined in Eq. (17), is now rewritten as:

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

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:

$$\begin{aligned} \text{at } V_{ocI1(ocI2)}(V) = 0.980 (1.1272), J_{scI1(scI2)}(mA/cm^2) = 27.06 (29.76), \\ \text{at } V_{ocII1(ocII2)}(V) = 0.980 (1.03), J_{scII1(scII2)}(mA/cm^2) = 24.2 (29.84). \end{aligned} \quad (43)$$

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:

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

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 $V_{oc} \geq V_{ocI1(ocII1)}$.

Therefore, the photovoltaic conversion effect occurs, according to:

$$\begin{aligned} J_{scl(sclII)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc}) &\equiv \\ J_{ol(olII)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x) \times (e^{X_{I(II)}(V_{oc})} - 1), \end{aligned} \quad (45)$$

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 $J_{ol(olII)}$ 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 $J_{scl(sclII)}$, into the electricity, by $J_{ol(olII)}$, 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 $V_{oc} \geq V_{ocI1(ocII1)}$, one can propose the general expressions for the PVCF, in order to get exactly the values of $n_{I1(II1)}(V_{ocI1(ocII1)})$ and $n_{I2(II2)}(V_{ocI2(ocII2)})$, as functions of V_{oc} , by:

$$n_{I(II)}(W, N_{d(a)}, T, r_{d(a)}, x, S; N_{a(d)}, T, r_{a(d)}, x, V_{oc}) = n_{I1(II1)}(V_{ocI1(ocII1)}) + n_{I2(II2)}(V_{ocI2(ocII2)}) \times \left(\frac{V_{oc}}{V_{ocI1(ocII1)}} - 1 \right)^{\alpha(\beta)}, \quad (46)$$

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 these $[X(x) \equiv GaAs_{1-x}P_x]$ -alloy junctions.

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

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

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

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

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 $V_{ocI(ocII)}$, 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, $T_H - T_C$, $T_C \equiv T = 300$ K, to the H-reservoir temperature, T_H , expressed as:

$$\eta_{I(II)}(T, V_{oc}) \leq \eta_{I\max.(II\max.)}(T, V_{oc} = V_{ocI(ocII)}) \equiv \eta_{Carnot} = \frac{T_H - T_C}{T_H}, \quad (49)$$

for a simplicity, noting that both $\eta_{I\max.(II\max.)}$ and T_H depend on $(W, N_{d(a)}, T, r_{d(a)}, S, N_{a(d)}, r_{a(d)}, V_{ocI(ocII)})$ -parameters.

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), 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 obtained, as those given in Table 2. Further, those of $n_I, J_{scl}, F_I, \eta_I$, and T_H , are computed, using Equations (46, 45, 47, 48, 49), respectively, and reported in the following 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 obtained, as those given in Table 4. Further, those of $n_{II}, J_{sclII}, F_{II}, \eta_{II}$, and T_H , are computed, using Equations (46, 45, 47, 48, 49), respectively, and reported in the following 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: $\eta_{I\max.}(\nearrow) = 31.18\%, 33.495\%, 35.99\%$, according to $T_H(K) = 435.9, 451.1, 468.7$, at $V_{ocI}(V) = 1.07, 1.06, 1.05$, 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: $\eta_{II\max.}(\searrow) = 33.05\%, 31.95\%, 31.37\%$, according to $T_H(K) = 448.0, 440.9, 437.1$, at $V_{ocII}(V)[> V_{ocI}(V)] = 1.20, 1.15, 1.12$,

respectively, suggesting that such $\eta_{I\max.}(I_{I\max.})$ -and- T_H variations depend on $V_{ocII}(V)[> V_{ocI}(V)]$ – values.

Then, in particular, as given in Table 3, for $x = 0$ and $r_{d(a)} = r_{Te(Mg)}$, one gets: $\eta_I = 23.48\%$ and 29.76% 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 29.71% , obtained with relative deviations in absolute values, 6.34% and 0.17% , and given respectively by Moon et al. (2016) and Green et al. (2022).

Finally, one notes that, in order to obtain the highest efficiencies, the single $GaAs_{1-x}P_x$ -alloy junction solar cells could be chosen rather than the single crystalline GaAs-junction solar cell.

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Appendix 1

Table 1. From Equations (5, 8a, 8b, 9) and in the n(p)-type $GaAs_{1-x}P_x$ -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)	↗	$r_{do}=0.118$	0.132	0.136	0.140
x	↗	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)	↗	1.21, 2.11, 3.34			
$\varepsilon(r_d, x)$	↘	13.1 , 12.1, 11.1	12.3, 11.4, 10.4	11.8, 10.9, 10.0	11.3, 10.4, 9.57
$E_d(r_d, x)$ meV	↗	5.21, 9.08, 14.3	5.91, 10.3, 16.3	6.38, 11.1, 17.6	6.99, 12.2, 19.3
$E_{gn}(r_d, x)$ eV	↗	1.52 , 1.92, 2.32	1.52, 1.92, 2.32	1.52, 1.92, 2.32	1.52, 1.92, 2.32
$E_{gin}(T = 300K, r_d, x)$ eV	↗	1.42 , 1.84, 2.25	1.42, 1.84, 2.25	1.42, 1.84, 2.25	1.42, 1.84, 2.25
Acceptor		Ga	Mg	In	Cd
r_a (nm)	↗	$r_{ao}=0.126$	0.140	0.144	0.148
x	↗	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)	↗	4.39, 7.01, 10.5			
$\varepsilon(r_a, x)$	↘	13.1 , 12.1, 11.1	12.4, 11.5, 10.5	12.0, 11.1, 10.1	11.5, 10.6, 9.74
$E_a(r_a, x)$ meV	↗	23.0, 36.6, 55.2	25.7, 41.0, 61.7	27.5, 43.9, 66.1	29.8, 47.6, 71.7
$E_{gp}(r_a, x)$ eV	↗	1.52 , 1.92, 2.32	1.52, 1.92, 2.33	1.52, 1.93, 2.33	1.53, 1.93, 2.34
$E_{gip}(T = 300K, r_a, x)$ eV	↗	1.42 , 1.84, 2.25	1.43, 1.84, 2.26	1.43, 1.84, 2.26	1.43, 1.85, 2.27

Table 2. In the HD [(Te; Sb; Sn)- GaAs_{1-x}P_x-alloy] ER-LD[(Mg; In; Cd)-GaAs_{1-x}P_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^{-21} (A/cm ²)	↘	3.2121	3.1031	2.9786
J_{Eno} in 10^{-23} (A/cm ²)	↘	5.7338	5.4613	5.1539
J_{ol} in 10^{-21} (A/cm ²)	↘	3.2179	3.1086	2.9837
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^{-21} (A/cm ²)	↘	7.4383	7.1859	6.8975
J_{Eno} in 10^{-23} (A/cm ²)	↘	3.8757	3.6185	3.3285
J_{ol} in 10^{-21} (A/cm ²)	↘	7.4771	7.2221	6.9308

Table 3. In the HD [(Te; Sb; Sn)- GaAs_{1-x}P_x-alloy] ER-LD[(Mg; In; Cd)-GaAs_{1-x}P_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, increase with increasing x for given $r_{d(a)}$, being new results

$V_{oc}(V)$	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 1.0824.				
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	33.13; 33.14; 33.15	88.59; 88.60; 88.60	31.11; 31.12; 31.13
1.07	1.027; 1.026; 1.025	32.88; 32.88; 32.89	88.59; 88.59; 88.60	31.16; 31.17; 31.18
			$V_{ocI} = 1.07 V$	435.8; 435.8; 435.9 = $T_H(K)$
1.08	1.037; 1.036; 1.035	32.52; 32.52; 32.53	88.58; 88.59; 88.60	31.11; 31.12; 31.12
1.1272	1.084; 1.083; 1.082	29.81; 29.82; 29.82	88.56; 88.57; 88.58	29.76; 29.77; 29.77
3	3.318; 3.315; 3.311	0.159; 0.160; 0.158	87.28; 87.29; 87.30	0.418; 0.416; 0.414
Here, $x=0.5$. For the (Te^+Mg, Sb^+In, Sn^+Cd) junctions, the value of α given in Eq. (46) is 1.0796				
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	0.688; 0.688; 0.687	27.06; 27.06; 27.06	91.04; 91.05; 91.06	24.14; 24.14; 24.15
1.05	0.734; 0.733; 0.732	34.95; 34.95; 34.96	91.08; 91.08; 91.09	33.42; 33.43; 33.44
1.06	0.741; 0.740; 0.740	34.68; 34.68; 34.69	91.08; 91.08; 91.09	33.48; 33.48; 33.49
			$V_{ocI} = 1.06 V$	451.0; 451.0; 451.1 = $T_H(K)$
1.07	0.748; 0.747; 0.747	34.23; 34.24; 34.24	91.08; 91.08; 91.09	33.36; 33.37; 33.37
1.1272	0.790; 0.789; 0.789	29.63; 29.63; 29.64	91.06; 91.06; 91.07	30.42; 30.42; 30.42
3	2.413; 2.411; 2.410	0.025; 0.024; 0.024	90.04; 90.05; 90.05	0.066; 0.066; 0.066
Here, $x=1$. For the (Te^+Mg, Sb^+In, Sn^+Cd) junctions, the value of α given in Eq. (46) is 1.0785				
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	0.539; 0.538; 0.538	27.06; 27.06; 27.06	92.62; 92.63; 92.63	24.56; 24.56; 24.56
1.04	0.569; 0.569; 0.568	37.12; 37.12; 37.13	92.65; 92.65; 92.66	35.77; 35.77; 35.78
1.05	0.575; 0.574; 0.574	36.98; 36.98; 36.99	92.65; 92.65; 92.66	35.97; 35.98; 35.99
			$V_{ocI} = 1.05 V$	468.5; 468.6; 468.7 = $T_H(K)$
1.06	0.580; 0.579; 0.579	36.56; 36.57; 36.57	92.65; 92.65; 92.65	35.91; 35.91; 35.92
1.1272	0.619; 0.618; 0.618	29.72; 29.72; 29.72	92.63; 92.63; 92.64	31.03; 31.03; 31.03
3	1.889; 1.888; 1.887	0.003; 0.003; 0.003	91.78; 91.79; 91.79	0.010; 0.010; 0.010

Table 4. In the HD [(Mg; In; Cd)-GaAs_{1-x}P_x-alloy] ER-LD[(Te; Sb; Sn)-GaAs_{1-x}P_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^+Snvvv
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^{-21} (A/cm ²)	↘	9.6698	9.0066	8.2559
J_{Epo} in 10^{-23} (A/cm ²)	↘	2.7337	2.4692	2.1708
J_{oII} in 10^{-21} (A/cm ²)	↘	9.6971	9.0313	8.2776
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^{-22} (A/cm ²)	↘	2.3368	2.1362	1.9118
J_{Epo} in 10^{-24} (A/cm ²)	↘	1.7488	1.4891	1.2139
J_{oII} in 10^{-22} (A/cm ²)	↘	2.3542	2.1511	1.9240

Table 5. In the HD [(Mg; In; Cd)-GaAs_{1-x}P_x-alloy] ER-LD[(Te; Sb; Sn)-GaAs_{1-x}P_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, decrease with increasing x for given $r_{a(d)}$, being new results

$V_{oc}(V)$	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; 31.23; 31.24	88.84; 88.85; 88.86	33.00; 33.02; 33.03
1.20	1.119; 1.117; 1.116	30.97; 30.98; 30.99	88.83; 88.85; 88.86	33.02; 33.03; 33.05
			$V_{ocII} = 1.20 V$	447.8; 447.49; 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	33.01; 33.02; 33.04
3	2.977; 2.973; 2.968	2.547; 2.539; 2.528	88.29; 88.30; 88.32	6.746; 6.725; 6.699
Here, $x=0.5$. For the (Mg ⁺ Te, In ⁺ Sb, Cd ⁺ Sn)-junctions, the value of β given in Eq. (46) is 1.0422.				
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	0.675; 0.674; 0.673	24.20; 24.20; 24.20	91.18; 91.19; 91.20	21.62; 21.63; 21.63
1.03	0.706; 0.705; 0.704	29.83; 29.84; 29.85	91.21; 91.22; 91.23	28.03; 28.04; 28.05
1.14	0.782; 0.781; 0.779	30.68; 30.69; 30.70	91.21; 91.22; 91.23	31.91; 31.92; 31.93
1.15	0.789; 0.788; 0.786	30.44; 30.44; 30.45	91.21; 91.22; 91.23	31.93; 31.94; 31.95
			$V_{ocII} = 1.15 V$	440.7; 440.8; 440.9=$T_H(K)$
1.16	0.796; 0.795; 0.793	30.16; 30.16; 30.17	91.21; 91.22; 91.23	31.91; 31.92; 31.93
3	2.176; 2.173; 2.170	1.390; 1.385; 1.379	90.81; 90.82; 90.83	3.788; 3.774; 3.757
Here, $x=1$. For the (Mg ⁺ Te, In ⁺ Sb, Cd ⁺ Sn)-junctions, the value of β given in Eq. (46) is 1.0369.				
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	0.531; 0.530; 0.529	24.20; 24.20; 24.20	92.71; 92.72; 92.73	21.99; 21.99; 21.99
1.03	0.556; 0.555; 0.554	29.92; 29.93; 29.94	92.72; 92.73; 92.74	28.58; 28.58; 28.60
1.11	0.599; 0.598; 0.597	30.43; 30.44; 30.45	92.73; 92.74; 92.74	31.33; 31.34; 31.35
1.12	0.605; 0.604; 0.603	30.18; 30.19; 30.20	92.73; 92.73; 92.74	31.34; 31.35; 31.37
			$V_{ocII} = 1.12 V$	436.9; 437.0; 437.1=$T_H(K)$
1.13	0.610; 0.609; 0.608	29.88; 29.89; 29.89	92.73; 92.73; 92.74	31.31; 31.32; 31.33
3	1.708; 1.706; 1.704	0.739; 0.735; 0.731	92.41; 92.42; 92.43	2.048; 2.039; 2.028